Short-Term Visit in Aachen (Richard Dronskowski Group)

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As part of the JST ASPIRE project, I conducted a research visit to Prof. Dr. Richard Dronskowski and his group at RWTH Aachen University, Germany, from January 31st to February 24th, 2025. The primary objective of my visit was to gain expertise in theoretical calculations, using Density Functional Theory (DFT) and LOBSTER package for analyzing local bonding states in materials of rock-salt and related structures, and to engage in in-depth discussions with the theoretical chemists there regarding my PhD research topics.

The Dronskowski group is well-known for its contributions to synthetic solid-state chemistry and solid-state quantum chemistry. Their research encompasses a broad spectrum of topics, including nitrides, carbodiimides, guanidine chemistry, neutron diffraction techniques, quantum chemistry, phase-change materials, and chemical bonding analyses, notably Crystal Orbital Hamilton Populations (COHP). Their publications have significantly advanced the understanding of chemical bonding and synthetic methodologies in the field of "Materials Science."

During my stay in Aachen, I received helpful training and guidance from Dr. David Schnieders, Dr. Peter Müller and Professor Dr. Dronskowski on computational setup and carrying out the calculations. On the first day, Dr. David Schnieders provided me with an introduction about the Dronskowski group’s computational protocols and tutorials. I frequently asked his assistance with my computational issues. I observed a distinct separation of people between computational and experimental research within the Dronskowski group. While my focus was on calculations, I am also interested in the experimental style of their work. The daily discussions with the group members, particularly those involved in the development of the LOBSTER package, were exceptionally fruitful because such discussions are not readily available in Kyoto. This direct interaction allowed me to perform detailed analyses and interpretations of computational results, providing fresh perspectives on my research. I was particularly impressed by the latest LOBSTER package update, which simplifies bonding state analysis by using intuitive “chemistry words” instead of complex computational terminology. During the stay, I also enjoyed spending weekends visiting several cities in Europe, taking advantage of Aachen's proximity to the border against Belgium and the

Netherlands. I would also like to thank the students and postdoctoral members for their hospitality, including the parties and lunches.

My visit to the Dronskowski group proved to be highly productive and served as an excellent kick-off for our ASPIRE project collaboration. I am confident that continued communication and interaction, including participation in conferences and research collaborations, will further strengthen the relationship between Kyoto (Kageyama group) and Aachen (Dronskowski group).

Lastly, I am thankful to all who contributed to setting up my visit, including Prof. H. Kageyama, Prof. Dr. R. Dronskowski, Ms. M. Marquardt (Dronskowski group secretary), and our group secretaries, Ms. S. Nojiri, Ms. M. Aoki and Ms. M. Taguchi. After returning to Kyoto, I am now looking forward to hosting several visiting students from the Dronskowski group this year. I am ready to contribute to their research and ensure they have a memorable and productive stay in Kyoto!

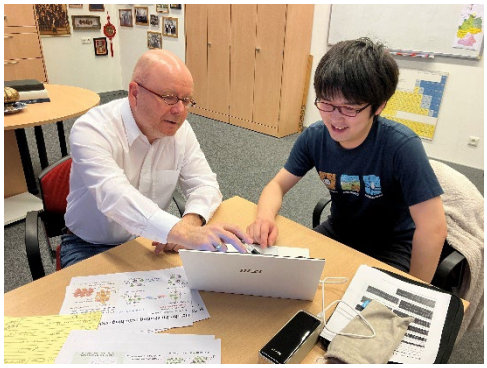

Figure. Prof. Dr. Richard Dronskowski (left) and me (right) discussing regarding the results of theoretical calculations.