

ASPIRE Young Lecture Tour (Oxford, Nantes, and Aachen)

Suguru Yoshida (Kyoto University)

I visited Oxford University (U.K., January 30 and 31), IMN Nantes (France, February 3–5), and RWTH Aachen (Germany, February 7 and 10) for an ASPIRE Young Lecture Tour, the first one under the Mixed-Anion ASPIRE project. This lecture tour took place immediately after the kickoff meeting for the ASPIRE project (also the final symposium for the Core-to-Core Mixed-anion project) in Lille, France (January 27–29). My lecture was titled “Atomic Displacements in Solids: What Occurs and Why,” and it was about how to determine and predict crystal structures of solid materials with a combined experimental/computational/group-theoretical approach.

Prof. Andrew Goodwin, the PI of Partner Team 1 Structural Science, supported organizing my visit to Oxford. I had an opportunity to discuss local structural analysis via the pair distribution function method, molecular dynamics simulations, and correlated disorder of mixed anion systems with Prof. Goodwin



and the group members, including Dr. Theodosios Famprikis and Dr. Nimrod Benshalom. The combined machine learning and PDF analysis was impressive and likely has a potential application to complex mixed-anion systems. The in-person discussion with Prof. Goodwin was critical for launching the ASPIRE project because he could not make it to the meeting in Lille due to his schedule conflict despite his important role in the project. I also had discussions with Prof. Simon Clarke (a member of Partner Team 2 Specialized Synthesis), Prof. Volker Deringer (random systems), Prof. Paolo Radaelli (condensed matter physics), Prof. Ludmilla Steier (photocatalysts), and Prof. Saiful Islam (energy materials). The professors also showed me around their research equipment,

thanks to which I was able to see the Oxford research facilities of the chemistry, physics, and materials engineering departments. My ASPIRE lecture was well received and gathered interest, for example, from a grad student from the Clarke group; the student has decided to stay at Kyoto University for 3



months in the summer of 2025, which will be supported by the ASPIRE project. His research plan is being discussed now and will be supervised by myself and Prof. Hiroshi Kageyama (PI of the Japanese team).

The visit to Nantes was hosted by Dr. Laurent Cario, a research director of CNRS and the PI of Partner Team 3 Specialized Synthesis. Dr. Shunsuke Sasaki (sulfide chemistry) guided me through the research facilities of IMN, well designed for the convergence of physical science and chemistry. After my ASPIRE lecture on the first day afternoon, I had detailed discussions with ASPIRE participants in Nantes—Dr. Sasaki, Prof. Olivier Hernandez (advanced crystallography), and Dr. Isabella Braems (genetic algorithm)—as well as Dr. Etienne Janod (out-of-equilibrium properties) and Dr. Stéphane Jobic (luminescent materials). Among them, Dr. Braems showed her strong interest in the structural exploration of mixed anion compounds via the integrated approach of phonon calculations and her expertise in genetic algorithms. Motivated by the discussion, she started to plan her month-long stay in Kyoto in 2025, and her visit is now scheduled for November 2025. We believe our collaboration will be accelerated during her stay in Kyoto and will



result in a useful methodology for the research community.

The last destination of the tour was Aachen, Germany, and the visit was hosted by Prof. Richard Dronskowski (a member of Partner Team 4 Theory). I discussed with Prof. Dronskowski and Dr. David Schnieders about real-space representation of periodic wavefunctions and fragment orbital



extraction from extended solids. These methods are surely useful in understanding the electronic structure and related properties of mixed-anion systems. Two graduate students from his group are staying in Kyoto from April 2025 under the ASPIRE project, and I detailed a plan together with them about their research themes in Kyoto. I felt unwell over the weekend probably because of the hard water in Europe, so unfortunately, could not visit the places in Aachen recommended by Prof. Dronskowski. Plus, European people didn't understand why hard water caused such trouble. It may be a specific problem for people living in soft water regions. Please keep it in mind when staying in Europe.

Overall, the lecture tour and visit were fruitful, extended my research network, and motivated some foreign researchers to stay in Kyoto for collaboration under the ASPIRE project. Some of my valuable experiences are missed in this report due to space constraints; I am happy to share more when we meet in person. I strongly recommend other young researchers involved in the ASPIRE project make use of the opportunity to have such a tour and definitely would like to have another one if allowed.