

Promoting Computational Materials Design in Europe: From Munich to Edinburgh to Hull

A Trip Report by Susan Menez Aspera

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August 30-September 13, 2012

The opportunity given to us by our laboratory, Kasai Laboratory, provided us an insight on the different current research trends in many European countries and gave us a chance to promote the research interest of our laboratory to other researchers from different countries. This was made possible by our recent trip in Munich, Edinburgh and Hull wherein the main purpose was to meet professors in Technical University of Munich and discuss each other's research interests, attend the European Conference on Surface Science in Edinburgh, and discuss ongoing collaboration with a professor in Hull. In this report, I will briefly discuss about the different activities that we had during the trip and the some insights that we gained from the trip.

1. Munich Part I : Introduction of Kasai Laboratory in Technical University Munich

August 31 – September 1, 2012. Our first stop was Munich. It was here that we met Prof. Notker Rösch (Figure 1), Academic Director of the Catalysis Research Center (CRC) of Technical University of Munich (TUM). He was our contact person and his office, with the help of Prof. Brenig, arranged the schedule of our stay in TUM and our meetings with other professors of the Catalysis Research Center (Appendix I). We started with him introducing CRC, the people/professors comprising CRC, and some of the different research interests of the center. He also mentioned some of the center's collaborators from different industries and universities. Right now, they have a big collaboration with National University of Singapore where he spends a large part of his time doing research for he has a laboratory in that university. They also have collaboration with one Japanese industry and right now they are eyeing on collaboration with a Chinese University. He also showed us the ongoing construction of the new CRC building, with funds amounting to 5-6 million euros, which would house about 500 hoods for experimental researches of the CRC. It is expected that the building will be ready for occupancy by the end of next year. He also told us that, unfortunately, Prof. Brenig cannot meet us during our stay for some



Figure 1. Triati, Prof. Notker Rösch and me in TUM. At our background is the poster of one of his student. The poster, he said, won an award in a conference.

family matters that he had to attend to.

Prof. Rösch said that his research group's interests are with heterogeneous catalysis and accurate calculation of the transition states for reactions. They also have developed their own software called paragauss, which they are still perfecting as of now. The underlying principle of that software, I

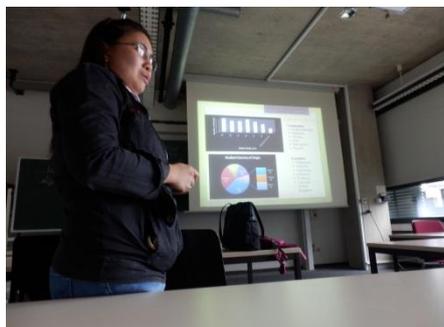


Figure 2. Me giving presentation in front of Prof. Rösch and the members of his laboratory.

I guess, is comparable to that implemented in Gaussian. But still many of their works uses VASP as seen by the posters that are hanging from their laboratory.

After that one hour meeting with him, we went to a seminar room where I gave a presentation about our laboratory, its research interest and my research work to him and the members of his laboratory (Figure 2). The audience was very much curious about Japan and some even said are interested to visit Japan sometime. The presentation went for almost an hour.

Prof. Rösch gave suggestions about my presentation particularly on “getting the feeling” of the amount of Van der Waals interaction between the O₂ adsorbate and the surface. As for the other researches of our laboratory, they were particularly interested in how we treat ionic conductivity and calculations involving ceria. They also admitted that they are not interested in the treatment of magnetic materials.

We also had a chance to visit a former member of Kasai Laboratory, Dr. Tanglaw Roman, who is now at the University of Ulm as a postdoc. He works with Prof. Axel Gross of the Institute for Theoretical Chemistry (Figures 3 and 4). We had lunch with him and after which he showed us around the university. Unfortunately, it was a Saturday and its vacation time as well so a very few people was around.



Figure 3. Me, Triati and Dr. Tanglaw Roman.

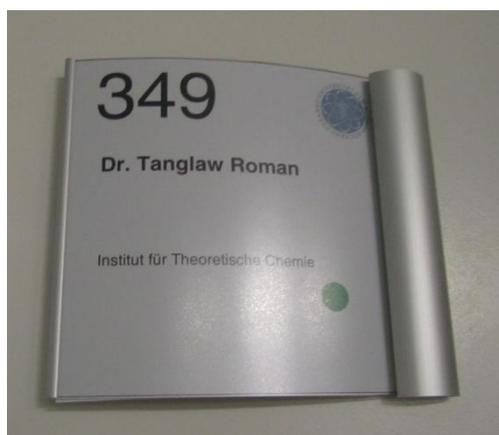


Figure 4. Tanglaw's room label.

2. Edinburgh: CMD-24, ECOSS-29, CMMP-12, ECSCD-11

September 3-7, 2012. The next leg of our trip is in Edinburgh where we attended and gave presentation in the 2012 European Conference on Surface Science (ECOSS). The venue of the conference is in Edinburgh International Conference Center (EICC), Edinburgh, Scotland, UK (Figures 5 and 6).



Figure 5. The façade of the conference site.



Figure 6. Front window of the conference site showing the name of the venue, Edinburgh International Conference Center (EICC).

It was mentioned by an avid participant that the event was previously for ECOSS only, but this year, the organizers merged four events wherein one could just imagine the increased number of participants. Diversity in participant's origin as well as in their research interest, which of course are all still related to condensed matter physics, was obviously seen in the conference. There were 9 parallel sessions simultaneously occurring at a particular time where most of the talks were just for 20 mins. For my research interest, which is mostly related to graphene and doped-graphene materials and its interaction with adsorbate or a metal surface, most of the "hot" topics are still on surface reconstruction/corrugation due to defects, treatment of Van der Waals interaction, and concentration/position of dopants and its interaction with an adsorbate. I say, these are also some of the issues that we are aware of and is currently treating in our laboratory, which is I say is still



Figure 7. Display in the conference site showing the poster session for ECOSS.

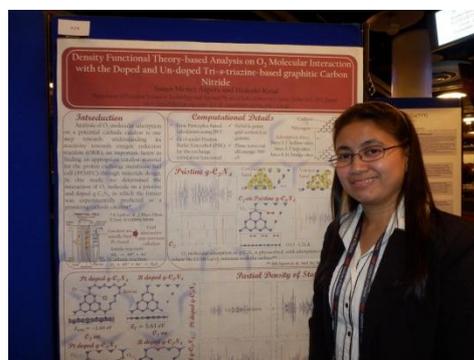


Figure 8. Me during the poster session. At my background is my poster.

on the international level.

Come September 5-6, 2012 where I gave my poster presentation on the topic entitled “Density Functional Theory-based Analysis on O₂ Molecular Interaction with the Doped and Un-doped Tri-s-triazine-based graphitic Carbon Nitride” (Figures 7 and 8). There were people coming to my poster and I explained to them my current research work. There were questions asked but the most relevant ones were: 1.) Did I take into consideration Van der Waals interaction?, 2.) Which dopant is better?, 3.) Would the same effect be seen upon changing the concentration of the dopant, and 4.) With the strong interaction of the O₂ molecule on top of the Pt in the Pt-doped g-C₃N₄ system, will this interaction provide a way for the Pt to be removed from the surface since it was shown that the Pt is somewhat elevated from the surface?. These questions, and some discussion with other participants, gave me insights regarding the relevance of my work and what other things are still needed to be considered to fully realize the objectives of my study. I also had the chance to see other posters of other researchers in a variety of condensed matter related topics. Most of the works in the conference deals with experimental studies, and the few discussions on theoretical results are not far from what we are doing in our laboratory.

On the third day of the conference, the organizers presented to a group of scientist an EPS

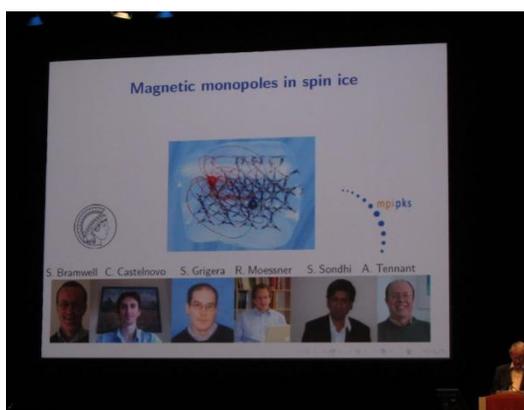


Figure 9. EPS Europhysics prize winners. This year’s winning research is on “Magnetic monopoles on spin ice”.



Figure 10. The winners of the EPS Europhysics prize with their picture takeduring the ceremony.



Figure 11. Friends we met during the conference.

Europhysics prize for their research on “Magnetic monopoles in spin ice”. After which, a representative of the group gave a lecture on their study (Figures 9 and 10). The lecture strikes me in such a way that the introduction of the speaker was from a clip of one of my favorite TV series wherein the main character discussed the definition of magnetic monopoles is such a funny situation. We also have met friends from different countries along the way (Figure 11).

3. Hull: Meeting with Prof. Carl Redshaw

September 9, 2012. After the conference, we went to Hull to meet Prof. Carl Redshaw (Figures 12 and 13). His laboratory and ours have a joint collaboration on a project. Our discussion with him is mostly based topics related to this collaboration. I guess the project is about molecular scaffolding for photosystem II reaction. After the discussion, he showed us around the university, which he is also a new comer. After which, we had lunch where he introduced us to his wife.



Figure 12. We visited university of Hull.



Figure 13. Me, Prof. Carl Redshaw and Triati at the University of Hull.

4. Munich Part II: Meeting other members of the Catalysis Research Group

September 11-12, 2012. The last part of our trip is back in Munich where we had meetings with the members of Prof. Rösch's group, Prof. Hubert Gasteiger and Prof. Ulrich Stimming. On the first day, we talked with members of Prof. Rösch's group regarding what they are working on and what are their research interests. Among them was Zhijian Zhao (catalysis) who works with reactions involving cleaving of fused rings, Dyugu Basaran (catalysis) who works with catalytic reactions involved in biomass processes, Astrid Nikodem (locating transition states) who works on finding methods for accurate determination of transition states in reactions, and Dr. Alena Kremleva (modeling of actinid adsorption on clay minerals) who's work on clay mineral is somewhat related to Triati's work on montmorillonite (MMT). The discussions were informative and interesting. We also noticed that most of their works are on reaction paths and mostly chemistry-based.

After the discussions with the members of Prof. Rösch's group, Triati gave a presentation on her research on MMT to Prof. Rösch, Dr. Kremleva, Clare and I. It was interesting and informative. She obtained suggestions.



Figure 14. Meeting with Prof. Hubert Gasteiger.
related to fuel cell research is still being installed.

We also had a meeting in the afternoon with Prof. Hubert Gasteiger (Figure 14) whose work is mostly on technical electrochemistry. He presented us with some of the works of his laboratory. Right now, his work is mostly on Li-S and Li-air battery, but he also had some fuel cell related works. We also presented to him some of the works of our laboratory. After which, he toured us around his laboratory where some his students are working. Since his laboratory is relatively new in that location, the equipment

The next day, we visited Prof. Ulrich Stimming of the Physics Department (figure 15). Their group is working with fuel cells but in experimental studies. The meeting was in a seminar room in front of his students and two other professors, Prof. Petra Bele and Prof. Oliver Schneider. The first presentation was about cathode material for PEMFC from Clare, then the succeeding discussions were from the members of their group. They are currently working with Pt on Au nanostructure for electrode, TiO_xC_y support for Pt for the electrode system, they also have works with organic materials as electrodes, and high temperature fuel cell such as direct carbon fuel cell.



Figure 15. Meeting with Prof. Ulrich Stimming. In this picture, Triati, Prof. Schneider, Prof. Stimming, Prof. Bele, and me.

Summary

In this trip, we therefore have:

1. Visited Technische Universität München (Technical University of Munich) in Germany where we met several professors from different laboratories where we introduced Kasai Laboratory and our research interest, and also know the research interests of their respective laboratories. These can be a way to open the door for possible research collaboration. The research group that we visited are:

- a. Prof. Notker Rösch's group working on Theoretical Chemistry from the Catalysis Research Center.
 - b. Prof. Hubert Gasteiger's group working on Technical Electrochemistry from the Catalysis Research Center
 - c. Prof. Ulrich Stimming's group working on Surface Science from the Department of Physics
2. Attended the CMD-24, ECOSS-29, CMMP-12, ECSCD-11 conference in Edinburgh, UK where we gave presentation of our research and heard presentation of other research groups.
 3. Met with Prof. Carl Redshaw in University of Hull in Hull, UK. Here, we discussed about the current state of our research collaboration with their laboratory.

Visit Schedule for
Susan Menez Aspera, Triati Dewi Kencana Wungu
and Mary Clare Sison Escano
Department of Applied Physics, Osaka University, Japan
Last update: September 20, 2012

Thursday, 30 August 2012

13:00 Arrival from Osaka

Friday, 31 August 2012

13:55 Pick-up by at the Main Entrance of the Department of Chemistry
Lichtenbergstr. 4, 85748 Garching, Phone 0049.89.289.13670

14:00 Meeting with Prof. Notker Rösch (Theoretical Chemistry)
Office CH 63105, Phone 0049.89.289.13620

15:00 **Seminar**
"Realization of Computational Materials Design: Introduction of Researches
in Kasai laboratory, Osaka University".
Seminar Room CH-63401

Sunday, 2 September 2012

Departure to Scotland

Monday, 10 September 2012

Arrival in Munich from Scotland

Tuesday, 11 September 2012

- 9:30** Meet the Group of Prof. Rösch
9:30 Zhijian Zhao (Catalysis)
10:00 Dyugu Basaran (Catalysis)
10:30 Astrid Nikodem (Locating Transition States)
11:00 Dr. Alena Kremleva (Modelling of Actinid Adsorption on Clay Minerals)
- 11:30** Presentation on "First Principles Study of Structural Stability and Electronic Properties of Lithium-Montmorillonite" to Prof. Rösch and Dr. Kremleva

Wednesday, 12 September 2012

- 12:45** Pick-up by at the main entrance of the Department of Chemistry
Lichtenbergstr. 4, 85748 Garching, Phone 0049.89.289.13670
- 13:00** Meeting with Prof. Ulrich Stimming and his Group
*Department of Physics, James-Frank-Strasse 1, 85748 Garching
Office PH 3079, Phone (Dr. Bele) 0049.89.289.12556*
- Presentation in Seminar Room xxx

Thursday, 13 September 2012

Departure to Osaka