

TRIP REPORT (29 August – 14 September 2012)

By: Triati Dewi Kencana Wungu

Date: September 19, 2012

Summary

The main purpose of this trip was to:

1. Attend the conference of CMD-24 (ECOSS-29, CMMP-12, ECSCD-11) which was held in Edinburgh International Conference Centre (EICC), Edinburgh, UK, 03 – 07 September 2012.
2. Meet several Professors of Technische Universität München (TUM)- Germany and to know the research interest of their laboratory. We visited the following three (3) research group and conducted several activities:
 - a. Theoretical Chemistry, Catalyst Research Center, TUM
Contact person: Prof. Dr. h.c. N. Rösch (Director of Catalyst Research Center)
 - b. Technical Electrochemistry, Catalyst Research Center, TUM
Contact person: Prof. Hubert A. Gasteiger
 - c. Technical Physics, Faculty of Physics, TUM
Contact person: Prof. Ulrich Stimming
3. Introduce the researches that Kasai Laboratory, Osaka University, is currently engaged in to the above mentioned research groups.
4. Meet Prof. Carl Redshaw in the University of Hull, UK and to discuss the current stage of join research proposal.

**CMD-24 (ECOSS-29, CMMP-12, ECSCD-11) Conference
Mon 3 – Fri 7 September 2012**



Edinburgh International Conference Center (EICC)

The 24th Conference of the EPS Condensed Matter Division (CMD-24), the 29th European Conference on Surface Science (ECOSS-29), the 11th European Conference on Surface Crystallography and Dynamics (ECSCD-11), and the 2012 UK Condensed Matter and Materials Physics Conference (CMMP-12) was conducted in parallel at the Edinburgh International Conference Centre (EICC).

The scope of the conference is:

ECOSS/ECSCD

- Metal Surfaces
- Semiconductor Surfaces
- Oxide Surfaces
- Biological Interfaces
- Surface Dynamics: Space-/Time-/Energy-resolved
- Surface Reactions, Kinetics and Catalysis
- Electronic Structure of Surfaces
- Liquid-solid Interfaces incl. Water and Electrochemistry
- Complex Systems: Large Organic Molecules, Self-assembly and Self-organisation
- Novel Methods: Instrumentation, Facilities and Computation

CMD/CMMP

- Nanostructures
- Semiconductors
- Polymers / Biology
- Magnetism / Spintronics / Inter-Metallic Phases
- Liquids
- Carbon including Nanotubes, Graphene, Diamond
- Low Temperature / Superconductivity
- Theory/Computational Physics
- Neutron / X-ray Diffraction

On Tuesday 4 to Wednesday 5 September 2012, I delivered a poster presentation on “First Principles Study on The Oxygen - Vacancy Migration in LaGaO₃. During my poster session, there were 4 participants listened to my presentation. The following questions were given to me during my talk:

- The agreement term written in my poster, which corresponds to the agreement energy barrier results between experiment and first principles calculation result, is not suitable to be used since it is not exactly the same (the difference between calculation and experiment is 0.02 eV and also the environment that influence the system in total)
- What is the effect of the number of oxygen vacancy and doping in pure LaGaO₃ to its property? Will it still be an insulator, semiconductor or metallic?
- If the migration path of oxygen vacancy is not an arch form, what would the result be?
- How long the calculation was conduct to reach the optimization?



Picture was taken during poster session.

For me the highlights of the conference were:

- Making professional connections and friendship with academician
- Learning about current issues and challenges in condensed matter science

During the conference I met several Japanese researchers such as Prof. Takanori Koshikawa, Prof. Kurahashi, Dr. Matsunaka, and Dr. Isamu Yamamoto. Also, met researcher from Indian and students from Indonesia, Malaysia and Ireland and made a good friendship.



Dinner with new friends after conference in the Indian Restaurant.



Clare, Triati, and Susan in front of EICC building.

Visit TUM
31 August, 11-12 September 2012



Date: Friday, 31 August 2012

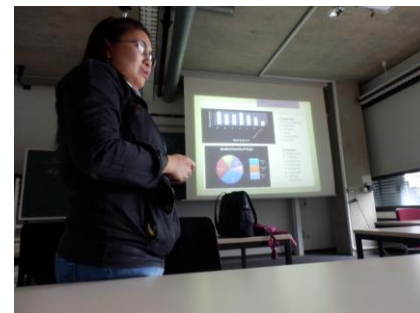


Picture was taken in front of Prof. Rösch office after Susan gave presentation. From left to right: Triati, Prof. Rösch and Susan.

research institute from Europe, USA, Singapore, and Japan (Osaka).

At 15.15, Susan Menez Aspera delivered presentation entitled “Realization of Computational Materials Design: Introduction of Researches in Kasai laboratory, Osaka University” in front of Prof. Rösch groups in the seminar room *CH-63401*.

We arrived in the Dept. of Chemistry at 13.40 and picked up by Dr. Miriam Häberle to be brought to Prof. Notker Rösch office (6nd floor, Dept. of Chem., TUM). At 14.00, we had a meeting with Prof. Rösch in his office. Prof. Rösch introduced the general of CRC including their staffs, research groups, students, new building, and collaboration in his presentation. Also mention a number of researcher and collaboration partner. There are 70 Post doctoral researchers and 230 Ph.D students in CRC. The CRC has an active collaboration with industries and



Susan was giving a presentation in front of Prof. Rösch groups.

Date: Tuesday, 11 September 2012

We had discussion related to catalysis, locating transition states, and adsorption of Actinid on clay minerals, with the member of Prof. Rösch research group in each of member's room. The following is the schedule of our discussion from 9.30 to 11.00 am.

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)

After discussion with them, I delivered presentation entitled “Montmorillonite as An Ionic Conductor Material: First Principles Study of Structural Stability and Electronic Properties” in front of Prof. Rösch and Dr. Kremleva. It was a pleasure for me to present this topic in front of the expert of clay mineral. They gave good comments and suggestions to my research results particularly to the model where the Lithium-montmorillonite exhibits metallic behavior, which is unacceptable in nature. The charge parameter should be taken into account in the input parameter during calculation so that the density of states analysis can indicate that Lithium-montmorillonite has an insulating property.

At 14.00, we continued our business to visit Prof. Gasteiger in TUM. Both Prof. Gasteiger and Susan gave presentations regarding the introduction of each laboratory (Prof. Gasteiger's laboratory and Kasai Laboratory). Also, we had a short laboratory tour and saw students who were doing experiment.



From left to right: Clare, Prof. Gasteiger, Susan, and Triati.

Date: Wednesday, 12 September 2012

We had a workshop in the Faculty of Physics, Prof. Ulrich Stimming research group. In this workshop, Mary Clare Sison Escano delivered presentation entitled “Quantum Simulation and Design Catalysis Materias for Fuel Cell Application. In general, the presentation given by Prof. Stimming research group was related to Fuel cell.



Prof. Oliver Schneider was giving a speech in the opening remarks



Clare was giving a presentation



One of Prof. Stimming student was giving a presentation.



Picture was taken after finish a workshop. From left to right: Triati, Prof. Schneider, Prof. Stimming, Dr. Belle, and Susan.

**Visit Schedule for
Susan Menez Aspera, Triati Dewi Kencana Wungu
and Mary Clare Sison Escano**

Department of Applied Physics, Osaka University, Japan

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

Visit University of Hull
Sunday, 9 September 2012



After we finished conference, we went to Hull-UK to visit Prof. Carl Redshaw in the University Of Hull. The main purpose of this visitation was to deliver the progress of join research proposal between Osaka University (Kasai Lab and groups) and Prof. Carl group.