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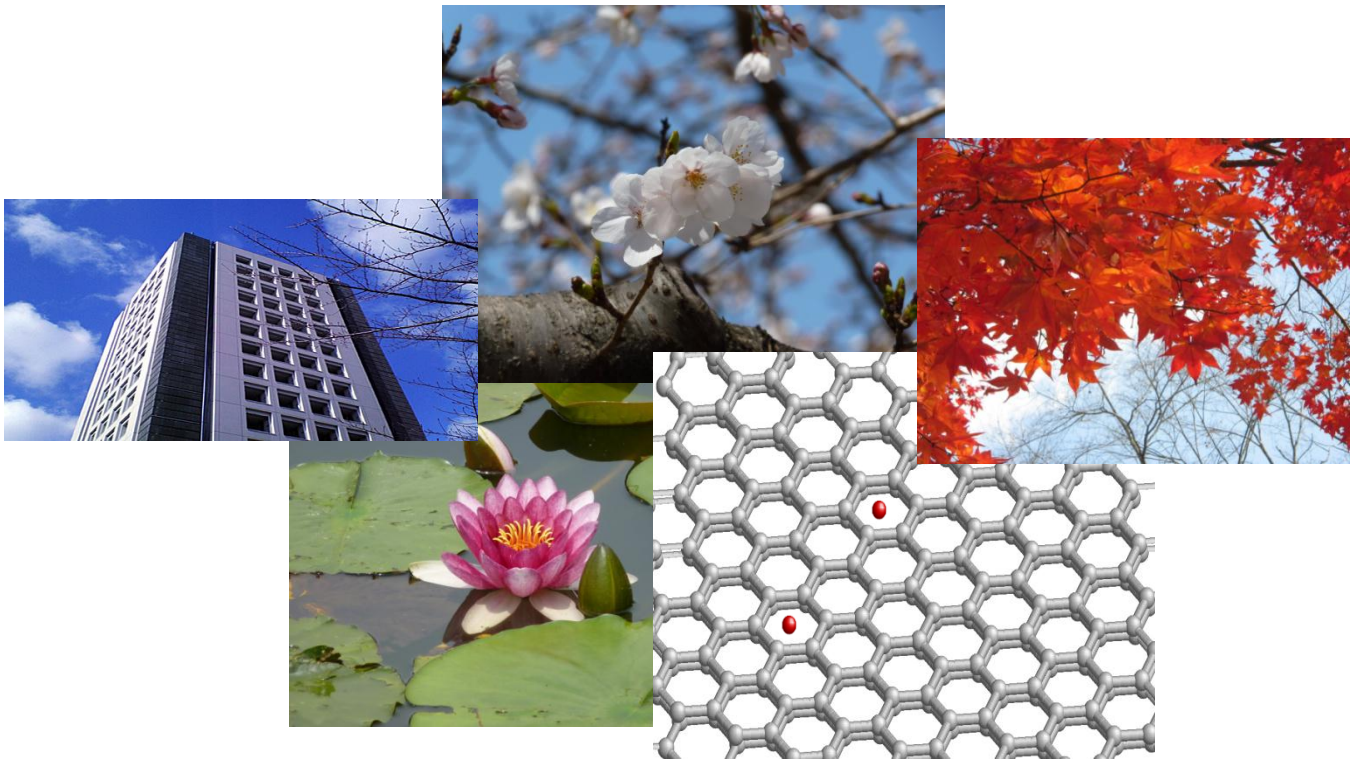

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【Quantum Engineering Design Research Initiative】

2011

Collaborative Research on Design and Creation of

New Green Nano Material

Graduate School of Engineering

Osaka University

The key scattering mechanisms in a polar modulation-doped heterostructure at low-temperature

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1. Introduction

We present a theoretical study on the effect of the key scattering mechanisms on mobility of two-dimensional electron gas (2DEG) in a polar modulation-doped heterostructure (MDHS). Owing to high-temperature Coulomb correlation among impurities, the low-temperature 2DEG mobility in a polar MDHS is limited not by remote impurities, but alloy disorder (AD) and roughness related scatterings, viz., surface roughness (SR) and polarization roughness (PR) that depend strongly on alloy composition and that are very sensitive to near interface values of the wave function. The 2DEG distribution is properly calculated within the realistic model of finitely-high barrier, incorporating into the theory all electrostatic sources.

Modulation doping was regarded as a successful technique for reducing the impurity scattering [1]. Moreover, owing to impurity correlation caused by Coulomb repulsion among ionized impurities during their diffusion in samples subject to a thermal preparation, their lateral distribution becomes more inhomogeneous, their scattering is more reduced. As well known [2], polarization is an important property of nitride-based HSs. Recently, we have shown [3] that the interface polarization charges take the three-fold role as the ionized impurities do. These charges on a rough interface are a carrier supply source into HSs, but also a confining source as well as a scattering mechanism for the carriers in polar HSs. Thus, the 2DEG mobility in a polar modulation-doped heterostructure at low temperatures is dominated not by remote impurities, but by AD and PSR scatterings. These key scattering mechanisms are very sensitive on the near-interface 2DEG distribution.

2. Results

2.1 Confining effects on 2DEG in polar MDHS

The carrier confinement in a polar HS is fixed by all possible confining sources located along the growth direction, viz., potential barrier, interface polarization charges,

Hartree potential created by ionized impurities and 2DEG. **We estimate the confinement effect on the electron wave function** from all electrostatic sources, viz., interface polarization charges, 2DEG, and remote ionized donors.

In the literatures [4-5] one often adopted the ideal model of infinite barrier, based on the standard Fang-Howard wave function. This simplified essentially mathematics of the transport theory and was a good approximation for some scattering mechanisms by, e.g., ionized impurities and phonons that are insensitive to the near-interface 2DEG distribution. However, in the case under study, the key mechanisms are AD and PSR (SR) that are very sensitive thereto. Therefore, **we examine the confinement effect within the realistic model of finite barrier**, based on the modified Fang-Howard wave function.

2.2 Form factor for unscreened scattering

The autocorrelation of unscreened scattering is specified by a form factor that is given in terms of the wave function, e.g., for alloy disorder and for surface roughness. Thus, the form factor $F(\sigma; n_s; N_I, L_s)$ depends on the charge density of the confining sources, e.g., interface polarization charges (σ), remote ionized donors (N_I, L_s) and 2DEG (n_s). To **illustrate conveniently the dependence of unscreened scattering on these densities**, we introduce a dimensionless form factor, defined as follows: $\Phi(\sigma; n_s; N_I, L_s) = \dfrac{F(\sigma; n_s; N_I, L_s)}{F(\sigma_0; n_{s0}; N_{I0}, L_{s0})}$.

3. Summary

The infinite barrier model is applicable, as a good approximation, only to scatterings that are ***insensitive*** to the near-interface 2DEG distribution. For scatterings ***sensitive*** thereto, the finite barrier model must be applicable. ***Our theory is able to explain experimental data*** about the dependence of 2DEG mobility observed in polar MDHSs, which has not been understood so far.

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Monolayer Controllable Fabrication of Metal Phthalophyanine by Layer-by-Layer (LbL) Technique

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1. Introduction

The layer-by-layer (LbL) method has become a leading option for fabrication of nanostructed thin films in a straightforward and low-cost manner. The sequential multilayer deposition can be conducted by immersing the substrate alternatively into the (poly)cationic and (poly)anionic dipping solutions. After depositing each layer, the substrate is immersed into the washing solution to remove unadsorbed atoms and subsequently dried under a nitrogen/air flow. The LbL technique can be employed for various substrate materials such as hydrophilic and hydrophobic glass, mica, silicon, metals, quartz and polymers. The LbL film fabrication is performed under mild conditions, which help to preserve biomolecular integrity of the materials. Consequently, the LbL technique is currently considered for many applications including catalysis, electrochemical sensing and biosensing.

2. Methodology

To obtain uniform LbL thin films, it is crucial to have controllable slow raising speed and drying time. An automatically controlled system is key to obtain these parameters. The constructed automatic tool consists of three main components: two stepping motors, two sensors and a programmable logic controller (PLC). The vertical stepping motor controls the up-down movement of the substrate. The first sensor is used to limit the movement within vertical boundaries. The horizontal stepping motor controls the left-right movement which allows the substrate to immerse into the selected solution. The position of each of the four solutions are marked and detected by the second sensor. The process is controlled by the PLC, which is advantageous for its simplicity, reliability and expandability. The motor speed, drying time and number of

layers can be adjusted on demand suitable for each substrate and dipping solution; for instance, the 0.042 mm/s raising speed and 60 second drying period result in evidently uniform copper phthalocyanine LbL film.

To prepare copper phthalocyanine LbL films, copper (II) phthalocyanine-tetrasufonatic acid tetrasodium salt (CuTsPc), poly (allylamine hydrochloride) (PAH) and 3A water are used as polyanion, polycation, and washing solutions, respectively. For nickel tetrasulfonated phthalocyanines (NiTsPc) films, the sulfonate ion of NiTsPc and the ammonia ion of PAH act as polyanion and polycation, respectively. The optical properties of the prepared LbL films containing 5, 7, 10, 20, 30, 40 and 50 bilayers are characterized by an optical spectrometer. The voltammograms are used to characterize the electrochemical properties of both films at various scan rates from 10 to 200 mV/s.

3. Results and Discussion

For CuTsPc films, the optical absorption peak is observed at the wavelenght of 627 nm and found to increase linearly with the number of bilayers. This indicates approximately equal amounts of CuTsPc are attached at each deposition. At different indicated scan rates, the voltammograms show similar shapes indicating the charge transfer is controlled by nanostructure of the LbL films. A pair of reduction-oxidation peaks is observed in all scan rates and for 5, 7 and 10 bilayer films. The couple peaks are due to the reduction of Cu^{2+}. For higher bilayers films, the high current can be conducted at only on forward bias; therefore, relatively small loops and peaks are observed. A narrow loop always appears on the reverse side while a larger loop in the forward side; and its width varies with the scanning rate.

For NiTsPc films, the optical absorption spectra exhibit two dominate peaks originated from soret and Q bands of NiTsPc layer. The optical absorbance at wavelength of 622 nm for Q band increases linearly with the number of deposited bi-layers, suggesting the equal amount of NiTsPc is adsorbed in each deposition. In addition, the scanning electron microscope image of the surface morphology of LbL films shows more dense grain with large numbers of bi-layers. The voltammograms show similar shapes at various scan rate, indicating charges transfer to nanostructure of the LbL films. These results show two redox processes associating with the redox of phthalocyanine ring and that between Ni^{2+} and Ni^{3+} ion coupling.

Acknowledgements

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First Principle Studies on Atomic Hydrogen Absorption into Graphite Edges

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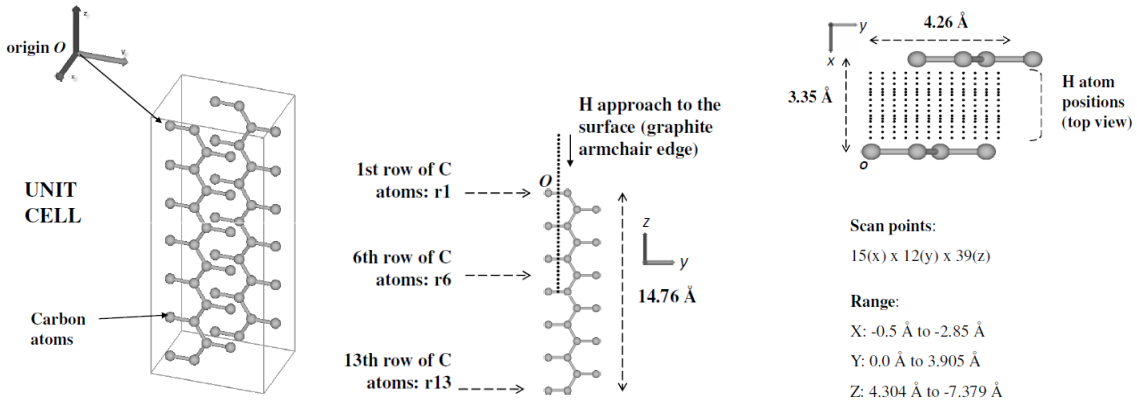
1. Introduction

The reportedly high hydrogen uptake of carbon-based nanomaterials makes them attractive as hydrogen storage devices in fuel-cell-powered electric vehicles [1]. DFT-based studies reveal that H_2 dissociative adsorption on the graphite zigzag (armchair) edge is non-activated [2] (activated [3]). Hydrogen is most likely to be found in its atomic form once inside the graphite layers [4]. VAS effect for H_2 is very weak on both edges, but the differing H_2 scattering behaviors can be used to identify unknown graphite edges [5]. TDS measurements reveal recombinative molecular H_2 (D_2) desorption in a main peak around 445 K (490 K) and a minor peak at 560 K (580 K). Desorption activation energies for H (D) was determined as 0.6 eV (0.95) eV [6].

2. Methodology



(a) (b) (c)

Fig. 1. Representations of the H-graphite systems and the dimensions of the graphite substrate: (a) The unit cell, the reference point *O*, and the positive x-, y-, and z-directions, (b) Side-view of the substrate consisting of 13 four-carbon atom rows and

the H approaching the graphite armchair edge, and (c) The various lateral positions of the hydrogen approach (dot) as seen from a bird's eye view (c).

DFT-based total-energy calculations are performed with VASP [7] using pseudopotentials and plane-wave basis sets. The ion-electron interaction is described by US-PP/PAW method, while GGA is utilized for the exchange correlation energy. The total energy is computed in a supercell geometry (see Fig. 1). The graphite substrate is represented by periodically repeated slabs (each 14.76 Å thick) composed of 52 C atoms or 13 four-C layers separated by 9 vacuum layers. The shortest C-C distance is 1.42Å. Potential energies along z- for various H lateral positions are determined to obtain the PES contour plots for H absorption into the graphite armchair edge along xz- and yz-planes. The C atoms were fixed during H absorption.

3. Results

H can enter the region between graphite sheets *via* the armchair edge through a reaction path with all points having negative potential energies. A strong H trap exists near the surface C atoms, suggesting that H termination of the edge C atoms' dangling bonds most likely occurs during absorption. Beyond the surface, the potential energy along the reaction path fluctuates and seems to approach zero, indicating that H absorption deeper into the subsurface through the armchair edge becomes more difficult without reconstruction. The H desorption barrier between rows is always less than that of the absorption. H stays near one of the graphite sheets during absorption. H motion parallel to a C row is possible while interlayer hopping is most unlikely to occur.

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Computational Study of DSC Sensitizer Originated from Ferrum (II)/ Ruthenium (II) with A Pyridyl-Quinoline-Framework Ligand

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Metal complexes, in particular, have been investigated intensively as sensitizer for DSC application because of their broad absorption spectra and favorable photovoltaic properties due to a metal to ligand charge transfer (MLCT) process. Among the metal complexes, Ru-polypyridyl complexes have shown the best photovoltaic properties i.e ruthenium black dye and N719. Here we report a computational study of sensitizer originated from ferrum (II)/ ruthenium (II) with a pyridyl-quinoline-framework ligand i.e 2-(2'pyridine-4'carboxylic acid)-cinchonine. The muliken gross atomic charge for both donor atom in the ligand are -0.0358 and -0.0425 respectively. Energy difference between its HOMO and LUMO is 3.76 eV. Comparison with the metal complexes will be presented.

Keyword: dye solar cell, photovoltaic, metal complexes sensitizer.

Computational Study of Zeolite Pore Formation using TBABr and TPABr as Organic Template

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We reported the computational model for the formation of pores in zeolite synthesis using TBABr and TPABr as organic templates. Computational studies indicates that the zeolite crystals in the first zeolite membrane (using TBABr as template) tend to have larger pore size than the pore size in the second membrane (using TPABr as template). The membrane pore size correlate with diameter of the ring formed by Si-O-Si or Si-O-Al network in the zeolite crystals. The larger number of rings Si-O-Si or Si-O-Al in the case of TBABr is more preferable than in the case of TPABr due to a lower energy system i.e -258,875 Hartree and -231,540 Hartree respectively. Thus, this computational study provides a qualitative information that permeat flux of the first zeolite membrane will be larger than the second zeolite membrane and this has been confirmed by experimental result.

Keywords : zeolite, organic template, permeate flux, pore size

Two weeks ago, I and Citra Deliana Dewi Sundari came to Japan to attend Quantum Engineering Design Initiative Workshop (at October 24 till October 27, 2011) and The Fourth International Symposium on Atomically Controlled Fabrication Technology (at October 31 till November 2, 2011). The topic of Quantum Engineering Design Initiative Workshop was about design and creation of new green nanomaterials. This was our first time came to Japan, especially Osaka. We were very surprised when we arrived at Osaka prefecture. It was very amazing, tidy, and clean city.

We left from Indonesia at October 22, 2011. We departed to Osaka from Soekarno-Hatta International Airport using Malaysia Airlines and arrived at Kansai International Airport at October 23, 2011. From Kansai International Airport, We took an Airport Limousine Bus to went to JR Ibaraki. After we arrived at JR Ibaraki, our colleague from Osaka University, Triati Dewi Kencana Wungu from Indonesia and Nguyen Tien Quang from Vietnam come after us. We waited for JICA Bus at bus stop near JR Ibaraki station. After the JICA Bus came, the bus take us to OSIC (Osaka International Centre). OSIC serves as the base for Japan International Cooperation Agency (JICA) program in the Kansai Region. After we arrived at OSIC, we checked in to the room number 301 for me and room number 808 for citra. Then, I took a bath and after that, I, Citra, and Triati went to barbeque party with other Indonesian students in Osaka. After I attended barbeque party, I came back to OSIC together with Citra, Triati, and Ganesh Shukri (also students from Indonesia). Because of tired, I slept very well until tomorrow morning.

On Monday, October 24, 2011, at 10.30 a.m., I went to the lobby in OSIC to meet other friends from other country who invited by Osaka University to attend QEDI workshop and The Fourth International Symposium on Atomically Controlled Fabrication Technology. They are Mr. Nelson Arboleda Jr. from De La Salle University (Philippines), Mr. Sujin Suwanna from Mahidol University (Thailand), Mr. Dinh Nhu Thao from Hue University (Vietnam), and Mr. Nguyen Thanh Tien from Can Tho University (Vietnam). I introduce my self to others, and they introduce their self to me. Then, we went to Kasai Lab. at Osaka University together. At 11.00 a.m. till 11.30 a.m., we met Prof. Dr. Hideaki Kasai at his office and we talked about ourself to Professor Kasai. After we met Professor Kasai, then we were given temporary office room by Mrs. Mayuko Aihara and we waited there for QEDI workshop at 13.00.

At 13.00, QEDI workshop was began and opened by Professor Kasai. Then, Nguyen Tien Quang as the first speaker gave some presentation to us at 13.10. He told us about oxygen dissociation on metal oxide-supported Pt cluster. By using first-principles method, he estimated the potential energy surface (PES) to find energy barrier for O_2 dissociation. He determined the reaction pathways and energy barrier by analyzing the PES curves and comparing it to the same reactions over an isolated Pt cluster to see how CeO_2 surface affects to the catalytic reactivity of Pt cluster. For the dissociation of oxygen molecule on CeO_2-supported Pt cluster, he found that O_2 goes from molecular adsorption state to atomic adsorption state with an activation barrier of 0,502 eV, while the activation barrier of O2 in the case of isolated Pt cluster was about 0,118 eV. After Nguyen Tien Quang, the second speaker was Ferensa Oemry. He told us about the effects of cluster size on Pt-O bonds formation in small platinum cluster. He told us that Pt_{10} cluster which undergo structural deformation during oxygen dissociation process was confirmed to yield negligible energy barrier which is opposite to Pt_4 cluster. His further investigation revealed that cluster reconstruction

which occurred in Pt_{10} can supress the external force induced by oxygen where it reacts by minimalizing the force which exerted on each atom in the system. He said that Pt_4 cluster could not experience the reconstruction because Pt-Pt Bond interaction in Pt_4 cluster stronger than in Pt_{10} cluster, the anti-bonding of Pt-5d and O-2p hybridization in Pt_4 cluster is found to be filled however in Pt_{10} cluster is almost unfilled. The third speaker was Hirofumi Kishi. The title of his presentation was Study of NO Oxidation Reaction over Pt Cluster Supported on γ-Al_2O_3 (111) Surface.

After Hirofumi Kishi finished his presentation, we took a break for ten minutes. Then, we continued the QEDI workshop to the next session. The fourth speaker was Mohammad Kemal Agusta. His research was about theoretical study of hydrazine adsorption. He studied about adsorption of hydrazine molecule on the metal surface such as Pt, Pd, Ni, Co, and Cu for application in direct hydrazine fuel cell technology, a non-platinum based fuel cell technology. He found that the most stable structure of hydrazine on the metal surface is anti conformation. The next speaker after Mohammad Kemal Agusta was Yuji Kunisada. The title of his presentation was A First Principles Study of Ortho-Para H_2 Conversion on the Ag (111) Surfaces with Coadsorbed O_2 Molecules. After Yuji Kunisada, the sixth speaker was Ryan Lacsao Arevalo. He studied the interaction of borohydride with 3d transition metals using Density Functional Theory method. The last speaker was Kohei Oka. He studied the spontaneous polarization and piezoelectricity on material $ATiO_3$, which A could be Pb, Sn, Ge, Bi, or Tl. After the last session finished, I, Citra, Mr. Dinh Nhu Thao, and Mr. Nguyen Thanh Tien came back to OSIC.

On Tuesday, October 25, 2011, I and Citra came to Kasai Lab. at 13.00 o'clock. The QEDI workshop day 2 was began at 13.30. The first speaker in QEDI workshop day 2 was Dr. Sujin Suwanna, invited researcher from Mahidol University. He talked about calculation of multiple-scattering amplitudes in the Anderson model. The next speaker after Dr. Sujin Suwanna was my friend, Citra Deliana Dewi Sundari from Bandung Institute of Technology. Her research was about computational study of DSC sensitizer originated from Iron(II) and Ruthenium(II) with a Pyridyl-Quinoline-Framework Ligand. The third speaker was my colleague, Triati Dewi Kencana Wungu. She studied the adsorption of water on Li-Montmorillonite using first principles calculation. After Triati, Kuniyuki Miwa gave presentation about spatial dependence of the STS profiles of Co-adsorbed molecules on metal surfaces. Then, Saputro Adhitya Gandaryus as the next speaker after Kuniyuki Miwa gave presentation about oxygen reduction reaction mechanism on Cobalt-(6) Pyrrole cluster using Density Functional Theory. The next speaker was Febdian Rusydi. He studied O_2 Adsorption on Zinc-Porphyrins and Iron-Porphyrins using first principle calculation. The last speaker was Wahyu Tri Cahyanto. He talked about a DFT study of OOH dissociation on platinum alloy catalysts.

On Wednesday, October 26, 2011, QEDI workshop was begun at 10.00 o'clock. The first speaker was Dr. Dinh Nhu Thao. He talked about some new efficient poisson solvers. The second speaker was me. I presented about computational study of Quinoline derivative as a sensitizer for Dye Sensitized Solar Cell. After me, Susan Meñez Aspera gave presentation about the role of surface distortion on molecular adsorption on the Tri-s –triazine-based Graphitic Carbon Nitride surfaces. After Susan finished her presentation, we took a break for ten minutes. After ten minutes, Joaquin Lorenzo Moreno gave presentation about DFT study on the adsorption of oxygen and hydrogen peroxide on Fe-filled single-

wallet Carbon nanotubes. After he finished his presentation, Nghiem Hoa Thi Minh gave presentation about tuning magnetic interaction in systems of dimers and trimers on a metal surface. After her presentation, the last speaker, Kazuki Kojima gave presentation about magnetic anisotropy in Co/Ni multilayer. After we finished QEDI workshop day 3, I, Citra, Dr. Sujin, Dr. Thao, Dr. tien, and Dr. Nelson came back to temporary office room and waited for visiting Institute for NanoScience Design (INSD) at 14.30. In INSD, we met Professor Akai. He told us all about INSD. After we met Professor Akai at INSD, we came back to Kasai Lab using shuttle bus and then we came back to OSIC.

On Thursday, October 27, 2011, QEDI workshop began at 13.00. The first speaker was Dr. Nelson Arboleda Jr. He talked about first principle studies on atomic hydrogen absorption into graphite edges. The second speaker was Allan Abraham Bustria Padama. His presentation was about dissociative adsorption of H_2 on Mn-modified Ni (111) surface using Density Functional Theory. After he finished his presentation, we took a break for ten minutes. Then, we continued the workshop. The last speaker was Dr. Nguyen Thanh Tien. He gave presentation about the effect of polarization charges on the electron mobility in the single heterostructures based on wurtzite materials. After he finished his presentation, we move to room P1-311 to attend review talk from Abdulla Sarhan. He gave presentation about theoretical study of electron-vibron interaction on surface adsorbed molecules.

On Friday, October 28, 2011, our schedule was visiting Ultra Clean Room (UCR) at 13.00. UCR is designed to realize some materials from computational modeling that have good properties. In UCR, we can realize some materials using condition same as in computational model. In UCR, we met Professor Yamauchi and he gave some explanation to us about everything in the UCR. After we finished our visit in UCR, we came back to Kasai Lab, and we waited for GET-together at 16.00. In GET-together, all of member of Kasai Lab came together with us to enjoy some food like sushi, sandwiches, and snack. After GET-together, we came back to OSIC.

On Saturday, October 29, 2011, we have no schedule at Osaka University. I and Citra have planned to go to Kaiyukan Aquarium. On Sunday, October 30, 2011, it was rainy day. I just stayed at room, but I have schedule at 16.30 to attend welcome party of The Fourth International Symposium on Atomically Controlled Fabrication Technology. On Monday till Wednesday, at October 31 – November 2, 2011, we attended The Fourth International Symposium on Atomically Controlled Fabrication Technology. Our contribution at the symposium was in poster session. On Thursday, November 3, 2011, it was national holiday. I and Citra have planned to buy some Japanese souvenir at Namba and Yodobashi-Umeda Camera for my colleague in Indonesia. On Friday, November 4, 2011, we visited SPring 8. On Saturday, November 5, 2011, I just stayed at my room and packed my luggage because on Sunday, November 6, 2011, I must leaved Japan and came back to Indonesia. I came back safely to my homecountry.

I got many experiences and many knowledge from this program. I want to say thank you very much to Prof. Dr. Hideaki Kasai who invited me, Ms. Mayuko Aihara who always sent important informations by email, buy e-ticket for me, sent an invitation letter from Professor Kasai, sent a letter of guarantee, and many things. I also want to say thank you very much to all of staff and member (Master and Ph.D students) of Kasai Lab for their kindness. And the last, I want to say thank you very much to Osaka University,

Quantum Engineering Design Research Initiative, Jenesys Programme, JSPS, GLOBAL COE, INSD Osaka University, and of course, my supervisor, Dr. Muhamad A. Martoprawiro who permitted me to attend this program.

October 2011

A Report about My Two-Week Visit in Osaka University

John Vincent S. Morales
Assistant Professor 1, DLSU Math Department

Introduction

I've been living for 25 years in the Philippines and yet I have never been out of the country before. Thus, the idea of visiting other places has become one of my greatest dreams. So when I learned from our department chair that JSPS is inviting young researchers to attend workshops in Osaka University, I never hesitated to apply and fortunately I was selected.

I always see Japan as one of the leading countries in terms of promoting science and technology. And to me, Japan is home to the world's greatest mathematicians. When I knew that I was selected, I felt very happy and somehow I knew that I was a step closer to achieving my dream – to obtain a Ph. D. in one of the universities in Japan. So, I decided to contact mathematics professors in OU's Math Department and to meet them if possible.

This is Osaka University's North Gate in Suita Campus, the closest gate to where we were staying – JICA.

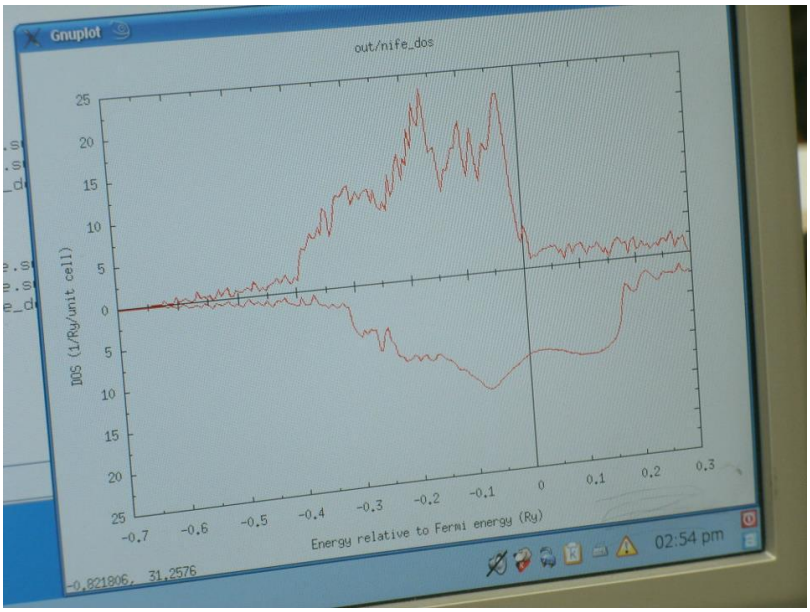
19th Computational Material Design Workshop

This is the Cybermedia Center in Osaka University Toyonaka Campus. We had the workshop in one of the laboratories in the third floor.

For the first week of my stay in Japan, we attended this event. The 19th CMD workshop was attended by people from different places in Asia. I, together with two other Filipinos, was enrolled in the seminar under the beginners' course. Under the beginners' course, participants got acquainted to computer programs that could calculate some properties of substances such as density of states, crystal symmetry space groups, impurities and many more. We had fun for each hands-on activity and it felt gratifying to see that my outputs are correct.

I, together with two other Filipinos, was enrolled under the beginners' course. Here, classes start at 9 am and end at 6 pm.

Aside from the hands -on activities, the workshop invited distinguished professors from different universities in Japan. These speakers discussed the theories behind how the calculations were carried out in the computer programs. As a mathematician, the theory means a lot to me. However, the speakers were talking in Japanese almost all the time that I was not able to follow the discourse. Other than that, the event turned out to be a satisfying learning experience.



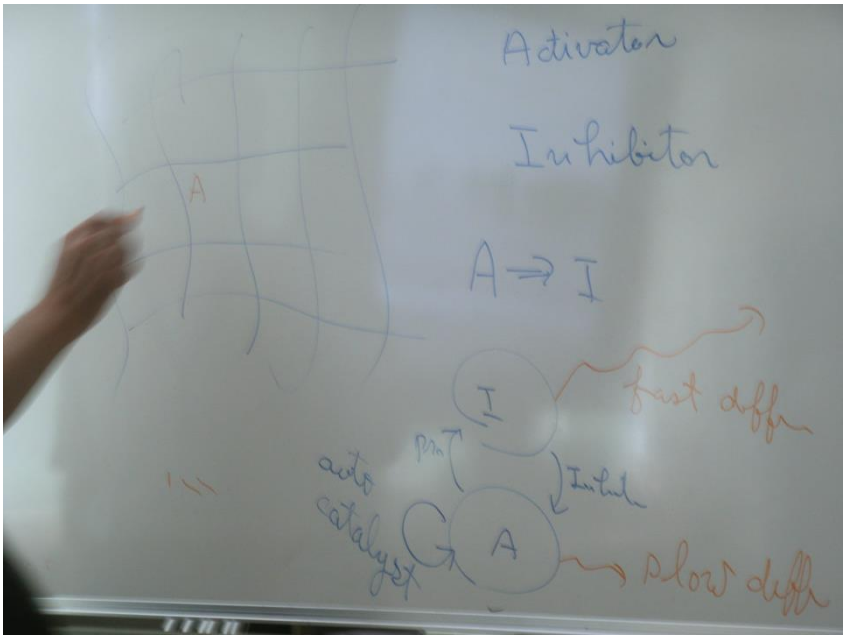
This is a sample output when we calculated the density of states (DoS) of a certain substance.

Research Group (Yagi Sensei)

For the second week, we were spread out into different research groups and I was put under Professor Atsushi Yagi's wing. Yagi sensei is working primarily on functional analysis, mathematical models and its application to biological phenomena. He authored a book entitled "Abstract Parabolic Evolution Equations and their Application", published numerous papers in reputable journals and worked with other notable people.

We were spread out into different groups. We were put under Yagi sensei's wing.

For the first meeting with Yagi sensei, he discussed the mathematics behind the diffusion behavior of Escherichia coli (E. coli bacteria) under the microscope. To do this, he used Nonlinear Diffusion System (NDS) and Continuous Dynamical System (CDS) to generate results. Other than this, he also discussed mathematical models explaining the dynamics of the black-and-white coating of animals using the same tools (NDS and CDS). In this topic, he assumed that there are two pigments causing the black and white color - the Activator and the Inhibitor. Under certain conditions, these pigments will diffuse and thus, the black-and-white phenomenon.



This is Professor Yagi's lecture on mathematical modeling of animals' black-and-white coating.

For the second meeting, Yagi sensei explained the mathematical models behind the forest health condition and spread of mangroves' roots. Using NDS and CDS, he explored the dynamics of the forest particularly the interaction of young trees and old trees.

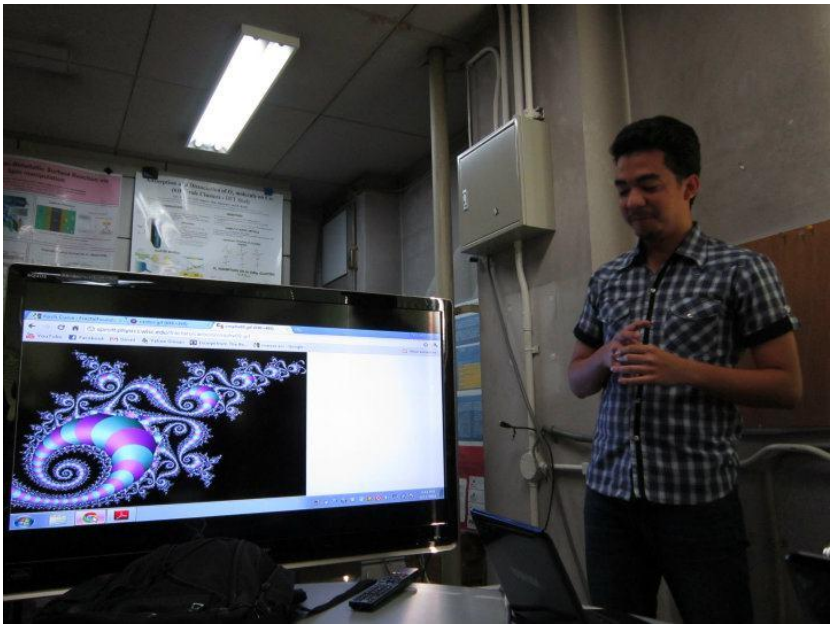
Overall, I found the meeting with Professor Yagi very fruitful and interesting. He made it clear to me that mathematics indeed has applications to real life. Though his research interest is different from mine, he made me see mathematics in a different light.

My Expository Work

After the first meeting with Professor Atsushi Yagi (Monday), Professor Hideaki Kasai instructed our group to prepare expository works from what we have gained from the meeting with Yagi sensei. I have chosen to discuss fractal dimensions and the report would be given on Thursday.

Fractal geometry is not one of my research interests so studying it was a challenge. I had to refer to soft introduction on the topic in order to digest big

information into small ones. I have decided to explain the fractal dimension of two sets namely, the Cantor set and the Koch Curve.



This is my lecture on fractals. I was discussing the notion of fractal dimension to students in the Kasai Lab.

The day came and we have prepared our presentations for the event. I was a bit nervous to see that Kasai graduate students were there to witness our discussions. And to my surprise, they were really asking questions. In my perspective, I think I have delivered properly what I have prepared. It was a wonderful experience speaking in front of experts and experts-to-be in the field.

Living in Japan

Staying in Japan for two weeks, I can say that life there is rather challenging but not entirely difficult. One of the greatest tests that I faced was taking very long walks. In the Philippines, we were used to taking rides from jeeps around the corner and getting to one's destination is easy. In addition, transportation expense is very cheap in my home town. Although trains and taxis are available for passengers in Japan, we find it very expensive and thus we opted to take hikes going from one place to another. We got used to it after a few days.

Each day we take this walkway going to Yagi sensei's laboratory. We also take this road going to Kita Senri where we usually buy our dinner.

Talking to some locals was another challenge. Whenever we buy things or ask for directions, we tried to make signs so they could understand us. I remember one time making gestures just to buy eye drops in a nearby drugstore. It was a wonderful experience though. Since I'm planning to take graduate courses in Japan, I understand that I need to study their native language. I guess it would be fun to learn another foreign language.

During the last day of the CMD workshop, I found time to meet some professors in the Mathematics Department. I grabbed the opportunity to talk to Professor Susumu Ariki and Professor Takayuki Hibi. It was an honor to meet these experts working in algebraic combinatorics – my research interest. They were very kind to explain to me the details of their graduate programs. It was nice to know that they accommodate people who are interested to study in Osaka University. I hope to see them again one day.

Report for Invitation Program – Citra Deliana Dewi Sundari (ITB, Indonesia)

For two weeks (October 23rd – November 6th), I lived in Osaka, Japan, as invited researcher for invitation program funded by JSPS. At October 22nd, I left my country and heading to Kuala Lumpur – Malaysia before flying to Osaka. It was a very nice flight prepared by Ms. Mayuko Aihara, I am so thankful for it. Sunday morning with a nice weather at October 23rd, I arrived at Kansai Airport, and then heading to JICA, check in there, and take a rest. From the first time arrived in Osaka, I was impressed by the city's tidiness, cleanliness, the air is much more fresh than in my country, not many cars and motorcycles in the road, rare traffic jam, and the citizen's attitude are so tollerants.

On Monday, October 24th, I and the other five researchers (from Thailand, Philiphine, Vietnam, and one other from Indonesia) went to Kasai Lab in Osaka University, Suita Campus guided by Mr. Nelson from Philiphine. Mr. Nelson know the way because he was used to be a students at Kasai Lab years ago. The Lab is near JICA building so we went there by foot. After that, we met with Kasai sensei in his room. He was so kind and caring, he even prepare space in his Lab for us to work.

After lunch (Monday at 1 pm), we attended the Quantum Engineering Design Initiative (QEDI) Workshop. This workshop was started by opening remark from Kasai sensei, and then continued by research presentation from graduate students from Kasai Lab. For today, we have seven presenters from Kasai lab, they were Nguyen Tien Quang, Ferensa Oemry, Hirofumi Kishi, Mohammad Kemal Agusta, Yuji Kunisada, Ryan Lacsao Arevaldo, and Kohei Oka. As I paid attention to the presentation, I learn many new things outside of my research field. I learned about oxygen dissociation on metal oxide-supported Pt cluster, effects of cluster size on Pt-O bonds formation in small Pt cluster, study of NO oxidation reaction over Pt cluster supported on γ-Al_2O_3 (111) surface, theoretical study of hydrazine adsorption on metal surfaces, a first principle study of ortho-para H_2 conversion on the Ag (111) surfaces with coadsorbed O_2 molecules, first principle study of spontaneous polarization and piezoelectricity on $ATiO_3$ (A = Pb, Sn, Ge, Bi, Tl), and I also learned about interaction of borohydride with 3d transition metals using DFT study.

All of this topic somehow still related to chemistry. Since my background is chemistry, I could understand the content of the presentation as long as I paid attention to it. All of the presentation topic was related to interaction between gas molecule with crystaline solid which can be applied to many application such as fuel cell electrode, photocatalysis, etc.

On Tuesday (October 25th), the QEDI workshop continued, and this day was schedulled for my presentation. First presentation was from Dr. Sujin Suwanna, invited researcher from Mahidol University, Thailand, and the topic was about calculation of multiple-scattering amplitudes in the Anderson model. The presentation was interesting but very mathematics, so many equations in it which I could not fast enough to realize the physical meaning of it. When a student asked him about the application, he answered that he did not really know about it. He researched about Anderson model because he just want to understand about it. That inspired me, actually, truly a spirit of a researcher.

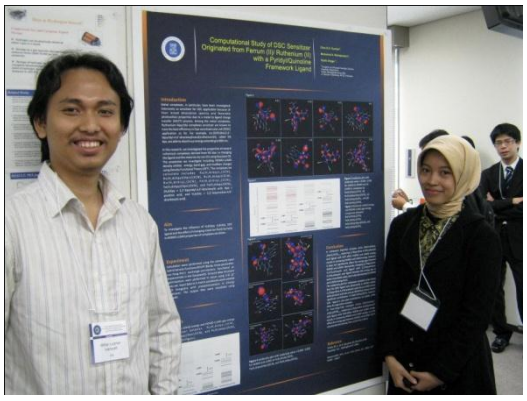
After Dr. Sujin was my turn to conduct the presentation. I explained about the effect of ligand and metal ion replacement in the famous N3 dye to its electronic properties based on DFT calculations. The presentation went smooth and I got two questions and one ally in debating. I was happy for having this

chance, sharing my research with everyone. After me, there were five other presenters from Kasai lab, four topics about molecular dynamics in solid and the rest is about O_2 adsorptions in complex molecules using DFT theory.

The QEDI workshop continued in Wednesday and Thursday. I found that all the presentation topic was interesting. The most interesting topic for me in this last two days of QEDI workshop was the first principle studies on atomic hydrogen absorption into graphite edges by Dr. Nelson Arboleda Jr. from De La Salle University, Philiphine, and the theoretical study of electron-vibron interaction on surface adsorbed molecules by Abdulla Sarhan from Osaka University. Dr Nelson's presentation was very understandable with a complete presented-data and reasoning. From his presentation, I learned about hydrogen atom behavior and why the hydrogen tend to do that, also the future application for graphite as hydrogen storage materials. But the model still use hydrogen atom, not hydrogen molecule we normally found and used in reality though, it was first principle study. Meanwhile, from Mr. Abdulla Sarhan's presentation, I found something that will support my research that is I-V curve calculation using Keldysh green function formalism. Since my research is about photovoltaic materials, I really need I-V curve calculation which I thought that it cannot be calculated before. I will explore about this function more, about how to use it, interpretate it, etc.

QEDI Workshop Participants

At Spring 8



Poster session at Aatomically Controlled Symposium

In front of UCR

I and the other invited researchers also have the chance to visit Institute for Nanoscience Design (INSD) in Wednesday (October 26th) after QEDI workshop, visit Ultra Clean Room (UCR) in Friday (October 28th), and visit Spring 8 (Super Photon ring – 8 GeV) in Friday, November 4th. In INSD we met with Prof. Akai.

After explained about INSD, Prof. Akai accompanied us to see the facilities in INSD. There, I found an ultra precision electron microscope, the precision is up to 10 Angstrom, and its very amazing. In UCR, Prof. Yamauchi assist, show, and explain to us about all facilities in UCR. There are a very precision etching machine, SEM, TEM, and 1 atmosfer room. And the last was visiting Spring 8. We went by bus, together with Ms. Mayuko Aihara, Kasai sensei, and students from Kasai lab, to Hyogo Prefecture. We even went to a tourist attraction site (shrine) and having lunch on the way to Spring 8. In Spring 8, I saw synchrotron facilities for the first time. We visited the main parts of Spring 8 and get explanations for the materials, machine, and how it works. It makes me want to try characterize my material using synchrotron radiation someday.

The last and the main activity I did in Osaka was The Fourth International Symposium on Atomically Controlled Fabrication Technology (October 31st – November 2nd). I took part especially in poster session, but I won't miss the chance to know and learn about the top researcher's research here. I and the other invited were also attend the welcoming party at Sunday night (October 30st) in Osaka University Nakanoshima Center. There, we met many researcher and also met Kasai sensei's family. At the symposium, there are many interesting topics and new invention presented. I especially interested in Mr. Tateyama's presentation about first-principle study on semiconductor electrode/liquid interfaces for photocatalysis and dye-sensitized solar cells, because it is related to my research. In the second day of symposium, my poster presentation went smooth. A few people interested to my poster and ask for further explanation.

Lastly, I left Japan and head back to Indonesia at Sunday morning, November 6th. I enjoyed Japan very much and wish to have a chance to live here longer. One important point that I learned from Japanese researchers here is that they can realized and can make something that theoretically undertandable in papers/calculation into real without thinking impossible! Its like "talk less and do more and impossible is nothing if we try", precious lesson for me to finishing the rest of my research. I want to thank especially to JSPS for the funding, to Kasai sensei for inviting us here, make me learn many things, and to Ms. Aihara for the very kind help and assistance.

REPORT FOR THE JSPS INVITATION PROGRAM

Personal information

- Name: Dinh Nhu Thao, Ph.D.
- From: Hue University's College of Education, Hue City, Vietnam.

Desired purpose of visit

- To attend "Quantum Engineering Design Initiative Workshop" Osaka University, Suita Campus, Oct. 23rd – Oct. 27th, 2011;
- To attend "The fourth international symposium on Atomically Controlled Fabrication Technology", Nakanoshima Center, Osaka University, Oct. 31st – Nov. 2nd, 2011;
- To visit Spring 8 "The world largest synchrotron radiation facility", Nov. 4th, 2011.

Period of stay

23 Oct. – 06 Nov., 2011.

Venue

Kasai Laboratory, Department of Precision Science & Technology and Applied Physics, Osaka University.

Expenses

- Travel expenses: Japan Society for Promotion of Science (JSPS);
- Living expenses: Japan Society for Promotion of Science (JSPS).

We have got a very good financial support from JSPS.

Accommodations

- Venue: Osaka International Center – JICA (OSIC).
- Service: We have been served with very good service with breakfast ticket. Staffs are friendly and whole-hearted.

Activities

We have arrived at Kansai International Airport (KIX) in the later evening of Oct. 23rd, 2011 because our flight from Ho Chi Minh City, Vietnam was delayed due to the technical problem.

On the first day after coming here we started our quite tight schedule. At 11 AM we had a meeting with Kasai Sensei at his Lab. We have a very nice talk with each other about ourself as well as about our research work. And then we attended the first session of Quantum Engineering Design Initiative Workshop held in Osaka University from 1 PM. The workshop lasted until afternoon of Oct. 27th. During the workshop I got familiar with DFT based calculation of hydrogen and oxygen storage and fuel, new topics that we have never had a chance to study before. Also, I have presented our research related to Poisson

solver for the Monte Carlo simulation of semiconductor devices. The workshop is really very useful for us to approach new fields of physics at recent stage and helps us to broaden our knowledge and view. This is very important for us to carry out new research results in the future. We expected the workshop would last longer and give us more details about the calculation technique.

In the afternoon of Thursday, Oct. 27th I had a meeting with Kasai Sensei to find a helpful suggestion and good assistance for our college. The meeting was initiated based on the following points:

1) The Department of Physics of Hue University's College of Education is currently in charge of a program named The Advanced Physics program. The program contains physics courses that are organized, and affiliated with the prestigious University of Virginia (USA). The courses are given in English and taught with the curriculum of University of Virginia (UVa, USA) by world-class professors all over the world, mostly from USA. Students have not only the good background of physics but also the excellent English skills, good teamwork ability, and promised potential. They often get ITP Toefl score of around 550 (corresponding to iBT Toefl score of 90) and they are very active in teamwork. We are looking for chances for students to study as well as to work abroad in developed countries as Japan. We hope our students will grow up quickly and accumulate enough knowledge and experience for the development of Vietnam in the future.

2) Professors from Osaka University have organized ACMD 2010 workshop at our college. Many students have joined this event. They like science very much in general and CMD in particular. Within their eye-shot, Professors from Osaka University are idols in reality.

3) Hue University's College of Education will soon, in this November, build up a center named Center for Theoretical and Computational Physics (CTCP – HUCE). I was proposed to become the Deputy Head of that center. The center is expected to carry out the worldclass research in order to promote our team of theoretical and computational physics and to make our college stronger in researching and training for the final results of raising up the level of students as well as the rank of our college. For that purpose, we are at first looking for the assistance for building up the center including financial support as well as technical support, and then the assistance for building up a strong team to carry out research.

4) Our college will change the administrative board in this November and I was proposed to become a leader of Department of International Cooperation of our college.

In that sense and from the points mentioned above, I have a duty to establish good relations with great universities as well as strong connections with great research groups around the world. I have presented our situation with Kasai Sensei and got an acceptance for assistance from Kasai Sensei thanks to his very kind consideration.

With the help of Kasai Sensei, Aihara Sensei and Mr. Nguyen Tien Quang – a doctoral student of Kasai Sensei, I had a chance to meet Zako Sensei who is in charge of Career Development Program for Foreign Students at 09:30 AM on Tuesay, Nov. 1st. We have achieved satisfactory result that is Zako Sensei will visit our college during Nov., 14th – 17th, 2011 in order to interview our students who are applying to the program that Sensei is the person in charge. Our college has sent an announcement to our

students and we are receiving the registration of our students to apply to the program. Mostly, students under consideration come from the advanced program that I have mentioned above. Moreover, our administrative board is very welcome Zako Sensei to our college and is waiting for his visit in order to get familiar with us and to interview our students. Also, we have agreed with each other about signing Memorandum of understanding (MOU) in the near future.

On Friday, Oct. 28th we have a nice visit to Ultra Clean Room (UCR) under the guide of Yamauchi Sensei in order to see how to "create what could not be created". Yamauchi Sensei is very gentle and Sensei taught us very carefully in details. We went to all rooms in the center and tried our best to get familiar with all equipments. The UCR has got the world record of accuracy that it can make in experiments. This is the first time in our life we have ever visited a laboratory like that. We all felt very excited with the top accurate equipments, complicated research topics as well as with the potential of UCR. We are now doing research on electron mobility in GaN/AlGaN single heterostructures taking into account some special scattering mechanisms however we have never been able to imagine how the samples are made, but now we can.

During Oct. 31st – Nov. 2nd, 2011 we were attending "The fourth international symposium on Atomically Controlled Fabrication Technology" held at Nakanoshima Center, Osaka University. We have been updated with the recent develop of scientific research worldwide. I was more interested in theoretical work than experimental one but I still focused on some experiments that I can understand. Especially, we were emphasized strongly with the DFT based first principles calculation. We have enjoyed very much oral presentation as well as poster session. In both sessions we have seen many PhD students and master students with excellent research results. We think in the future we should manager our research toward application edge as oxygen and hydrogen storage, photonics, substainable energy materials and devices, and protein based electronics devices. I also made a network with young researchers attending the symposium. We have many chances to discuss with each other through tea-break, especially through poster session, and many extra activities such as welcome party, making okonomiyaki, and banquet.

On Thursday, Nov. 3rd, I and Dr. Suwanna from Thailand have enjoyed Japanese culture very much and have had a very nice time with JICA's Wadaiko team. We have done performance together with many Japanese students in front of Osaka castle and we have got big hands and compliments from viewers.

On Friday, Nov. 4th, we have visited Spring 8, the world largest synchrotron radiation facility. We have been introduced about the facility through watching video clip and stepping inside it. We were very happy and lucky that we have had a very nice chance to visit such as a gigantic place ever. The facility is really very modern, complicated and has great potential in doing research at the top. We have enjoyed very much our time there. After visiting that facility, on the way coming back, we have decided to push strongly our research straight toward to new stage.

Besides, on Oct. 29th I visited my advisor – Katayama Sensei in Nomi shi, Ishikawa prefecture. He has been a professor of JAIST when I got a PhD degree in 2004. This time we have had an emotional meeting fulfilled with happiness and big smiles thanks to your kind invitation and kind arrangement.

On Saturday, Nov. 5th, we come back home. The flight from HCM City to Hue City has been delayed because the bad weather condition and we have a flood in our hometown even at the airport. Thank God I am safe!

Evaluation

I strongly evaluate and recommend this program and I expect very much this program will continue in the future.

Acknowledgement

We would like to express our many thanks indeed to Kasai Sensei, Aihara Sensei and all members of Kasai Lab for the invitation and for the very kind help during the time we were being there in Osaka University. And we would like to thank OSIC for the good service. Finally, we would like to thank very much indeed JSPS for the very good financial support.

Report on Invitation Program for East Asian Young Researchers

Sujin Suwanna

Introduction. The Quantum Engineering Design Research Initiative (QEDRI) in conjunction with the Global Center of Excellence (GCOE) of Osaka University has kindly invited and financially supported young researchers from Southeast Asia countries to take part in a research outreach entitled "Invitation Program for East Asian Young Researchers." I am the only participating researcher from Thailand, where I work as a lecturer at Mahidol University in Bangkok, but I am joined by two Vietnamese, two Indonesian and one Philippine researchers for two weeks of workshop and symposium in Osaka, Japan.

The QEDRI is a great idea, and I have learned that it is funded by the Japanese government. Once again, I am humbled by the Japanese hospitality extended to developing countries in Asia and worldwide. This time, I am right at the receiving end of Japan's kindness as Osaka University has many researchers in the field of my interests, and I have been looking for an opportunity to discuss research with them.

At first, I was afraid that the QEDRI program is strictly limited for material scientists or physicists who have interests in material designs. But I am a theoretician (even a mathematical physicist) with little background in material physics, so I was pleasantly surprised to be selected to participate in the program. After three weeks in Japan, I have learned very much not only in the subject of my interests but also on the frontier development of related fields. More importantly, I have made many research connections that can only beneficial for me in the future.

Program Activities. The program is designed for two weeks of research discussion with researchers at Osaka University. In the first week, we had a workshop entitled "Quantum Engineering Design Initiative Workshop: Design and Creation of New Green Nanomaterials" at Suita Campus. Participants at this workshop were mostly students and researchers from Prof. Kasai's laboratory, a big and active research group. The workshop lasted for five days, from October 24^{th} to 28^{th} , which included twenty four talks, and two visits to other research centers. I gave a talk entitled "Calculation of Multiple Scattering Amplitudes in the Anderson Model." While my talk was perhaps too theoretical for the students' interests, I received some interesting questions and comments, and thought it was a stimulating discussion.

Most of other talks focused on the study of material properties in one fashion or another, in which researchers commonly used computational methods in their work. Topics included surface sciences, hydrogen storage in fuel cells, and solar cells. These topics were new and interesting to me, and I had a wonderful learning experience.

For our visits to two research centers, Ms. Aihara had kindly arranged the visits for us (as she had kindly prepared our programs and lodging). On Wednesday October 26^{th}, we visited the Institute for NanoScience Design (INSD) where Prof. H. Akai is the director. The Institute is impressive and has many high-power research equipments, such as an electron microscope which a resolution about a few nanometers.

We learned that the Institute was built for educational and research purposes and for bridging industrial research and academic research together. On Friday October 28th, we visited the Ultra Clean Room (UCR), under the direction of Prof. Yamauchi. We were all impressed with the equipments there, and had a lot of fun touring the laboratory in a white uniform which covered every part of our body, except eyes. For us, it was difficult to imagine our countries being able to build such a high-tech facility, so it was a great experience to have seen it at Osaka University and to know what kind of research requires the ultra clean room.

In the second week of our program, we attended the Fourth International Symposium on Atomically Controlled Fabrication Technology at the Nakanoshima Center of Osaka University near downtown Osaka. The Symposium was sponsored by the Osaka University Global COE Program. There were many oral presentations as well as poster sessions, with topics ranging from photonics, surface and interface nanoscience, novel semiconductor devices, innovative technologies for post-silicon materials to devices and sustainable energy materials. While most speakers were Japanese, there were many invited speakers from abroad, and they all gave interesting talks. The Symposium really stressed the important issues that we are facing today in terms of sustainable energy and environmental friendly materials.

The Symposium had also provided us with opportunities to experience Japanese culture and sightseeing. After the symposium talks on Monday October 31st, there was an excursion session, when the Symposium organizers took us walking around the busiest part of Osaka including the largest underground mall. It was early in an autumn evening, but light display could be seen everywhere on the street. With the weather being so nice, we enjoyed walking, talking and meeting new friends from the Symposium. I have learned so much from talking to Prof. Saditt, from Germany, while we were walking from the subway station. After a while of walking, we arrived at an authentic Japanese restaurant, where we would learn how to cook "Japanese pizza." It was my first time to cook a Japanese meal, and I was excited about it. The restaurant was packed by participants from the Symposium, and that made it even more fun. At the table, we discuss science, education and culture. All and all, it was a great experience.

I presented my poster at the Symposium on Tuesday November 1st. It went well, but the session was short in time, so I did not receive many questions. Nonetheless, it was very well organized and some posters were very interesting, and I learned much from them. The Symposium was finished on Wednesday November 2nd, and therefore our academic activities were formally concluded.

On additional and tangential remarks, Thursday November 3rd was Japan's national holiday, so people did not go to work. Dr. Tao, from Vietnam, and I had learned two lessons of Wakaido, "Japanese drums," at JICA, and we were scheduled to perform in front of the Osaka castle on this day. I was nervous but excited. With only two practices, I hoped we would not make many mistakes in front of the audience. The performance went okay; I enjoyed it and made many more friends than mistakes. There were other performances at Osaka Castle on that day, and a huge crowd. The Wakaido experience had taught me many lessons: determination, unity and friendliness. I was most impressed with the young Japanese drummers and how they concentrated on their jobs, and really performed amazingly and harmoniously.

On Friday November 4th, Prof. Kasai took us along with his students to visit SPring-8, the world largest synchrotron facility. It was more than a hundred kilometers from Osaka, so in one bus we went sightseeing along the way. At Ako Castle Ruin, I learned about forty-seven ronins and their sacrifices which I had heard from a samurai movie. The samurai's honor code has always fascinated me, and I was glad to visit their site on this trip. SPring-8 is big as advertised and we got to see many parts of the facility. Being a theoretician, it was hard for me to imagine how much valuable a facility like this is to experimentalists.

After two weeks, our program was concluded. My new colleagues returned to their countries, and I stayed one more week in Japan to discuss a research on the Anderson model. I had scheduled a meeting with Prof. Keith Slevin at Toyonaka Campus of Osaka University. In addition, Prof. Akai had kindly arranged for me a meeting with his Ph.D. student (Mr. T. Nagata) who had carried out transport properties calculations in quantum systems. This is my research interest, and I am thankful for the given opportunity. My meeting with Prof. Slevin went very well. We discussed my work on the Anderson model on the first day that we met, and later we discussed other methods, numerical methods, to study disordered systems. During the week, I was introduced to many topics--topics that otherwise I would not have learned--such as Anderson transition in plasma oscillations, quantum hall effects, and topological insulators. These topics are new to me, and I can explore them for my future research. Moreover, I had learned from Mr. Nagata how to employ the AkaiKKR package to calculate conductivity from the Kubo-Greenwood formula. The calculation, which is based on Butler's formulation, is much more difficult that I had previously imagined. During the time that I was at Toyonaka campus, I had studied this formulation a little bit, but not enough, and I think I should study more before I can discuss this topic further with Prof. Akai.

The meetings at Toyonaka campus gave me much insight for my future work. Additionally, I have made connections with experts that I could exchange knowledge in the future, and this is valuable for my trip. Before the end of my stay in Japan, I decided to attend the 7th Handai Nanoscience and Nanotechnology International Symposium at Icho Kaikan on Suita Campus on November 10th. While this was a short participation, I got a sense of a direction of research in nanoscience, and actually learned some applications of physics, especially as it related to chemical and biological sciences.

Research Opportunity. I am interested in studying transport processes or non-equilibrium phenomena in a quantum mechanical system, particularly in mathematical modeling of Anderson localization and its transition. Thus far, my work has been mainly in mathematical physics, rather than in computational physics. Earlier this year when I met Prof. Akai and Prof. Kasai in Bangkok at the Computational Material Design (CMD) Workshop hosted by Mahidol University, I had learned about the KKR technique and the AkaiKKR package to compute many physical properties of system such as band structure, density of states, magnetic properties and so on. The package can be used to calculate Green functions, and subsequently conductivity of the system; I had hoped that it would help me to study the Anderson metal-insulator transition. My participation in the

QERDI is helpful in that regards, but the Anderson model is difficult to solve and requires more than the existing computational package.

At any rate, I can say with certainty that my participation in the QEDRI program has benefited me in various ways. (1) I have learned about latest developments in the fields of nanoscience and material physics, both theoretically and experimentally from talks at workshop and the Symposium. (2) I have had a fruitful research discussion with Prof. Akai and Prof. Slevin on conductivity calculations and on disordered systems. More importantly, (3) I have created a research network with colleagues from nearby countries and with experts at Osaka University.

After three weeks in Japan, I return to Thailand with a better sense of what to do in my research, and which direction my research should be extended. For these reasons, and other experiences I have gained, I am thankful for the opportunity given to me by the QEDRI program, and especially grateful to Prof. Kasai for his support and hospitality to make it possible for our participation.

Conclusion. I participated in the QEDRI program for three weeks at Osaka University, where I learned various research developments, discussed a research problem in the Anderson model, and created a research network with young researchers from ASEAN countries and with experts at Osaka University. I also had experienced some wonderful Japanese cultures and hospitality.

Recommendation. In the closing of this report, I wish to make a few recommendations which may help improve the program.

(1) I think the program would benefit young researchers more if they are paired up with experienced researcher at Osaka University. This means they will work closely in a small group which may include doctoral students and a faculty mentor. It also means that, upon being accepted to the program, a young researcher has to identify his research problem to be carried out in the program. Therefore, his/her time in Osaka will be supervised by a mentor and his research problem will be intensely discussed. In the current format, while I have learned much about other people research problems from our exchange and workshop presentations, I am basically working on my research by myself with my own methods. I think it is more beneficial to see a new approach or get some critiques for my work.

(2) The two-week period is too short to carry out a serious research discussion and see evidence of progress. In my case, I would prefer to spend longer time, and perhaps during the months of March to May.

(3) With existing computational tools available at Osaka University, I would recommend that the program adds a short workshop on how to use these tools and software. This can be done in terms of a lecture series given by Ph.D. students whose research work has been based on these methods. I think it e will benefit new students in the group and new researchers, like myself, very much.

Research Progress

By

Lukman Nulhakim

Institut Teknologi Bandung

Indonesia

1. Sep 5 Mon – 9 Friday :

Attending 19th Computational Materials Design (CMD) Workshop in Osaka University Toyonaka Campus Cuber Media Center.

Learning some program for material computation such as Machikaneyama, OSAKA2K and ABCAP. (begginers course)

- 5 sep (Mon)
  - ✓ CMD Introductory Lecture (Yoshida)
  - ✓ CMD Copy mart
  - ✓ Crystal Symmetry and electronic structure
  - ✓ Fundamentals of ab-initio calculations
  - ✓ UNIX crash Course
  - ✓ Get together
- 6 Sep (Tue)
  - ✓ Machikaneyama Introductory (Akai, Sato, Ogura)
  - ✓ Machikaneyama Hands-On
  - ✓ Case study
- 7 Sep (Wed)
  - ✓ OSAKA2K introductory Lecture (Shirai)
  - ✓ OSAKA2K Hands-on
  - ✓ Case study
- 8 Sep (Thu)
  - ✓ ABCAP Introductory Lecture (Hamada)
  - ✓ ABCAP Hands-on

    ABCAP:
    - Environment variable
    - Preparation
    - Calculation of ferromagnetic Ni and the others atom

- AIP
- Si (nonsymmorphic)
- Ferromagnetic Fe
- Antiferromagnetic Cr
- Space group
- Crystal structure
- Examples and exercise

✓ Case study

- 9 Sep (Fri)
  - ✓ Hands on all of study about programe
  - ✓ Special lecture I, II, III

2. Sep 12, Sep 14, and Sep 15, 2011

Visit laboratory: Akai research group

12 Sep 2011: Introduction, group discussion with Akai Sensei

14, 15 Sep 2011: study **my research** about Al doped ZnO nanostructure for etanol application

Abstract:

" Ethanol is one of the chemicals are categorized as VOCs (Volatille Organic Compounds). Ethanol at high concentrations may cause skin irritation, gastrointestinal tract damage, poisoning and even death. Because it is very necessary tool of early detection of the sensor to know its existence.

ZnO is a semiconductor metal oxide that can be used for gas sensor applications. Currently ZnO gas sensors typically work at high operating temperatures, with selectivity and low sensor response. To improve the sensor response, selectivity and reduce the operating temperature can be done by adding a certain amount of doping. CBD (Chemical Bath Deposition) is one method that can be used to fabricate ZnO nanopori. In this research has been conducted by making doping ZnO with Al using CBD method. This method is relatively easy in the process and the process is cheap in comparison to other methods.

Substrates used for film deposition using the precursor is alumina with $Zn(NO_3)_3.4H_2O$ (zinc nitrate tetrahydrate) and $Al(NO_3)_3.9H_2O$ (aluminum nitrate nonahydrate). Analysis of the crystal structure, chemical composition and morphology of samples carried out by using XRD, EDS and SEM. XRD results show that the phase formed is polycrystalline ZnO. EDS measurements show that there is the Al composition in the coating is 1:48 at% Al, 2.90 at% Al and 3:55 at% Al. SEM results showed flowerlike and sheet-shaped microstructure, characterized by the formation of sheets of transparent structure for the samples in Al doped ZnO. From the measurement data obtained by the sensor response to pure ZnO sample at a concentration of 2.5%, 5% and 7.5% by volume of ethanol, respectively 70.88%, 78.21% and 88.57%.

While the sensor response to Al doped ZnO samples, the optimum value is obtained at sample of 2.90 at% Al. For this sample, at concentrations of 2.5%, 5% and 7.5% volume of ethanol obtained value of each sensor response was 95.29%, 95.67% and 96.68%. ”

3. Sep 13, 2011

International Workshop On Collaborative Research On Design And Creation Of New Green Nano Materials (Suita Campus), Osaka University.

We study more about research roadmap in Kasai Group Laboratory and attending group presentation about:

- ✓ First principle study on spontaneous polarization and structural phase transition of the perovskite oxide
- ✓ Interference effect on the STS profile of a coadsorbed molecule
- ✓ First principles calculations of the Adsorption of water on Li-Montmorillonite
- ✓ Interaction of trivalent transition metal ions with water molecules
- ✓ Magnetic ordered states induced by O2 adsorption on Ag (111)

4. Sep 16, 2011

Visiting RIKEN AICS (Advanced Institute for Computational Science)

following the presentation of the RIKEN AICS on a new building with advanced computer research center. Listening exhibition at the RIKEN AICS together all members JSPs and Kasai member group. traveled around the RIKEN and familiar computing system that is in place. Banpaku visited park, one of the green parks recreation with all members.

CMD workshop is very important in developing knowledge in the field of materials design.

Life as a short term student in Osaka University

By

Lukman Nulhakim

Institut Teknologi Bandung

Indonesia

Japan is a country that is very interesting for research. a comfortable environment for research. all is supported by research facilities are very complete and adequate and comprehensive research reference source. I am very happy as a student in Japan. despite its short residence time but I can take advantage of keesempatan and time to be used with the best.

The first day I arrived at Kansai airport. I was very impressed with the airport environment neat and clean. then I went by bus to Osaka to stay at the hotel Ishibashi. Along the way I was impressed with the Japanese environment. I use the bus to the scheduled departure and arrival is very timely. transport a pleasant, clean, no smoke and comfortable. then I use other means of transportation is the train. as well as buses, trains also very timely. Japanese people are very friendly and polite

I live in Ishibashi for 1 week and next week we moved into the dorm JICA. we had a lot to learn to interact with many people from different backgrounds. While in Japan, I was so safe and comfortable. someday I want to stay longer in Japan or working in Japan. I want to develop a career in Japan.

Empty time I use to get to know the area around Osaka. My study of the Japanese culture and society. I really love Japan.

Thank you for Osaka University, Kasai Group and JSPS program. I hope someday I can further study in Japan or to work and develop a career in Japan.

The Short Visiting Report

NGUYEN THANH TIEN

I am a lecture at Cantho University (CTU), Vietnam. CTU is widely recognized as a premier university in the Mekong Delta (MD) of Vietnam. As a leading multidisciplinary university located in the heart of the MD, CTU enjoys a special niche among higher education institutions in Vietnam. I was invited as a guest researcher at Prof. Hideaki KASAI's Lab, Osaka University. The period of visiting is from 23 October to 6 November, 2011. I worked with many others at the lab. They are visistors come from the Southeast Asia and the members of lab. During my stay, I was

i) met Prof. Hideaki Kasai and attended the Quantum Engineering Design Initiative workshop;
ii) visited the institute for NanoScience Design and met Prof. Hisazumi Akai;
iii) visited the Ultra Clean Room and met Prof. Kazuto Yamauchi;
iv) attended the fourth international symposium on Atomically Controlled Fabrication Technology;
v) visited Spring 8 "The world largest synchrotron radiation facility";
vi) and met Prof. Masaru Zako.

Here is the first time I come the Osaka university. This visit has left deep impressions for me.

Nguyen Thanh Tien, 9 Nov 2011.

I have always wanted to visit Osaka University as I have known the Department of Applied Physics, Osaka University focuses on the education and investigation aiming at the development of advanced science and technology, which is based on the fundamental and applied physics and is connected with the revitalization of next-generation industrial foundation. Especially, the research here focuses on the properties of surfaces and interfaces, and other systems in the nanoscale regime. This is the field which I am studying. It is also suitable for my university and my ability. I think that I will try to promote the assistance of the professors to strengthen my studied ability and my university.

I gave my talk on thursday, 27, oct 2011 about the effect of polarization charges on the electron mobility in the single heterostructures at the Prof. Kasai's lab. I had some very good interactions with people at the seminar. I found people very active and interested in upgrading their capabilities. I was impressed that the members of group worked very dynamic and effective. The researchs of group focuse on the design and creation of new green nano materials. I have been very impressed that the Prof. Kasai manages to do and the large number of students in the lab is able to finish their working very good. I also had lunch and dinner with a little the member of group. They are very friendly. I exchanged views on our common concerns.

I was visited the institute for NanoScience Design and met Prof. Hisazumi Akai. He discussed with us about the nanoscience and nanotechnology design in graduate-level education and research training program. I think that this program is very useful for me. I am very interested in two fields: computational nanomaterials and nanodevice design; nanolab hands-on practices for refresher program. I will register to study this program if possible and will introduce this program with the staffs of my university.

I was visited the Ultra Clean Room and met Prof. Kazuto Yamauchi too. This is first time which I vistit a modern laboratory like that. This laboratory researches the giant-scale nanotechnology that enables us to fabricate atomically controlled surfaces with the size of more than several hundreds of millimeters. Here, the cutting-edge products or instruments contribute to the many scientific fields including biology, medical and pharmaceutical sciences, semiconductor device technology, and X-ray free electron laser optics etc. Prof. Kazuto Yamauchi introduced with us modern devices and new methods to study nanoscience and nanotechnology. Although I can not understand whole problems but I can understand some physical mechanisms and some processes of nano-scaling. I pay special attention to the way to reduce the surface roughness. After this visiting, I will orient the next researchs in near future.

Attending the fourth international symposium on Atomically Controlled Fabrication Technology is an important activity in this visit. The aim of this symposium is present the creation of new fabrication processes beyond the current limitations, the systematization of the fabrication processes as science. This symposium highlights the recent achievements in the program. The symposium consisted of keynote lectures, contributed talks and poster presentations and provided an opportunity for scientists and engineers to exchange information and ideas. Some invited talks were presented by scientists come from the top universities and institutions in the world. Interdisciplinary studies and discussion on the future directions of the fields were strongly encouraged. This is good opportunity for me to have a good knowledge of this interesting field.

I also visited the Spring 8, is a large synchrotron radiation facility which delivers the most powerful synchrotron radiation currently available. Consisting of narrow, powerful beams of electromagnetic radiation, synchrotron radiation is produced when electron beams, accelerated to nearly the speed of light, are forced to travel in a curved path by a magnetic field. Here, I was known that SPring-8 is the world's largest third-generation synchrotron radiation facility, provides the most powerful synchrotron radiation currently available. SPring-8's ultra-brilliant synchrotron radiation gives researchers exciting opportunities for advanced research in materials science, spectroscopic analysis, earth science, life science, environmental science, industrial applications and so forth. It is wonderfull ! I can not image this before. I was watched the video of history of Spring 8 and its operative state now. I was looked the facility of Sping 8 and the other facility. We discussed about the mechanism to create the X-ray laser. I also didn’t forgot to take some photographs here. I will discuss with my colleagues and students about the extremely power of Spring 8.

In addition, I and Dr. Thao disscused with Prof. Masaru Zako about the Advanced Education Program for Master's Degrees. From there, we known the aim of this program is to promote the acceptance and employment of exceptional foreign students into Japan with the goal of fostering innovative human resources in Asia. I will inform this program with my students and my leads. I will choose the excellent students apply this program if possible.

To learn about Japanese history and culture is very enjoyable. I recorded many interesting things in this visit. I will not forget to relate those events with my family, friends, and students. I hope that Osaka university in general and in Department of Applied Physics particular will cooperate and help us more in the future. I know that Osaka university and my university are preparing to establish long-term relation in many fields in the near future.

Hello my name is Nguyen Van Chinh. I come from Vietnam, I'm a second year master's degree at the University of Natural Sciences, National University of Hanoi in Vietnam. Currently I'm doing the calculations in materials science. Come to the JSPS program I found very interesting.

Very surprisingly the first time we buy a bus ticket vending machine. The machine in the country we do not have. Although the automatic machine but has instructions specific images, which helps a lot for me to use. When the bus to the hotel, we have the opportunity to observe traffic streets and Japan in the evening. We have heard much about the traffic of the country of Japan, but this is the first time I've seen firsthand. With a massive transportation system scale and modern power makes me wonder. I go to the hotel by . This time is 9 pm. We leave a day before the meeting at the Toyonaka Campus Cyber Media Center.

We entered the 21st Century witnessing several remarkable progress in Science and Technology. Novel materials and devices that were once considered the stuffs of science! fiction are, one after the other, becoming a reality. First-principles method is a method to calculate accurately material properties from fundamental equations of quantum theory only. By using this method, we are able to study not only static properties of materials (crystal structure and band structure), but also dynamic properties such as diffusion and phase transition at finite temperatures, in which most experimentalists are interested. Our study is not limited to study the electronic properties of existing materials. It is our mission to predict unknown or non-existing materials. More-over, it is also important to give guideline to experimentalists how to synthesize such materials. I attended the workshop to learn about first-principles method and application.

The opening ceremony will be started at 12:00 at CALL1 room of Cyber media center(3rd floor). After, they begin CMD. All the texts will be prepared by English, aside from some will be given by Japanese (Crystal Symmetry& Electronic structure, Case studies). However, hands-on training including UNIX Crash course will given by both. There are many tutors to support the training. They can support to me by English. I have questions in all lectures and trainings, I can ask the teacher and tutors by English. This helped me a lot. Workshop begin with a lecture about KKR-Green's function method by Kazunori Sato (June 1998) modified by Masako Ogura and Hisazumi Akai (August 2008). In this lecture, how to use Machikaneyama2002 (AkaiKKR), a KKR-CPA-LDA package, is briefly guided. The KKR method is one of the methods of electronic structure calculation and is also called "Green's function method". KKR indicates the initials of Korringa, Kohn, and Rostoker, who invented this method. CPA means the coherent potential approximation, which can deal with random systems. Green's function might be difficult to understand if you are trained with ordinary band structure calculations, which solve an eigenvalue problem by diagonalization. However, you can apply KKR-CPA to much wider range of situation than ordinary band structure calculations can do. For example, it can deal with finite temperature magnetism and partial disorder systems since CPA can treat not only periodic systems but also random systems. I use it to calculate the electronic structure and put some defects, some donors or accepters, some magnetic impurities in zinc-blende GaAs. More wonderful, you can download KKR program directly from internet. The lecture is very interesting when I first learn the code OSAKA 2K. This program has the ability to find the

minimum geometry. This is very attentive to me. With “Osaka2k”, we are the leading members of the computational materials design consortium under conduction of Osaka University. This activity includes a series of regular school (twice of year), special lecture on demand, publication, etc. In the regular school, five-day treaning of program codes including “Osaka2k” is intended for users skill up for computation. Many case studies by experts increases experiences for materials design. Exchange of knowledge of individuals stimulates new ideas of materials design. Next the lecture, I learn All electron Band structure CAlculation Package (ABCAP). We have study the symmetry of crystal (symmetry operations), study the symmetry of wave function (irreducible representations), and study the optical transition between valence and conduction bands (dipole allowed). I use code ABCAP to calculate band structure, DOS (density of state) for Ni, AIP, Fe, Si, Cr. The section have Density Functional Theory (DFT), FLAPW method, Full potential, crystal structure.The end lecture, Prof. HAMDA introduce the web http://crystdb.nims.go.jp/index_en.html. This web is very useful for me to search information of atom.

Case study I of Prof. Ons Egami begin on tuseday.
(1) Outline of Computational Method for Electronic Structure & Transport Simulation:
(1) Real-space finite-difference method
(2) Overbridging boundary matching method
2. Applications
(1) Conduction property of sodium nanowire
(2) Conduction property of aluminum nanowire
(3) Conduction property of helical gold nanowires
(4) Conduction property of fullerene nanowires
(5) Tunnel current in STM system
(6) Leakage current through gate dioxide
The section introduce calculation method of the bulk wave functions. For example: Conduction properties of sodium nanowires, Al nanowire under elongation, conductance of Al nanowire, leakage current through silicon oxide films, conductance of C_{60} wires, charge distribution of the incident electron, conductance of Li@C60 chain, Density of states in C_{60} and Li@C_{60} wires.

Case study II of Prof. Yoshiyuki Miyamoto has name:Time-dependent First-principles code and its application to excited state dynamics .You give me a lecture about your strategy of program-development in addition to your example of computation. Could you tell us how to get budget, human resource and how you could do in private company? Your comments on future architecture of supercomputer to which we must adopt ourselves would be very welcome.” This lecture have out line
1. Strategy of code development
2. Strategy of computational target
3. Example of Applications
4. For Next Generation Supercomputers

when I finished the lesson, I get answer for questions why we (don't) need supercomputer? Because I can understand everything without experiments but I can't understand everything without experiments. We need supercomputing to simulate large and complex phenomena which are hard to understand by our own brain.

Case study III of Prof. Hideaki Kasai: Many body effects elementary processes at meta surfaces.

The end workshop I get result

+ I can achieve an understanding of first-principles method and application

+ I use KKR program, code OSAKA 2K and ABCAP. I calculate band structure, DOS, … for my research.

Invitation Program for East Asian Young Researcher

I am the second year of master degree student from Mahidol University, Thailand. JSPS and Osaka University offered me the one of the greatest opportunity in my study life. In this program, I had chances to open my scientific view point and to have new experience which was invaluable for me. When I was in Thailand, my viewpoint of the material and quantum design research was very limited, but this journey taught me and extent my scientific boundary. Many things, I have never heard or seen before, was discover here – It impressed me very much.

On the schedule activities

On the first week, I attended Computational Material Design Workshop Fall 2011 at Toyonaka Campus, Osaka University. CMD workshop was very interesting and useful for me. There are many gainful topics, for example, Basic knowledge for computational material design research and quantum calculation, practices for Machikaneyama, OSAKA2K, ABCAP, and others special topics and case studies. Unfortunately, most of the workshop was in Japanese language which I could not understand, but the hand out and example made me understand some of them. This workshop was very beneficial to my thesis. Because I am new in this field of research, this workshop taught me a lot and gave me the opportunity to learn how to think and how to work in this field. In addition, I had a chance to meet other young researcher and the program developer who I can talk to and answered my doubts about quantum calculation. I had been attended two parties in this workshop and I talked to Japanese students, professors, and other participants from Vietnam, Philippine, and Indonesia – they were wonderful. Not only the benefits in scientific that I got from these, but also the social and cultural study. This kind of workshop is not familiar in Thailand, therefore; there are a lot of knowledge and experience.

Now, I am working with Machikaneyama about the electronics structure and magnetic properties of the iron, nickel, and cobalt - ternary compound, thereby; Computational Material Design Workshop in Osaka helps me a lot for the better use of the Machikaneyama program in my work and the understanding of the basic knowledge and the calculation process.

The Monday of the second week, I spend most of the time working out with paper of the Evaluation of Schottky Barrier Diodes Fabricated Directly on Processed 4H-SiC(0001) Surfaces by Y Sano, Y shirasawa, T Okamoto, K Yamanuchi because Prof. Yamanuchi went abroad to international conference. I spent Saturday and Sunday night studied about this paper and what is the research of Prof. Yamanuchi's laboratory interested in. This is the abstract of the paper that I read which gave me general idea about the SiC one of the interested material in this laboratory.

Evaluation of Schottky Barrier Diodes Fabricated Directly on Processed 4H-SiC(0001) Surfaces

Yasuhisa Sano[1,*], Yuki Shirasawa[1], Takeshi Okamoto[1], and Kazuto Yamauchi[1,2]

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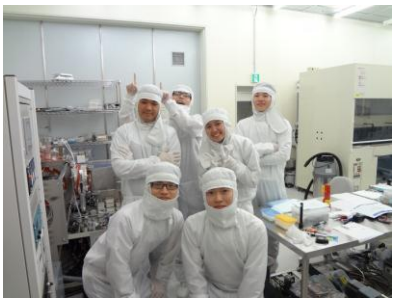
[2] *Research Center for Ultra-Precision Science and Technology, Graduate School of Engineering, Osaka University, 2-1 Yamada-oka, Suita, Osaka 565-0871, Japan*

Silicon carbide (SiC) is a suitable substrate for low-power-consumption power devices and high-temperature applications. However, this material is difficult to machine because of its hardness and chemical inertness, and many machining methods have been studied intensively in recent years. In this paper, we present a simple method to evaluate the electrical properties of the processed surface using the ideal factor *n* of a Schottky barrier diode (SBD) fabricated directly on the processed surface. Upon comparing the values of *n* for SBDs fabricated on a damaged SiC surface and a non-damaged SiC surface, we found that there is a significant difference in the dispersion and magnitude of *n*. Furthermore, by combining this technique with slope etching, we were able to estimate the thickness of the damaged sub-surface layer.

On Tuesday of the second week, I attended the special meeting which students in Prof. Kasai's laboratory were the speaker. The topics were their researches that made me understand what kind of research they are working. There are a lot of foreign students in Prof. Kasai's laboratory such as Indonesia and Vietnam, but there is no Thai student there.

The next two day – Wednesday and Thursday, I went to Prof. Yamanuchi's Laboratory. The students presented their name, hobby and research briefly, in the first morning. This laboratory is working about X-ray mirror, X-ray focusing lens, microscopy, surface processing with ultra-precision technique, etc. In the afternoon, I went to ultra-clean room which was my first time for entering clean room. At first, we toured around the ultra-clean room and discussed about abilities and duties of some machines. Not only the researches here that different from Thailand, but also the tools and machine were high technology and complete. In my research field, mostly, I used only high performance personal computer, so I am not familiar with the experimental equipment. However, I can know at first sight that there was a huge gap of the science between Thailand and Japan. The experience of the visiting Ultra-Precision laboratory told me that the boundary of the science is extended at every moment. Their work about the x-ray mirror and surface processing was amazed me a lot because this was the new information for me that we can process the surface to be smooth in atomic

range! Some of the machines are in Thailand, too, but most of them were not being seen in my university laboratory. For this two day, we (I, Vera, and students in Prof. Yamanuchi's Lab) processed the surface by using elastic emission machining (EEM) and then we investigated the surface by Atomic force microscope and interferometer. After that we processed new surface by Catalyst-referred etching (CARE) technique. The surface was examined by AFM. Later, we used ion beam figuring machine and investigate the result on substrate by interferometer. At last, we watched the demonstrate of the sputtering process of the Platinum on the Silicon substrate. In the evening, we had a party in the Yamanuchi's Laboratory. Everyone is very kind to me and I hope someday in the near future I will come and visit them at Osaka University, Japan again. The scientific experiments were very impressive. It was one of the greatest experience and rarest opportunity in my student life.

On Friday, we visited the biggest supercomputer "K-computer" at RIKEN, Kobe. This was my first time visiting the supercomputer, too. It was very excited me about how large and powerful it was. I have only been working in computational simulation for a few months with my personal computer, but supercomputer might help the scientists and the researchers a lot in their simulation. It was the valuable chance for me to visit "RIKEN". I would like to thanks JSPS for giving this opportunity for me.

Free time activities

I hoped this visiting Japan could be very valuable for me because not only scientific knowledge and research work, but also culture and society. That is all true for me I got the knowledge a lot, met new friends from various countries, experience new culture and society, etc. The time I spent in Japan, now, becomes one of my favorite memories.

On the first weekend, I went to the downtown by Hankyo train for touring with my Thai friend who was studying biotechnology in Suita campus, Osaka University. I try some Japanese food at Umeda and took a subway to Namba for sightseeing. I spent most of Sunday evening traveling around, taste Japanese food, and visiting department store.

The next Saturday, I went to Kobe and visited many places with my two Thai friends (both were studying in Osaka University), for instance, Kitano, Tenmangu Shrine, Mount Rocco, and Kobe Port.

For the last weekends, I traveled to Kyoto on Saturday. I tried some Japanese food and brought some souvenirs and amulets from the temple.

On Sunday, I wandered around Osaka Port and visited museums such as Osaka Museum of Housing and Living, Osaka Maritime Museum, and Osaka Aquarium Kaiyukan with the group of Thai student who was studying in the city around Osaka.

The last day in Japan – Monday 19th, I wandered around Osaka for visiting Osaka Castle, Osaka Science Museum, Osaka museum of history, Shitennoji Temple, Osaka Municipal Museum of Art, and Tennoji Zoo. At the end of my journey, I went to Kansai international Airport and come back home safety.

I had visited many places in Japan in this trip. Not only the science, but also culture and history I was experience. I felt very enjoy staying in Osaka Japan, and I, myself, be confident that in the future I will visit Japan again.

Conclusion

There are many things that I learn from this long trip in Japan. In science, I know that there are a huge gap between Thai and Japanese science society. It is my responsibility to improve the science in Thailand because I have got the government scholarship and, in the future, I will work for Thai government as the lecturer or the researcher. This visiting give me the inspiration to improve myself and Thai scientific research. I have been to many countries, Malaysia, Myanmar, Singapore, and Japan, Japan is my favorite place because of the orderly and the cleanness. I interested in history and culture not less than science and technology, so this visit give me a chance to wander around by myself, study Japanese lifestyle, and history better than last time that I visited Tokyo three years ago. I feel very thankful to the JSPS for the funding and I would like to thank Osaka University for my visiting. I would like to thank Prof. Akai, Prof. Kasai for inviting me and give me this invaluable opportunity to attend this program, and thanks Mrs.Mayuko for coordinating. I promise I will do my best to keep going forward in my scientific work. Thank you from my heart.

Krit Charupanit

Mahidol University, Thailand

Life as a short term student in Osaka University

This is the first time, I go to the Japan country.

In Jica We have a party with other friend

In the lecture

2011-09-10_Osaka in 2 weeks

Life as a Short Term Student in Osaka University

Hanifadinna

Master Students, Department of Engineering Physics

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I was so grateful to have an experience about living in Japan because until now Japan is still well known for its advance in science, technology, and industry while maintaining high belief in traditional cultures. Especially Osaka, the place that I never realized I have been there for some times. I was happy and grateful for having an opportunity to get the 19th CMD course and laboratory visiting program in Osaka University, one of the best university in Japan.

I feel so overwhelm to get a lecturer directly from the expert of computational material field during the CMD. Here, within this writing I want to express my gratitude. Thank you very much to Kasai Sensei and their administrative secretary in giving me a chance to visit Osaka University via the JSPS Inviting Young Researchers Program. Thank you very much for the facility I got during my time. Everything is well prepared and well arranged.

Through the CMD workshop I can learn some code which developed directly by the author. I've got two intensive classes during the CMD workshop. The lecturer was very kind and the teaching assistant also very patient in teaching me. The workshop that I got has broadened my knowledge about the code of material design and the first principles study.

I also want to address my gratitude to Yoshida Sensei, a person who gave me a chance to know about the research activity in his Laboratory. I've been there for three days and I've got a very nice welcome when staying. At the first day laboratory visit, I attend the Laboratory weekly meeting to see some of the research progress of the laboratory member. That was so interesting that I could see the presentation. Although I couldn't understand the language, I saw that every member was so enthusiastic in giving a response to those who present the progress. I felt that everybody is support each other to give an intern improvement. The Laboratory is the comfort laboratory I've ever felt. It just like home in campus with very nice member. Thank you so much also for every kindness and easiness during my time there. I got so many inputs to know about the research of some laboratory members. Those have brought me into a new perspective about the research in the area of magnetism and computational design of nano material.

The everything that I got has persuaded me so much to knows the research about the magnetism and the first principle calculation.

Bandung, October 2011

To know that I accepted as QEDC short term students made me not only happy but very happy. To be here, at Japan it just like my dreams becoming true. Honestly at the first three month I was confused what should I do?, everybody has busy with his own project and I think I am nothing and not enough smart to be here and wasn't good compared to another. It's Ok!! Those of bad feeling were fading away. People just need sometimes to know their surrounding right?

I have been living in JASSO dormitory for almost eleventh month until now. There, I could knowing each other from different country, different culture, different language and different life style, but we realized we are united, were living in Japan, we appreciate those of Japanese culture which anything well arranged and everybody well behave.

The most grateful is I'm being a part of Kasai Laboratory Member. At the first sight I was proud to be here, I met Kasai Sensei, and I felt that sensei to much kind like my Lecturer in Indonesia Prof. Hermawan. Every student in Laboratory has a schedule of face to face meeting with Kasai Sensei in every week. Until now I'm about feeling guilty to sensei because sometime I didn't stick to my work, he is too kind and humble. I would like to thank to Kasai Sensei for giving me an opportunity to be a part of Kasai Laboratory Member. Otsukaresama sitsurei shimasu

Although I have finished all of my credit semester for finishing my bachelor degree in my home university ITB-Indonesia, here in Osaka University I took some undergraduate class. The class I attended are presented in Nihongo which sometimes it feel so hard to understand but as I explain above, Japanese always trying to give their best to another, again I'm so grateful I met another kindly person Lecturer namely Goto Sensei. He always translated for every single word he wrote on green board in English and explains with very patient.

I have been doing my research for Fe-polypryrrole, which in fact I have been started since my last semester in ITB and today I still got tide up to report it into the paper worked. I have difficulties to arrange word by word. I realized I need to much learn, effort and consistence to be able to write. Japan is well known for its advance in science, technology, and industry while maintaining high belief in traditional cultures. With this his condition, soon I believe, is become high motivation for another future students in pursuing QEDC program in Osaka University, one of the most pride university in Japan.

It’s not that much hard to well adapted in Osaka. I met so many Indonesian and moreover they are my senior in the same major from ITB. Here I feel so amazed to see so fast rescue and work of secretary in Kasai Laboratory. Thanks To Tanaka-san who always taking me care for a bunch of administration problem that I can’t handled it only by me and also all of member and staff of Kasai Laboratory.

I’m enjoying every single time in Japan. I have a look so many events, I can attend to international class seminar, I can even join to CMD workshop in Kyoto with free of accommodation. I finally accustomed to present my research and to be brave to talk with the stranger.

I don’t know how many word to describe my grateful and, I feel these so wonderful, happy and overwhelming has got experience to live abroad. These preliminary experiences were brought me in highly regarded country Japan and escaped in friendly Suita-shi Osaka-fu. Someday I believe I will miss this place missing the discipline people, full of smile and fast paced in action.

Osaka, August 16, 2010

Life as a short term student in Osaka University

My life is very lucky because I could visit Japan twice. At the first time, I went to Tsukuba, Ibaraki to attend Asian Science Camp. But then I spent most of my time in Conference room and hotel. So I did not understand much about Japan. At the second one, I had more time to travel around and learn more about Japan. This helped me to realize that Japanese people and Japanese culture are very very nice!

In this program, I attended many workshops. Those were good chances for me to understand better about the serious academic atmosphere in Japan. Besides, I could meet some great sensei who are the leading professors in Materials Science, and I could learn a great deal from them.

After CMD Workshop, we had a free weekend. Ms. Linh, I and two other Vietnamese guys decided to go to Kyoto, an ancient capital of Japan. Kyoto is a city for tourism, where

Japanese culture has been preserved so well that I could gain a lot of cutural facts. The first place we ran into is a hand-made store in which everything is made meticulously and sophisticatedly. After that we went to Gion, an area where geisha lived in the past. At this place I was totally satisfied when coming across a geisha who has very charming beauty and owns a refined manner. I must love her at the first sight! Kyoto brought to me an impressive feeling that I could not stand introducing to my friends when I came back.

Beside Kyoto, we also enjoyed views in Osakajo (Osaka Castle) and Kobe. When walking around the Osakajo, I saw a traditional dacing performed by high-school students. It was such a lively dance that I was really excited and relaxing. The inside of Osakajo has been coverted into a museum that shows history of the castle and Osaka. However the inside is not as antique as it should be. The other interesting place is Kobe city. Because it is a port city, we could see the mixture of many cutures

there. For instance, you might come across an European architecture, or a Chinese store in the street. Food is also influenced from other countries. Thus, the city is an ideal place for a foreigner to recall his/ her motherland.

Japan is also famous for its various kinds of delicous food. Among many dishes I tried such as sushi, takoyaki, barbecue, onigiri, and so on, I like udon and seafood soup the best. Japanese foods are not only delicous but also very good for one's health. As I looked at any food, I could easily find the amount of nutrition it contains.

Japanese people are very hospitable, helpful and studious. Aihara-san and other secretaries helped us a lots in visa application, accommodation, and many many more. Some Japanese friends whom I met in train station were so enthusiastical to show us the way. This is a picture of a Japanese man whom I ran into when I walked around JICA. I like him so much. He has a generous love to his family, so he tries to work the most as he can (usually from 5a.m to 7 p.m) to support them. It is more respectful that while he is working as a driver, he tries to learn English, and he speaks English very well. All of the Japanese I met gave me a big lesson of how to live meaningfully.

This time was also a good chance for me to meet lovely friends. Other invited students in the program are all friendly and very very excellent. We had an unforgettable time together. And I hope that it is good base for good connection between scientific researchers around East Asian in the future. Besides, I met some Vietnamese students who are studying in Osaka University. They are very active, hard-working, and lovely. Without hesitation, I can say that I am very pround of you!

The second visit to Japan gave me an absolutely interesting experience. I could not only study useful knowledge in Materials Science, but also learn the beautiful culture and meet many great people. The experience really encourages me to go back Japan for my futher studying. Hopefully, Japan will welcome me in a near future.

Duong Thi Diem My

Carlo Antonio T. Ng

De La Salle University - Manila

The opportunity I had to be a short term student in Osaka University was a wonderful one which I enjoyed and learned a lot from. Life in Japan and in the campus was very different from back here at home in the Philippines and was a pleasant one.

My visit last September 3-19 was my first time to go to Japan. On our first week we attended the CMD workshop at the Tonoyaka campus and stayed in a hotel near the area; and on the second week, we were assigned to visit a professor's laboratory, which I was assigned to the Akai Laboratory also in the Toyonaka campus, attended a day of seminars at the Suita campus and visited the RIKEN Institute on our last day of the program.

I was able to visit two campuses of the Osaka University and I saw a different side of the university from both of them. Compared to our university's campus, they were very different from each other and I enjoyed the two Osaka University campuses despite than. Both De La Salle University and Osaka University are composed of a lot of buildings housing different facilities in the campus. The difference however was the space the campus occupied. Since the De La Salle University back here is situated in the heart of the city of Manila, the buildings are built very near to each other such that space is maximized. Because of that, there are only few open spaces in our campus. Comparing Osaka from our home university, I was able to appreciate the open spaces in the campus for students to use in various activities. During my first week at the CMD workshop, during the breaks, I would go out of the Cybermedia building and just enjoy the fresh air and it would refresh me and my mind. The campus, for me was very conducive to learning. Aside from that, I was also able to see students enjoying the open areas of the campus, since we were there during the summer break, I expected to see an empty campus; but to my surprise, there were a lot of students enjoying the campus that time. Students were playing different sports activities in the big open field beside the Cybermedia center; students were enjoying each other's company in barbeques both in the afternoon and at night. Students were using bicycles to get around the campus which I also found very convenient.

When we visited the Suita campus on the second week, I was able to see a campus which was slightly different from the Toyonaka campus. I think that the Suita campus was larger and had more trees in it. Despite the big size of the campus, there were a lot of signs inside the campus which helped a lot for me in finding the places I had to go then.

On the second week of the program, I was assigned to visit the Akai laboratory again in the Toyonaka. In the second week of the program, we transferred lodging from the Ishibashi area near the Toyonaka campus to the JICA-Osaka International Center which was located just at the back of the Suita campus. In going back to the Toyonaka campus, I was able to enjoy morning walks from the JICA-OIC to the monorail station in front of the Osaka University Hospital. I enjoyed the walk early in the morning when it was not that hot yet and with the fresh air. The closeness of the monorail stations were also very convenient since both campuses were very near to the monorail stations, so when I alighted from the train, it would just take me a short walk to reach the other campus. In the three days I rode the monorail, I was amazed at the complex, but convenient set-up of the rail lines. After the laboratory visit, before going home and during the weekends I would try our riding the other train lines to go to one place to another. The changing of trains and the changing of the train lines were hard to understand at first, but after a few rides I got the hang of it and appreciated the train lines and how they were connected from one to the other.

By having the privilege to visit Japan and Osaka University in this two week program, I was able experience living and studying in Japan even for a short time. I was able to appreciate Osaka, the places we stayed and visited, and the campuses of Osaka University. This experience gave me something to look at if I would decide to continue further studies in Osaka University.

By talking to the professors who were also in the program, students currently studying in Osaka University, including some of my friends taking up their PhD studies there, I was able to learn more on the life as a student and researcher in the university. They gave us things on what to expect and life in the university. The programs offered were also discussed, both for short-term studies and longer studies such as Master's and Doctorate studies, by the professors. And from this, I would consider taking up possibly doctorate studies in Osaka University after I finish my Master's degree; like what the previous graduates in our university has done after obtaining their Master's in Chemistry degree.

LIFE EXPERIENCE DURING STAY IN JAPAN

Fadjar Fathurrahman
Computational Science Master Program
Institut Teknologi Bandung, Jl. Ganesha 10, Bandung, Jawa Barat, Indonesia

Saturday, September 3rd, 2011. We arrived at Kansai International Airport. It was rainy even though I heard that it was summer in Japan, then. We went to Hotarugaike via airport's limousine bus. We stayed at Ishibashi Hotel.

Sunday, September 4th, 2011. I just spent my whole time in my room. I just realized that crows are very common in Japan. I learned how to use chopsticks from internet.

Monday, September 5th, 2011. 1st day of Computational Design Material (CMD) workshop. We were very late to meet up at Kasai-lab for overview of the program. I also met three Indonesians in the workshop. They came from LIPI and I had already met one of them in the previous CMD workshop in Bandung (2010). Whoa, that's unexpected. I thought that only sixth of us would be Indonesian. We also met another person from Indonesia who studied in Akai-sensei's lab.

I attended advanced course on RSPACE by Ono-sensei.

Tuesday, September 6th, 2011. 2nd day of CMD workshop. I continued the advanced course on RSPACE.

Wednesday, September 7th, 2011. 3rd day of CMD workshop. Course on RSPACE had ended and I attended advanced course on Machikaneyama-Akai-KKR. Akai-sensei told us that in KKR method, we does not need to diagonalize the Hamiltonian matrix. I did not yet understand the details yet (because I have to study the theory and read the code to fully understand why this is the case), but this is very interesting. I think someday I will also try to study this KKR method.

Thursday, September 8th, 2011. 4th day of CMD workshop. From this day course, I learned several interesting application of Akai-KKR to calculate Curie temperature of magnetic materials.

Friday, September 9th, 2011. 5th day of CMD. We had several interesting lectures this day, especially from Sato-sensei and Oshiyama-sensei. We checked out from Ishibashi Hotel and went to JICA.

Saturday, September 10th, 2011. I did not go outside JICA this day. I spent my time to review my cureent research on diagonalization of Hamiltonian matrix. I still tried to adapt with the food here. Fortunately, in JICA food was more conditioned for foreigner. Even so, I still wonder where I can get sweet tea here?

Sunday, September 11th, 2011. I went to Suita campus in the afternoon. I want to familiarize myself with the environment before going to Morikawa-sensei lab tomorrow. I also went to a supermarket to buy some food and drinks. The environment is very different from Bandung (city). It was very cozy. There were no irritating noise of cars or motorcycles here. There were no traffic jams. The pedestrian like me will be very happy to live in the situtation like this. In Bandung, I have to be VERY CAREFUL whether I want to cross the street or just walk by.

Monday, September 12th, 2011. I, Raymond (from Philipine), and Nam (from Vietnam) visited Morikawa-sensei's lab. He talked to use about the researches we are doing now. He introduced us to his staffs and students. He also invited us for dinner. My friends though that I got lost because I was late and the fact (?) that my sense of direction is bad.

Tuesday, September 13th, 2011. We attended workshop that was held by Kasai-sensei's lab. My lecturers, Pak Nugraha and Pak Supri also gave their talks.

Wednesday, September 14th, 2011. We visited Morikawa-sensei's lab again. This time, Goto-sensei gave his talk about direct energy minimization method. I also discussed with Morikawa-sensei about Davidson diagonalization in his STATESENRI code.

Thursday, September 15th, 2011. We visited Morikawa-sensei's lab again. Ono-sensei gave his talk about electron transport calculation of nanostructures. Saito-san gave his talk about GeO_2/Ge interface. Marcus gave his talk about spin-orbit effect and noncollinear magnetism in PAW formalism. Huoooo, finally I could find sweet tea in Japan. Pak Supri told me where I can find the sugar in the dinner room. Combined with oolong tea, I can finally taste my favorite drink.

Friday, September 16th, 2011. We, the invited students, and Kasai's lab members went to Kobe to visit K-computer. After that we had lunch together. Then we visited Banpaku Kinen Koen. We had tea ceremony there. Hoa, they have very beautiful garden of flowers here. There were also some flowers for sell. If I brought my mom here I must bring her here.

Saturday, September 17th, 2011. I, Kak Hani, Kak Lukman, Vera, Pak Nugraha, and Pak Supri went to Kyoto. We visited Kinkaku and Ginkaku-jin. Both were very nice places. Too bad that we only had time to visit those two. I think I will visit the other places in Kyoto when I have opportunity to stay in Japan again. By the way, it was a very hot day (although Japanese said that summer will end soon). The sun did not shine brightly but I sweated a lot.

Sunday, September 18th, 2011. We checked out from JICA and went to Kansai International Airport.

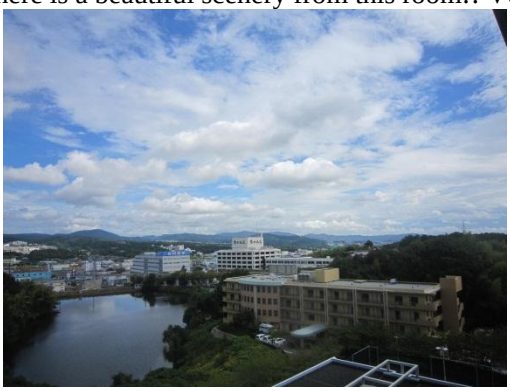
LIFE AS A SHORT TERM STUDENT IN OSAKA UNIVERSITY

I and my friends (Hani, Vera, Lukman, Wahyu, and Fadjar) from Indonesia have invited by Osaka University to visit Osaka University for two weeks. I didn't know them before this program. Fortunately, I could enjoy this program with them. We have the same flight from Bandung to Osaka. "Oh My God, unfortunately, I come here in the summer season, it is very hot season, I don't like it!!", that's my first impression when I arrived in Kansai airport. But Osaka is one of the big cities in Japan. So many people, high building, fly over, etc. Great!
Hani was our guide, because she had lived in Osaka for a year. From Kansai, we went to Ishibashi hotel around Toyonaka campus Osaka University, because we had to join CMD workshop for a week in Toyonaka campus. In the Ishibashi hotel, we lived on a small room for three of us (Me, Vera, and Hani). But it made me chummy each other.

On Monday, September 5th, we had to come to Kasai Laboratory on Suita campus in the morning first for opening ceremony, before we attended the CMD workshop in the afternoon. But we got miscommunication with our friends, so we came late, whereas Japan famous in "on time" custom. Fortunately, they are (Kasai Sensei and Kasai laboratory member) very kind, the opening ceremony started after we arrived. We met another short term students from different country, 3 people from Vietnam, 3 people from Philippines, and 1 person from Thailand. After the opening ceremony, they pick us up to Toyonaka campus to attend CMD workshop.

CMD workshop held from September 5th until September 9th. I joined advance course, learnt HiLAPW and ESOpt. Oguchi Sensei and Kusakabe Sensei are very kind. They teach us well. Oguchi Sensei was very attractive when he was teaching us. I like the way he teach.

On September 9th after CMD workshop, all members of short term students (13 people) moved out from Ishibashi hotel and moved in to JICA. Different from Ishibashi hotel, JICA is the good place. Each student got one room. I slept at room 811. There is a beautiful scenery from this room!! Very beautiful! Love it!



The 2nd week we spent in Suita campus. I, Wahyu, My, and John got lecture from Yagi Sensei. But he gave us lecture only 2 times, Monday 12th and Thursday 15th. Yagi Sensei's room was in the same floor and the same building with Kasai Sensei Laboratory. So, we were given room that we can use while we didn't receive lecture from Yagi Sensei. We were given paper from Kasai Sensei, and he asked us to review that paper.

Thursday came, and we shocked when we had to make a small workshop and invite the all members Kasai Laboratory. Fortunately, I became a moderator only in that small workshop. In that situation I could feel this laboratory, how they learnt from another student and how to discuss a problem.

Friday! September 16th, we tripped to Riken in Kobe and Banpaku park. Riken is the largest supercomputer in the world. After we visited Riken, we went to a luxurious hotel for lunch.

After that, we back to Osaka and went to Banpaku park. Unfortunately there is no special leaves or flower, so we saw a huge park with green leaves only. On Banpaku park, we learnt tea ceremony and drank it.

From Banpaku, we went to Kasai Laboratory for closing ceremony. We received certificate and Kasai Sensei's books with his signature. Happy! But that closing ceremony gave us sign that the program finished.

Saturday is our last day before we leaved Japan on Sunday. I went to Kaiyukan with my friend from Kanazawa. Kaiyukan is a beautiful aquarium with animal within.

Staying in Osaka for two weeks is the great experience for me. Someday I want to come to Osaka again, so many place that I have to visit.

RESEARCH PROGRESS REPORT

CMD Workshop and Experiment in Yamauchi Lab

A. CMD workshop

There were two program in Advanced Course that I chose in CMD Workshop. First was HiLAPW and the second was ES-opt. HiLAPW was taught by prof. Oguchi and Esopt was taught by prof.Kusakabe.

Band calculation was often called first-principles or ab initio calculation. This meant that a theoretical study on the basis of band calculation became calculating not only band structure but also several physical quantities directly from first principles. There had been three important issues in progress of the first-principles calculation. The first was the establishment of the basic theory, typically density-functional and related theory. The density-functional theory provides a practical approach of one-electron theory through local-density approximation (LDA) and more recently generalized gradient approximation (GGA). The second was the highly-developed band-structure calculation methods which made possible a realistic calculation for a very complicated material system with reasonable computer resource. The third was rapid progress in high performance computing.

The Hirosima Linier-Augmented-Plane-Wave (HiLAPW) program package was designed to perform band-structure calculations based on density functional theory (DFT). Main features included:

- scalar-relativistic spin-polarized calculations within the local (spin) density approximation (LSDA);
- all-electron self-consistent calculations;
- total-energy and atomic-force calculations for determining the equillibrium structure and phonons;
- electron density-of-states (DOS) calculations;
- electron density and potential function calculations for 2D or 3D drawings.

I learned how to use this program from basic step, installation. There were some package that we had to install. There were some executable files which had different functions, input and output files. They were xsets, xlapw, xdoss, xnewa, xwbox, xpbox, xspin, xwcon, xsymm, and xrept. It was the first step to use this program.

There were two examples case in this course. Cu were first example case of calculations in this course. We used Cu with fcc structure. HiLAPW allowed us to calculate density of state and band structure from Cu. Total density of state Cu was gotten by extracting the fermi energy from file using getfermi. Furthermore, the PSP plotted the result. The band structure was calculated by script JOB-EK and JOB-SYM. The shell-script JOB-EK demands energy-eigenvalue calculations for k points along the high symmetry lines of the fcc Brillouin zone. The script JOB-SYM requests to extract the irreducible representation for each eigenstate. The second case was Si with diamond structure. An SCF calculation of

Si was carried out and DOS and band structure were plotted in a similar manner to the calculations for fcc Cu. To start the SCF calculation, we was able to use script JOB-SCF.

This course also explained extensively about the basic theory of HiLAPW calculation. This program was calculated by using the Full Potential Linearized Augmented Plane Wave method (FLAPW). FLAPW calculation method was one of the most precise and efficient method which able to solve the DFT Kohn Sham equations with periodic boundary conditions.

After running for a simple case, we were free to choose a case to run using HiLAPW. One of selected case was ZnO which had form of crystalline wurzite. Running ZnO material was done by using a PC cluster that existed at Cyber Media Center. The results of running produced band gap of ZnO about 1.3 eV. Large band gap indicated that this material was included in insulator material. In fact, experimental results showed ZnO band gap around 2 eV. In addition, the results of running program also obtained density of states of ZnO. The result of running program was showed in Figure 1 and Figure 2.

Figure 1. Density of State

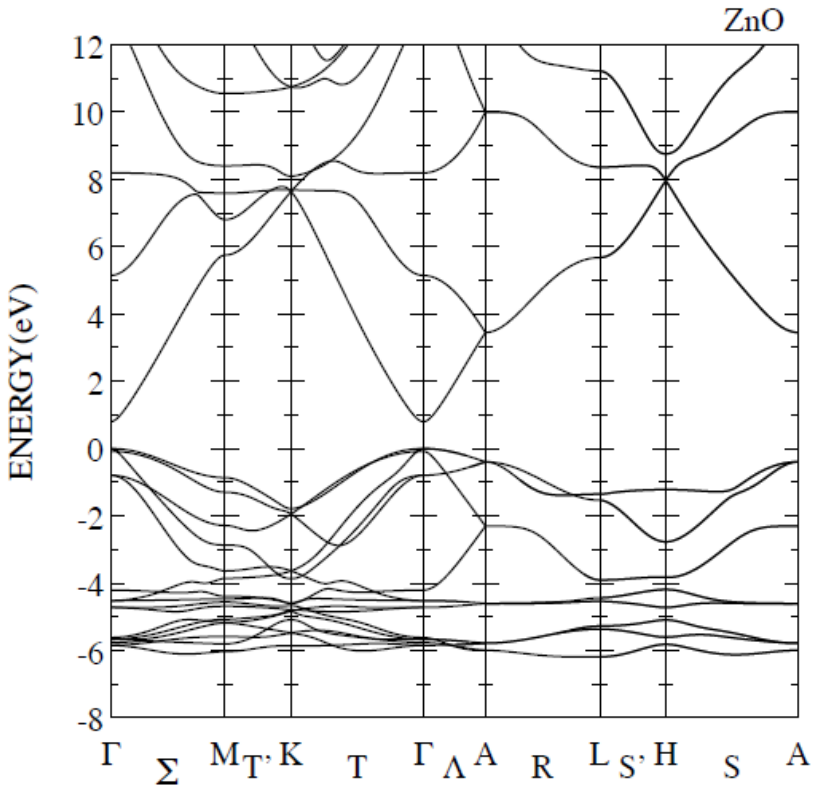


Figure 2. Band Sructure of ZnO

The second program was ESopt. ESopt was program package for the electronics structure calculation based on the density functional teory (DFT). The word "ES" was from electronic structure and "opt" because this program adopting the plane wave expansion method was originated from the package developed in the the Institute for Solid State Physics (ISSP), University of Tokyo. The original "opt" had two characteristic features, high readability of the source code and realization of CG (conjugate-gradient method) to optimize all degrees of freedom wavefunction. ESopt was revised program from opt. ESopt was produced by choosing functions selectively and by applying the Fortran 95 sceme.

At the beginning of the training program we studied the case of static systems, then proceed to study the dynamic system. We can manipulate the material we want, such as simple SWCNT material. Simple SWCNT contained of twenty carbon atom. We studied how to run optimation of the simulation. Preparing pseudo potential was the first step. The second step, we had to create CORD and SOPT.CNTL. The last step was changing the DESTDIR and "do make". The INPUT_DATA/CORD part determined the atomic coordinates in the internal coordinates,which was the relative coordinate with respect to the unit vectors. SOPT.CNTL performed the fixed cell mode. The cell was not necessary the same as the unit cell of a crystal,but might be super cell. If we wanted to use dynamics case we use ALLOPT.CNTL to perform variable cell mode. The full structural optimization and the constant-pressure molecular dynamics were realized using this mode.

We was also able to modify our simple structure SWCNT with one atom addition or more. We also modified the simple SWCNT with double unit cell. We were able to modify unit cell, k point, cut energy

and convergence criteria for interatomic force or CG interaction in input data. We were able to make the simulator of molecular dynamics performance with or without nose thermostat control.

The most interesting part of this program a dynamic process that can be displayed by using the application Xcrysden. Xcrysden was able to perform dynamics process of simple SWCNT. It performed atom-atom interactions SWCNT per unit of time specified. We could manage the dynamic case simulation view from Xcrysden. We could see the interaction between carbon atoms in SWCNT.

B. Doing experiment in ultra precision machining laboratory (Yamauchi Laboratory)

According to the motto "creating what can not be created", They tried to handle a large scale nanotechnology where the structure was controlled on an atomic scale over a large area spanning several 100 mm. In recent years, Yamauchi laboratory had developed a nanoscale machining and nanoscale measurement system such as EEM, PCVM, MSI, RADSI, UPW-ECM, and CARE. Using this system they had succeeded in "creating what can not be created" such as high performance electronic devices and optical devices substrate, X-ray devices, and X-ray nanoscopes. Furthermore, this laboratory was also contributing to pioneering new science and technology in collaboration with various field such as biology, medical science, drug discovery, semiconductor devices, and X-ray free electron lasers.

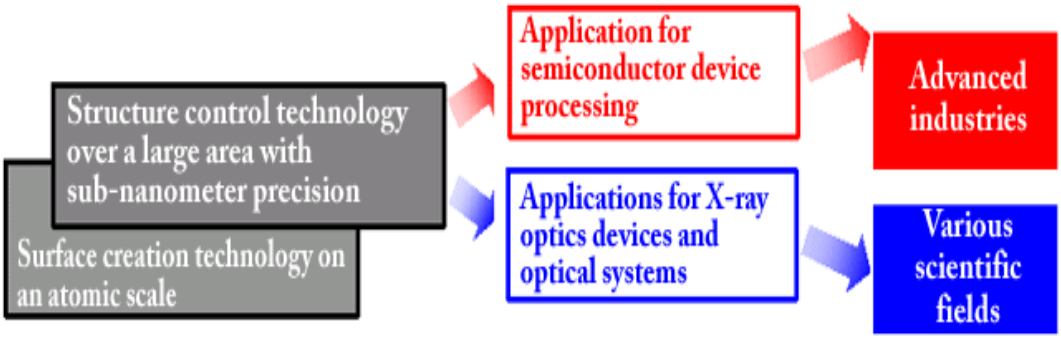


Figure 3. Yamauchi Laboratory work scheme

During a visit to the Lab Yamauchi we were given the opportunity to perform experiments on Ultra Clean Facility (UCF). UCF was equipped by world class facilities, including a clean room, an air supply system processes were ultra clean and ultra pure water supply system. UCF had four classrooms 1. Class 1 meant that 1 cft of the air content of less than one particle diameter exceeds 100 nm. Each clean room has three floors that maintained by vertical layer flow. The circulation of water was supplied by a local system that had low energy consumption. The average circulation of air around 120 cycles / h. It was achieved by using 250 units of Fan Filter.

The first apparatus was used in the experiment was CARE (Catalyst Referred Etching). This tool was in use to refine the surface of Si or GaN wafers with chemical polishing methods. Using this method Si

wafer was irradiated by UV and oxidized by photo electrochemical. The results of chemical oxidation was removed using a polishing plate which had function as a solid acid catalyst in a phosphate buffer solution. The plate which commonly used was SiO_2. Furthermore, Wafer and plate were rotate freely. Pressure exerted on the sample was 200 hPa and the rotation at 12 rpm. The result was a smoother surface of wafer which its pattern like a terrace. The result was much better than the commercial wafers.

The second apparatus was electron beam evaporation (ULVAC). The Electron Beam Evaporation (also know as e-beam evaporation) process fell into a larger category of Micro-Electro-Mechanical Systems (MEMS) processes known as Physical Vapor Deposition (PVD). Deposition processes were used to release a material from a source and transfer that material to a substrate, forming a thin film or coating. PVD processes were commonly used for the deposition of metals, because they can be performed at lower process risk and cheaper in regards to materials cost that Chemical Vapor Deposition (CVD).

In the evaporation process, a block of the material (source) to be deposited was heated to the point where it starts to boil and evaporate. Then it was allowed to condense on the substrate-the material that we wanted to coat. This process took place inside a vacuum chamber, enabling the molecules to evaporate freely in the chamber, where they then condensed on all surfaces. For e-beam evaporation, an electron beam was used to heat the source material and caused evaporation.

Electron beam evaporation was a commonly used process for coating lenses and filters with anti-reflection, scratch-resistant or other specialized coatings. The process was also commonly used for coating insulating and resistor films on electronic components.

REPORT

Life as a short term student in Osaka University

I had been living as short term student in Osaka University for two weeks with tight schedules. There was CMD (Computational Material Design) Workshop in the first week. CMD workshop was held in Cyber Media campus at Toyonaka. I took advanced course in CMD workshop. There were two group in Advance course that I chose before, HiLAPW and ES-opt. Beside that, there were several special lecture from some professors. Furthermore, There were International workshop on collaborative research on design and creation of new green nano materials on Tuesday and then I visited Yamauchi Lab on Wednesday and Thursday. They were held in Suita campus. In the end, we visited RIKEN advance Institute and Banpaku Park before invitation program closing ceremony.

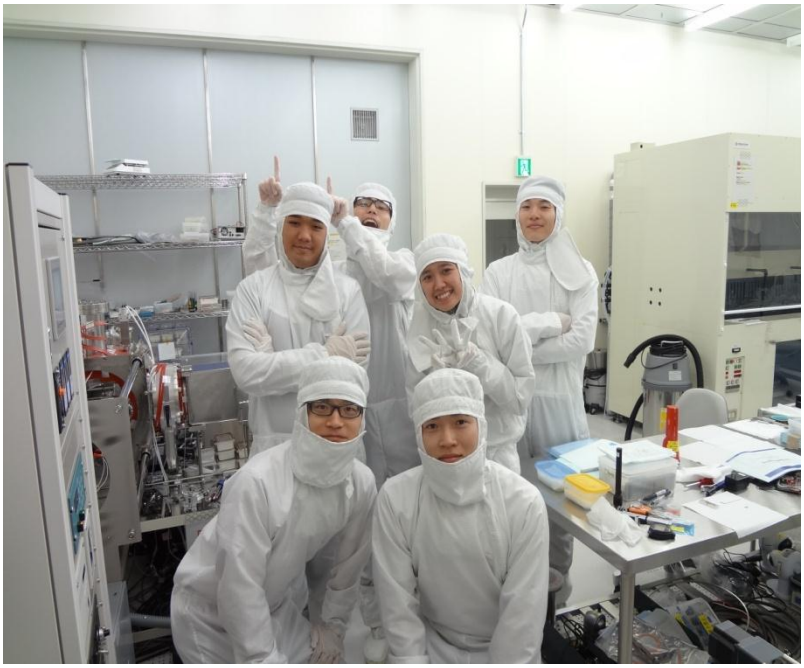
HiLAPW was given in Oguchi sensei's class. I was very enjoyed his class. He taught me well. He taught with schematic procedure so I could fast understand about his lecture even I was new in DFT. I felt free to ask everything that I did not know and he explained very well. I thought that his class was my favorite class. There was discussion session in his class. We were free to running material as we wanted and then we gave presentation about the result. We chose our own material and we ran that on PC Cluster, then we waited for the result and analyzed it. He would give me explanation if I did mistake to explain my result. In this session I could compare my material case with the others case, so we could share our problem and our knowledge using HiLAPW. It was the best way to know much about HiLAPW. It was very interesting. I really hoped that I could attend in his class again.

ES-opt was given in Kusakabe sensei class. He was very patient in teaching. We learned about DFT (Density-functional-theory). He gave us not only static case but also dynamic case in his lecture. He explained us step by step using ES-opt software. He showed us about the process of dynamic case with Xcrysden. Simple SWCNT (single wall carbon nanotube) was the example. The simple SWCNT contained of twenty carbon atom. We could manage the dynamic case simulation view from Xcrysden. We could see the interaction between carbon atoms in SWCNT.

We also received some special lectures in Toyonaka campus. Professors who gave us lecture were Prof. Tomoya Ono, Prof. Miyamoto, Prof. Satoshi Itoh, Prof. Fumithosi Sato, and Prof. Hideaki Kasai. They presented about their interesting topic that related with Computational Material Design. One of their lectures was about Computational Material Design application. In the end of CMD workshop, there were certificate awarding and photo session with all CMD workshop participant.

I visited Yamauchi lab for two days in Wednesday and Thursday. Unfortunately, Prof. Yamauchi was not in Lab because he had to attend in international conference in USA so I did not meet him. I just met Assistant professor Matsuyama. Assistant professor Matsuyama and all Yamauchi lab members welcomed me well. They introduced them self and their great projects. They were very friendly people. It was very nice to be here. I got a lot of friends from this lab. In the middle of break time, they explained me

about Japanese culture and recommended place to go in Japan. They also explained me about Japanese character, Hiragana, Katakana and Kanji. I was very happy because they gave me beautiful Kanji name meant “good wind picture”. I also told them about Indonesian culture and they appreciated it very much.



The best experience in Yamauchi lab was able to do experiment in Ultra Clean Facility. They showed me about their latest project. I impressed about their motto, to “create what could not be create”. It was amazing motto. There were a lot of modern apparatuses in Ultra Clean facility such as ULVAC, EEM, Wet Bench, CARE, X-ray multilayer fabrication apparatus, FIB-HITACHI FB-2100, and some modern measurement apparatuses. We have made terrace surface in Si wafer with CARE in Ultra Clean Facility. It was great experience although the result was not good enough because of contamination and short experiment time.

I went to Kobe port island with all Kasai lab member on Friday. We visited super computer in RIKEN advanced institute. It was one of latest masterpiece in Japan. They claimed that K computer was fastest computer in the world. It was really amazing. Furthermore, we went to Banpaku park. We followed “Chato” or Japanese tea ceremony in Banpaku park. Chato was unique tradition from Japan. They taught me how to drink green tea in Japanese tea ceremony.

In the end of invitation program, there were closing ceremony with Kasai Lab members. Prof. Kasai awarded us Invitation program certificate and gave us his books. I got his signature in his book. It was impressive moment. I was very thankful having a valuable chance to have two great week in Japan. Dino sensei told us that Everything was possible and impossible just took no longer. It gave me motivation to be a good researcher someday. I really hope that someday I will go to Japan again and doing my research or doctoral program here.

REPORT

Life as a short term student in Osaka University

Today is the second day CMD workshop in Osaka University. In this day, the schedule is lecture with Prof. Tamio Oguchi about HiLAPW method (Full Potential Linearized Augmented Plane Wave). The FLAPW is among the most precise and efficient first-principles methods which are able to solve density-functional-theory Kohn-Sham equations with the periodic boundary conditions. After this lecture, we continue to study case with Prof. Tomoya Ono. In the Prof. Ono lecture's we study about Real-space finite-difference (RSFD) method and Overbridging boundary matching (OBM) method. With this method we can found The grand-state electronic structure is obtained by solving the Schrödinger (Kohn-Sham) equation.

Today is the second day CMD workshop in Osaka University. In this day, the schedule is lecture with Prof. Tamio Oguchi about HiLAPW method (Full Potential Linearized Augmented Plane Wave). The FLAPW is among the most precise and efficient first-principles methods which are able to solve density-functional-theory Kohn-Sham equations with the periodic boundary conditions. After this lecture, we continue to study case with Prof. Tomoya Ono. In the Prof. Ono lecture's we study about Real-space finite-difference (RSFD) method and Overbridging boundary matching (OBM) method. With this method we can found The grand-state electronic structure is obtained by solving the Schrödinger (Kohn-Sham) equation.

Today is the third day CMD workshop in Osaka University. In last day, I was learned with Prof. Kusakabe about ESopt. 'ES' is meaning Electronic Structure and 'opt' is meaning that the program/tool adopting the plane wave expansion method from the package developed in the Institute for Solid State Physics (ISSP), University of Tokyo. ESopt is a program package for the electronic structure calculation based on density functional theory (DFT). After that lecture, we continued study case with Prof. Miyamoto. In Prof. Miyamoto lecture's, we study about the application of Computational Material Design.

Today is the fourth day CMD workshop in Osaka University. In this day, the schedule is lecture with Prof. Koichi Kusakabe about ESopt. Yesterday, we learned about calculation in a static system case, today we try to calculate in dynamic case. It is very interest because we can create a system, by manipulate materials, and after that we can see the atom interaction in 'xcrysden application'. After this lectures, we continue to study case with Prof. Hideaki Kasai. He give us a lectures about surface science. He said that one of the ultimate goals of surface science is to be able to design and control reactions as they progress on surfaces.

This day is the end of CMD workshop. It is very memorable moment for me, becauce it can increase my knowledge about computational material design and more new knowledge from all sensei in CMD workshop, especially for Prof. Kusakabe, who very patient to give me explanation and show how to operate and make that tools (ESopt). I hope some day I can see him again. Besides lectures from Prof. Kusakabe, we get the special lectures from Prof. Satoshi Itoh and Prof. Fumithosi Sato. after that closing workshop with photo section.

Today I went to suita campus, Osaka University. My schedule is meet with Prof. Atsushi Yagi. He is professor in department of information and physical sciences, graduate school of Information science and technology. He is Chair of 1st core in Quantum Engineering Design Research Initiative (QEDRI). 1st core in QEDRI is creation of frontier mathematical methods. Today, Prof. Atsushi Yagi give a lecture for us about mathematical methods for engineering, self organization, mathematical model, mathematical analysis and numerical computations. It is so interesting lecture because with mathematic, we can learn another subject, like biology, physics, et al. I hope I can follow this until I back to Indonesia.

Today my schedule is go to suita campus, Osaka University. I want to follow International workshop on collaborative research on design and creation of new green nano materials. The program opened by vice president of Osaka University, Prof.Akira Takahashi and Prof. Hideaki Kasai from Dept of precision science & technology and allied physics. After that continue with the lecture from Dr. Nugraha and Dr. Suprijadi from ITB, Indonesia. I amvery proud because they represent Indonesia. After their lecture the program continue with the explanation of QEDC orientation. QEDC is Quantum Engineering Design Course. After that continue with presentation from the student of department of precision science & technology and applied physics until finish this program.

Today my schedule is go to suita campus, Osaka University. My schedule is prepare for make a presentation to Prof. Hideaki Kasai. He asked us to read a paper, and after that asked us to presentation. I think it is like proposal presentation, so I must prepare this with very well. We study about a paper from 10.00 am until 05.00 pm to prepare, so I hope I can give the best to Prof. Hideaki Kasai tomorrow.

Today, I went to suita campus. The schedule is presentation to Prof. Hideaki Kasai. I am very disappointed today, because I didn't prepare a presentation with good. This is my fault, because I doesn't understand the papers provided by Prof. Hideaki Kasai. This is a very valuable experience for me, and I hope I get a second chance to fix all this. For me and for person who provide an opportunity for me.

Today we visited the RIKEN super computer in Kobe port island. It is a fantastic place. RIKEN is the world's fastest computers. I hope if one day I can try to use the facilities there for my research. After visiting RIKEN, we went to lunch and after that, we went to Japan Banpaku-Garden Park. It is a very beautiful place. there we followed the procession to drink tea, the Japanese tradition. I hope this is not the last day of my visit to Japan. and I hope someday I can come back here to learn about science at Osaka University and also studied Japanese culture.

REASEARCH PROGRESS REPORT

Lecture with Prof. Atshusi Yagi, Osaka University

Today I went to suita campus, Osaka University. My schedule is meet with Prof. Atsushi Yagi. He is professor in department of information and physical sciences, graduate school of Information science and technology. He is Chair of 1st core in Quantum Engineering Design Research Initiative (QEDRI). 1st core in QEDRI is creation of frontier mathematical methods. Today, Prof. Atsushi Yagi give a lecture for us about mathematical methods for engineering, self organization, mathematical model, mathematical analysis and numerical computations. It is so interesting lecture because with mathematic, we can learn another subject, like biology, physics, et al. I hope I can follow this until I back to Indonesia.

Self-organization is the process where a structure or pattern appears in a system without a central authority or external element imposing it through planning. This globally coherent pattern appears from the local interaction of the elements that make up the system, thus the organization is achieved in a way that is parallel (all the elements act at the same time) and distributed (no element is a central coordinator).

The most robust and unambiguous examples of self-organizing systems are from the physics of non-equilibrium processes. Self-organization is also relevant in chemistry, where it has often been taken as being synonymous with self-assembly. The concept of self-organization is central to the description of biological systems, from the subcellular to the ecosystem level. There are also cited examples of "self-organizing" behaviour found in the literature of many other disciplines, both in the natural sciences and the social sciences such as economics or anthropology. Self-organization has also been observed in mathematical systems such as cellular automata.

Sometimes the notion of self-organization is conflated with that of the related concept of emergence. Properly defined, however, there may be instances of self-organization without emergence and emergence without self-organization, and it is clear from the literature that the phenomena are not the same. The link between emergence and self-organization remains an active research question.

Self-organization usually relies on three basic ingredients :

1. Strong dynamical non-linearity, often though not necessarily involving Positive feedback and Negative feedback
2. Balance of exploitation and exploration
3. Multiple interactions

Mathematical analysis, which mathematicians refer to simply as analysis, has its beginnings in the rigorous formulation of infinitesimal calculus. It is a branch of pure mathematics that includes the theories of

differentiation, integration and measure, limits, infinite series,[1] and analytic functions. These theories are often studied in the context of real numbers, complex numbers, and real and complex functions. Analysis may be conventionally distinguished from geometry. However, theories of analysis can be applied to any space of mathematical objects that has a definition of *nearness* (a topological space) or, more specifically, *distance* (a metric space).

Chemotaxis is the phenomenon in which somatic cells, bacteria, and other single-cell or multicellular organisms direct their movements according to certain chemicals in their environment. This is important for bacteria to find food (for example, glucose) by swimming towards the highest concentration of food molecules, or to flee from poisons (for example, phenol). In multicellular organisms, chemotaxis is critical to early development (e.g. movement of sperm towards the egg during fertilization) and subsequent phases of development (e.g. migration of neurons or lymphocytes) as well as in normal function. In addition, it has been recognized that mechanisms that allow chemotaxis in animals can be subverted during cancer metastasis.

Several mathematical models of chemotaxis were developed depending on the type of

- migration (e.g. basic differences of bacterial swimming, movement of unicellular eukaryotes with cilia/flagellum and ameboid migration);
- physico-chemical characteristics of the chemicals (e.g. diffusion) working as ligands;
- biological characteristics of the ligands (attractant, neutral and repellent molecules;
- assay systems applied to evaluate chemotaxis (see incubation times, development and stability of concentration gradients);
- other environmental effects possessing direct or indirect influence on the migration (lighting, temperature, magnetic fields etc.)

Cell-Chemotaxis Model Mechanism

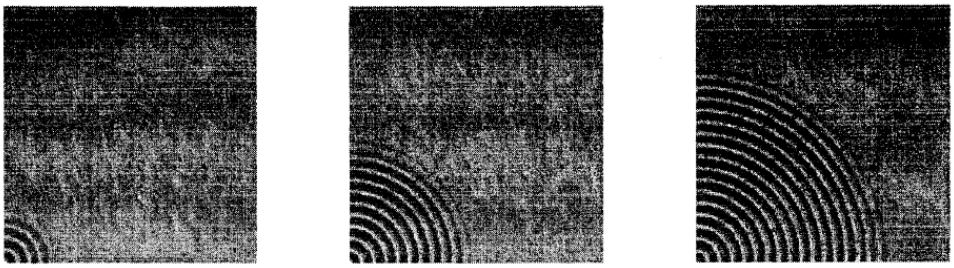
The model we consider here involves actual cell movement. Pattern formation models which directly involve cells are potentially more amenable to related experimental investigation. There is also some experimental justification from the evidence on pigement cell density variation observed in histological sections which we described above. Also, Le Douarin (1982) speculated that chemotaxis may be a factor in the migration of pigment cells into the skin. Heuristically we can see how chemotaxis could well be responsible for the rounding up and sharpening of spots and stripes. In the model, we propose that chromatoblasts both respond to and produce their own chemoattractant. Such a mechanism can promote localisation of differentiated cells in certain regions of the skin which we associate with the observed patterns on the snake integument. The cells, as well as responding chemotactically, are assumed to diffuse. It is the interaction of the cell mitosis, diffusion and chemotaxis which can result in spatial heterogeneity.

The relatively simple mechanism we propose is

$$\frac{\partial n}{\partial t} = D_n \nabla^2 n - \alpha \nabla \cdot (n \nabla c) v - r n (N - n),$$
$$\frac{\partial c}{\partial t} = D_c \nabla^2 c + \frac{Sn}{\beta + n} - \gamma c,$$

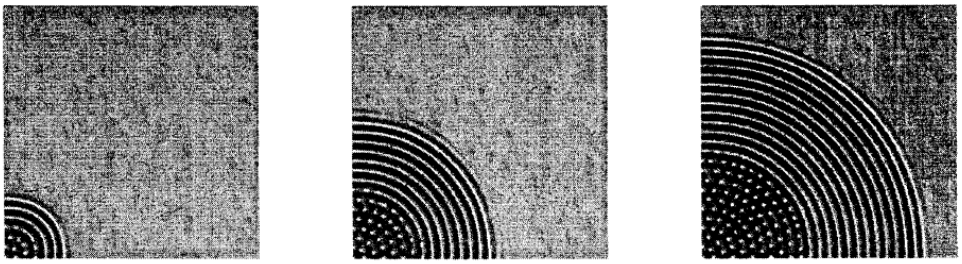
where n and c denote the cell and chemoattractant densities respectively; Dn and Dc are their diffusion coefficients. We have taken a simple logistic growth form for the cell mitotic rate with constant linear mitotic rate r and initial uniform cell density N. The chemotaxis parameter α is a measure of the strength of the chemotaxis effect. The parameters S and γ are measures, respectively, of the maximum secretion rate of the chemicals by the cells and how quickly the chemoattractant is naturally degraded; β is the equivalent Michaelis constant associated with the chemoattractant production. This is the specific model discussed by Oster andMurray (1989) in relation to developmental constraints.

EXAMPLE : MATHEMATICAL ANALYSIS FOR CHEMOTAXIS GROWTH SYSTEM



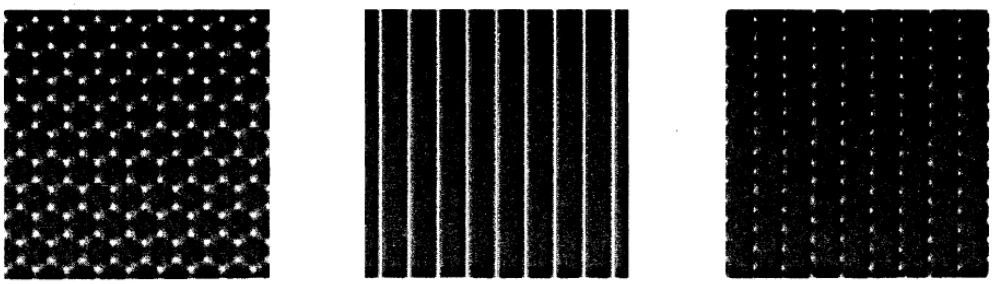
(a) $t = 16$ (b) $t = 32$ (c) $t = 48$

FIGURE 1. Target pattern with continuous rings for $\nu = 11.0$.



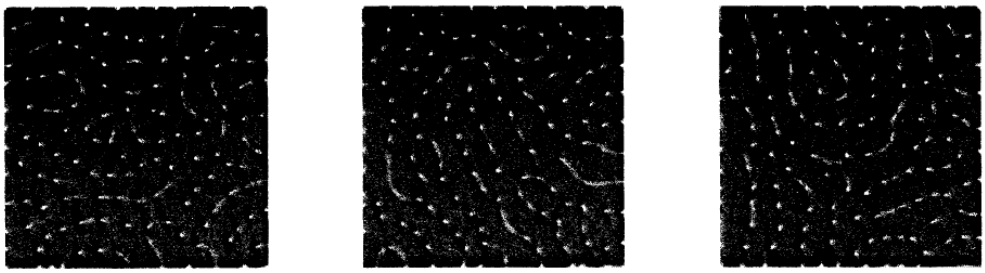
(a) $t = 8$ (b) $t = 16$ (c) $t = 24$

FIGURE 2. Target pattern with perforated rings for $\nu = 32.0$.



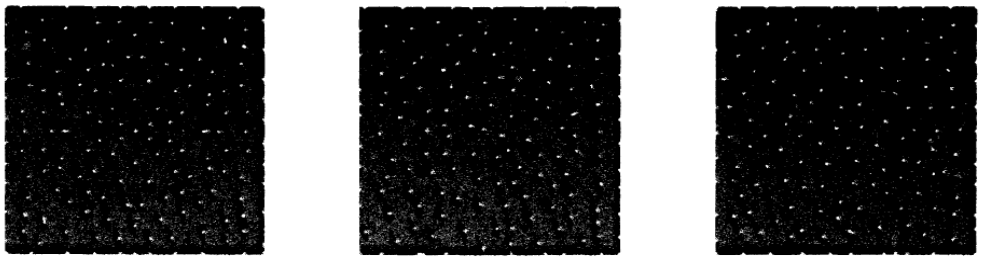
(a) Honeycomb ($\nu = 6.2$) (b) Stripe ($\nu = 7.2$) (c) Perforated Stripe ($\nu = 8.5$)

FIGURE 3. Stationary patterns for $\nu = 6.2$, $\nu = 7.2$ and $\nu = 8.5$.



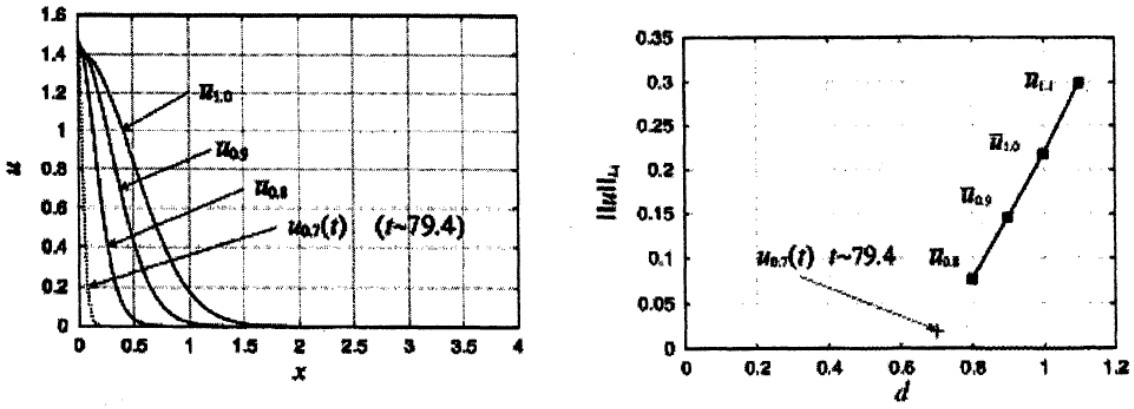
(a) $t = 1024$ (b) $t = 2048$ (c) $t = 4096$

FIGURE 4. Moving perforated labyrinthine pattern for $\nu = 9.0$.



(a) $t = 64$ (b) $t = 128$ (c) $t = 256$

FIGURE 5. Chaotic spot pattern for $\nu = 11.0$.



(a) Graphs (b) L_1-norms

FIGURE 6. Stationary solutions $\overline{u}_d$ and $u_{0.7}(t)$ $(t \sim 79.4)$.

Reference :

- Yagi A, Tsujikawa T, Mimura M, *Mathematical Analysis for Chemotaxis Growth System*, 数理解析研究所講究録, 1499 巻2006 年126-134
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OSAKA UNIVERSITY

Suita, Osaka, 565-0871, JAPAN

DEPARTMENT OF APPLIED PHYSICS

GRADUATE SCHOOL OF ENGINEERING

JSPS INVITATION PROGRAM FOR EAST ASIAN YOUNG RESEARCHERS

INTERNATIONAL MINI WORKSHOP ON NANDEMO

Preface:

JSPS Invitation Program for East Asian Young Researchers works to establish and expand networks from Asian country. It also helps to create generations with high knowledge quality and regional communities based on knowledge. With this purpose, we were invited to Osaka University and attended many activities. One of those interesting activities was International Mini Workshop on Nandemo held by ourselves with the help of Wilson sensei. By mean of this mini Workshop, we learned a great deal of things such as how to work in a team, to organize a workshop, to present a scientific problem, and so on. My report is presented as a proceeding of the Workshop. The proceeding includes three presentations of which topics vary from Pure Mathematics, Applied Physics to Applied Mathematics. In this small proceeding, content of each presentation is replaced by a picture.

PROGRAM

INTERNATIONAL WORKSHOP ON NANDEMO

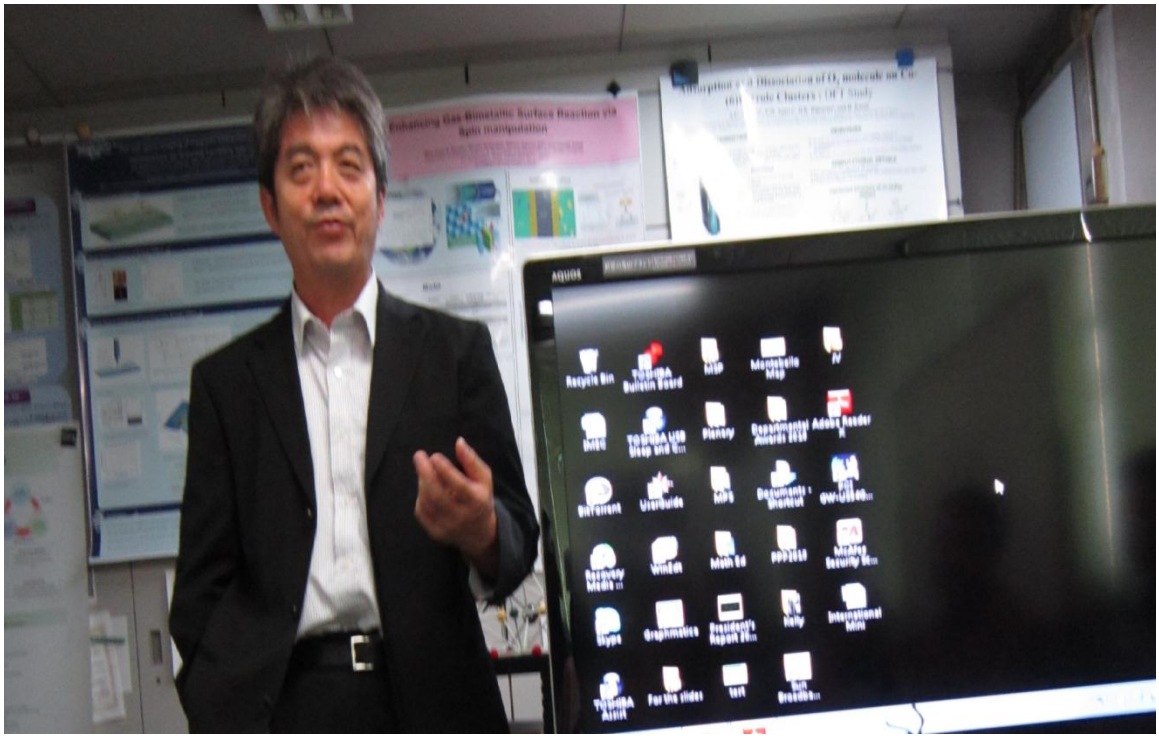
September 15th, 2011

Kasai Laboratory, Suita Campus

Moderator:	Nyayu Siti Nurainun	
Opening Remarks:	Prof. Kasai	(4:30 – 4:35)
Speaker:	John Vincent Morales	(4:35 – 4:50)
	Introduction to Fractals	(15 minutes)
Speaker:	Wahyu Aji	(5:05 – 5:20)
	Design Principles for Oxygen-Reduction Activity on Perovskite Oxide Catalysts for Fuel Cells and Metal-Air Batteries.	(15 minutes)
Speaker:	Duong Thi Diem My	(4:50 – 5:05)
	Modeling the Dynamics of Marital Interaction: Divorce Prediction and Marriage Repair	(15 minutes)
Closing Remarks:	Nyayu Siti Nurainun	(5:20 – 5:22)

The Workshop is instructed by Moderator Nyayu Siti Nurainun

Opening Remarks is given by Kasai sensei



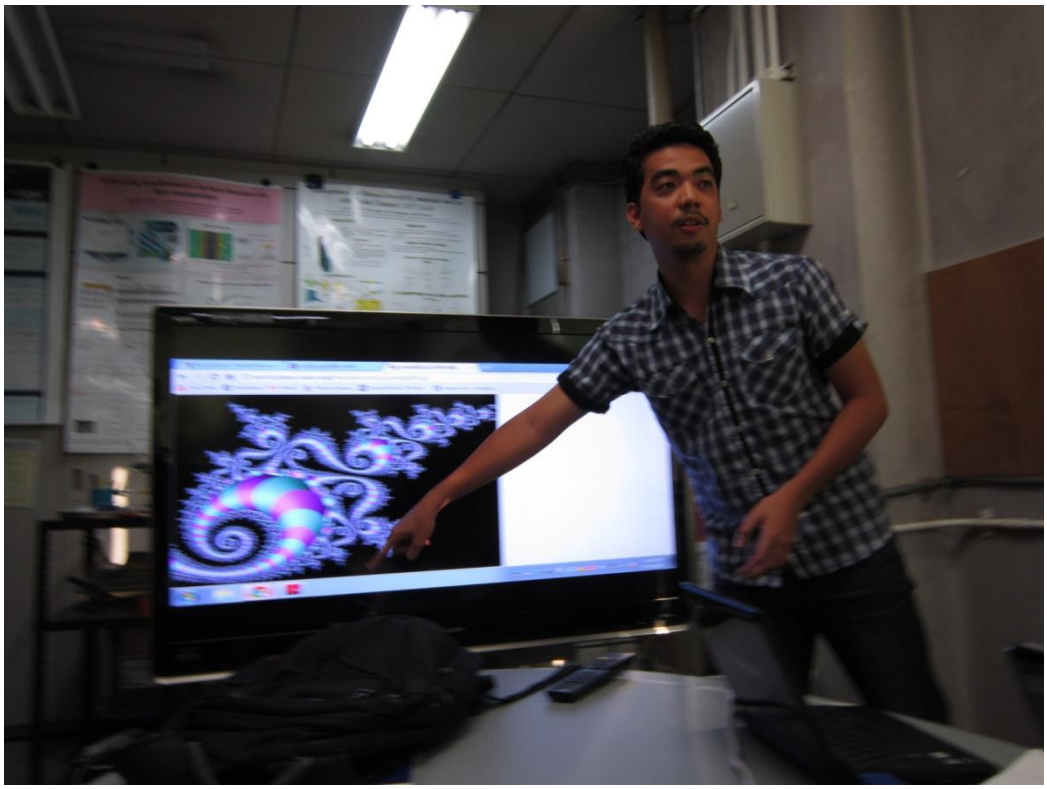
INTRODUCTION TO FRACTALS

John Vincent S. Morales

Assistant Professor 1, DLSU Math Department

Abstract:

A fractal is defined as a rough or fragmented geometric shape that can be split into parts, each of which is a reduced-size copy of the whole [1]. Even though fractal can be expressed by mathematical equation that undergoes iteration, they are found in nature. Studying of fractal has many applications in medicine, soil mechanics, seismology, and technical analysis. In my presentation, I will give a soft introduction on fractal, which is its definition and two common sets namely, the Cantor set and the Koch curve.



DESIGN PRINCIPLES FOR OXYGEN-REDUCTION ACTIVITY ON PEROVSKITE OXIDE CATALYSTS FOR FUEL CELLS AND METAL-AIR BATTERIES.

Wahyu Aji Eko Prabowo
Graduate School of Engineering Physics
Bandung Institute of Technology
Bandung, Indonesia

Abstract:

The prohibitive cost and scarcity of the noble-metal catalysts needed for catalysing the oxygen reduction reaction (ORR) in fuel cells and metal-air batteries limit the commercialization of these clean-energy technologies. Identifying a catalyst design principle that links material properties to the catalytic activity can accelerate the search for highly active and abundant transition-metal-oxide catalysts to replace platinum. Here, we demonstrate that the ORR activity for oxide catalysts primarily correlates to σ*-orbital (eg) occupation and the extent of B-site transition-metal-oxygen covalency, which serves as a secondary activity descriptor. Our findings reflect the critical influences of the σ* orbital and metal-oxygen covalency on the competition between O2 2–/OH– displacement and OH– regeneration on surface transition-metal ions as the rate-limiting steps of the ORR, and thus highlight the importance of electronic structure in controlling oxide catalytic activity [2].

MODELING THE DYNAMICS OF MARITAL INTERACTION:

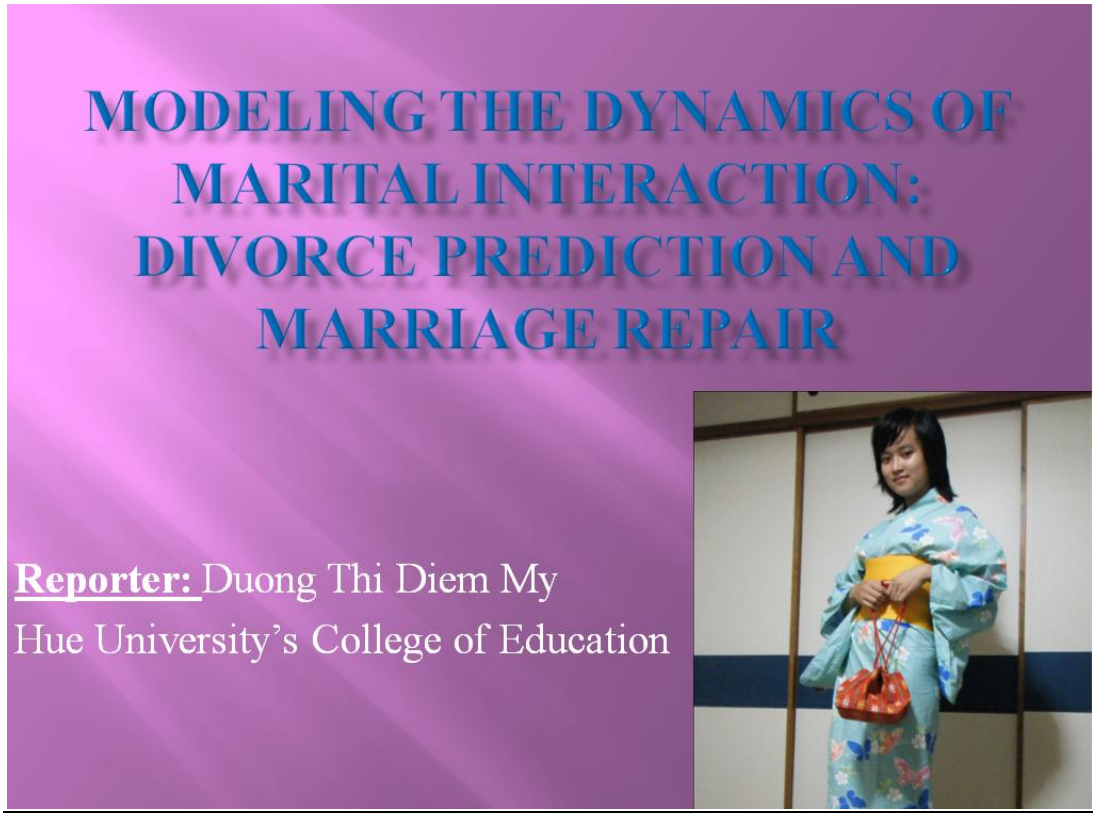
DIVORCE PREDICTION AND MARRIAGE REPAIR

Duong Thi Diem My

Hue University's College of Education, Vietnam

Abstract:

Mathematical model is a description of a system using mathematical concepts and language [1]. It is applied in such many aspects as natural sciences, engineering, and even social sciences. In my presentation, I will demonstrate the literature application of the mathematical model which is modeling the dynamics of marital interaction. This research has been developed for only short time; thus, it has not shown any clear result yet. However, this topic is a promising one, and will open a new broad direction for researching in psychology science.



Reference:

[1] http://en.wikipedia.org

[2] Jin Suntivich, Hubert A. Gasteiger, Naoaki Yabuuchi, Haruyuki Nakanishi, John B., Goodenough, Yang Shao-Horn, "Design principles for oxygen-reduction activity on perovskite oxide catalysts for fuel cells and metal–air batteries", *Nature Chemistry*.

Research Progress Report

Hanifadinna

Master Students, Department of Engineering Physics

Institut Teknologi Bandung Jln., Ganesha 10, Bandung 40132, Indonesia

CMD Progress Report

RSPACE code

Lecturer: Tomoya Ono

This code was using real space finite difference (RSFD) method for electronic structure and transport calculation. The ground state of electronic structure is obtained by solving the Schrodinger equation

$$\left(-\frac{1}{2}\nabla^2 + V(r)\right)\psi_i(r) = \varepsilon_i\psi_i(r).$$

Using RSFD method is dividing the space into equal spacing of grid points ($x_i y_j z_k$) while the wave function (ψ_{ijk}) and potential are defined at those grid points. This code is providing the arbitrary boundary condition for bulk model.

Some simple calculation were been done during this course using the massively parallel computer in which the result are transferred via the networks cable. It has been providing by Cyber Media Center (CMC), Osaka University.

Molecular calculation

The first experience was optimization calculation of CO molecule. There are two directories we need to modify. The thing first thing to start the calculation was creating the parameter file with “param.f” under the source directory of CO. When the compilation is completed, the check and confirm would be created under the “kukan40, “pre”, “ele” and “pop”. Another directory is exe which should contain “job.j”, “read.inp”, “atom.xyz” and “pre”. The execution condition is represented by “read.inp” and the information of atomic coordinates is created by “atom.xyz”. When the program is completed, the information is kept by “mdresult”, it contain the information on the electronic structures at each molecular dynamics step.

The calculation within this method can be performed by using parallel processing (nodes). The key is using "lda0" when compiling the job.

This method also allow us doing the calculation for supercell for example is calculating the electronic stricter of lithium crystal and lithium surface. For more accurate first-principles calculation, this method was provide use to considering the spin and increasing the number of sampling k-points.

Machikenayama Code

Lecturer: Hisazumi Akai, Kazunori Sato, Masako Ogura

This code is using Koringga-Kohn-Rostoker Method (Green's Function) to calculate the electronic structure. This method allows us to consider a complex energy, to get a band structure calculation with considering finite temperature magnetism and partial disorder of random system.

The exercise is started by calculating the electronic structure of bcc iron with a given lattice constant then tried up some of various lattice constant given. The calculation of density of state also performed to plot the band structure system. The little difficulties I faced during the exercises were to read some of the band structure, to determine the half metallic or non half metallic. The experience to read the band structure is indeed should be learn.

This code is allowed to calculate the disordered system with using impurity of transition metal and the random alloy with modifying the concentration of atoms.

Visiting Yoshida Laboratory

Hiroshi-Katayama Yoshida

Environment, energy, aging society, security

The industrial society nowadays tries to search the energy with having a respect of the social problem. Some considerations were taking into a challenge in 21st century, such us:

- nano-electronics
- environment-friendly materials
- high-efficiency energy conversion
- life-science-related materials
- security-related material

From those mentioned above, the focus chosen was a solar cell because of a number of considerable advantages. The first important challenge trends now is nano-electronic material. The use of nanostructures in solar cell offers the potential for high efficiency by either using new physical mechanisms or by allowing solar cells which have efficiencies closer to their theoretical maximum; 91% with nano scale material. The multiple potential uses for nanostructures show why there is large interest in these approaches, since they may be able to improve on the conventional solar cell of Silicon base solar cell. The computational material design now is try to give the solution in design the material for highly efficiency solar cell product. The detail calculation result can predict theoretically what the contribution needed to fabricate the material for solar cell in the future.

The first principles study has been proposed a material design for high efficiency photovoltaic solar cell by using with the coherent-potential approximation (KKR-CPA) within the local density approximation (LDA) using the program package MACHIKENAYAMA202 to calculate the mixing energy of CuIn1_xGaxSe2 *(Tani et al)*[1]. The calculation performed with LDA and self interaction correction (SIC), developed by Filipetty and Spaldin.

From those slightly presentation I've seen the result of two dimensional spinodal nanodecompotition under layer by layer is point out to the characteristic model of dilute magnetic semiconductor (DMS). The phase called "Konbu phase" means seaweed in Japanese. The DMS itself considered as a substitutional alloy and calculation of the system performed by coherent potential approximation.

Fig. 1: CMOS-free MRAM structure made by the spinodal nano-decompositoin.

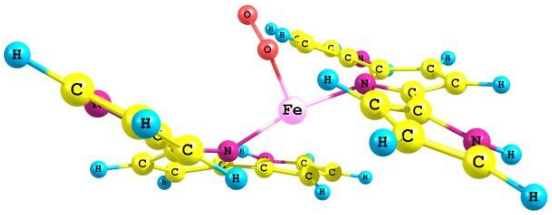
Most of the member of Yoshida Laboratory is doing the research about the magnetism. The mostly talking was about the DMS. Some of the research is focusing a first principle investigation of the electronic structure of transition metal doped III-V and II-VI semiconductors and the magnetic properties of an impurity in DMS for spintronic application. The accurate investigation about Curry Temperature, T_c is became important since the high T_c is still one of the considerations in designing DMS material. The Hamiltonian and Monte Carlo simulation have been suggested to calculate the Curie temperature of DMS.

Current Research

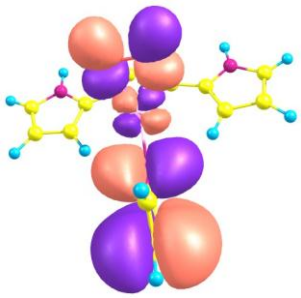
Adsorption of O_2 on Fe-(n)pyrrole Molecules from First-Principles Calculations

Inspired by iron-porphyrin as organic compound hemoglobin that contains four pyrrole rings to bind the metal Fe which have responsible for binding the oxygen, now recently a researcher has synthesized a possible development of Fe and Co based catalyst. Bahsyam and coworker has developed a cathode catalyst using non platinum based catalyst and made from a cobalt-polypyrrole-carbon composite which exhibiting high ORR activity with stable performance. Following this Lefèvre and coworkers used active iron cation coordinated to pyridinic groups within micropores of the carbon support and notes that after extended use in a fuel cell, the catalyst's high initial activity decrease significantly.

In this work, density functional calculations were performed to determine a possible model for Fe-polypyrrole and hence to understand the interaction of O_2 molecules on Fe-polypyrrole cluster to clarify the oxygen reduction reaction at the cathode side. Following this, another goal was to develop a predictive scale of Fe-polypyrrole reactivity based upon structure, and calculated properties. In the process of carrying out these calculations a number of basis sets were tested.



O_2/Fe(6)-pyrrole interaction



HOMO-4 for optimized configuration of O_2/Fe-(4)pyrrole.

Fe-polypyrrole is expected to have good activity in oxygen reaction reduction. In this study we performed a DFT based calculation on the adsorption of O_2 molecule on Fe-(n)pyrrole cluster using Gaussian 03 [3)]. The hybrid functional B3LYP was employed for the exchange-correlation energy and 6-311+G(d,p) basis-set was used for the basis function. The stable adsorption site of O_2 molecule on Fe-(4)pyrrole is found to be at the O_2 center of mass located on the top of the Fe atom.(side-on configuration) while Fe-(6)pyrrole at-end on configuration The elongation mechanism of O_2 on Fe-(n)pyrrole is induced by the interaction between the Fe d-orbitals and O_2 anti-bonding π^* orbital, which results in charge transfer from Fe atom toward the O_2 molecule.

Electronic structure analysis indicates that the elongation of O_2 on Fe–(n)Ppy is induced by the interaction between the Fe d-orbitals and the O_2 anti-bonding orbital. The large elongation of the O_2 bond when adsorbed on Fe–(n)Ppy is due to the formation of a side-on configuration especially for Fe–(4)Ppy with 13.3% elongation as compared with the Fe–(6)Ppy cluster. This will ease O_2 dissociation and enhance the ORR mechanism.

References

Journal:

APEX/Applied Physics Express Vol. 3, No. 10, 101201-1-3 (2010)

APEX/Applied Physics Express Vol. 4, No. 1, 015203-1-3 (2011)

APEX/Applied Physics Express Vol. 4, No. 2, 021201-1-3 (2011)

Allen M. Barnett[1], Douglas Kirkpatrick[2]Christiana B. Honsberg, 1-4244-0016-3/06/$20.00.,

Review of modern physics, volume 82, April-June 2010

APS/123-QED. *Spinoidal nano-decomposition in spintronics materials*

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Kazunori Sato, Masako Ogura & Hisazumi Akai. *Band structure calculation using KKR-Green's function method.* August 2008

Tomoya Ono. *First-principles calculation code based o real-space finite-difference method*. Dept. Prec. Sci. & Tech., Grad. Schl. Eng., Osaka University. 2009

Website:

http://www.suzukilab.mp.es.osaka-u.ac.jp/index_e.html

http://kkr.phys.sci.osaka-u.ac.jp/

RESEARCH PROGRESS

Computational Science Master Program

Institut Teknologi Bandung, Jl. Ganesha 10, Bandung, Jawa Barat, Indonesia

Visiting Laboratory

I visited Morikawa-sensei's Computational Physics group, Precision Science and Technology Division, Graduate School of Engineering, Osaka University.

Talk given by Yoshitada Morikawa:

Morikawa-sensei discussed about Davidson diagonalization. This method is used to obtain several extreme eigenvalues and the corrensponding eigenvectors of diagonally-dominant symmetric matrix. This method is originally motivated by configuration interaction method that usually used in quantum chemistry to calculate correlation energy of molecules. Now this method is used on many standard first-principles software packages.

Talk given by Hidekazu Goto:

Goto-sensei gave talk about direct enery minimization of total-energy functional on the basis of variational principle without imposing constraint of orthogonality and normalization on one electron orbitals. This method is implemented in real-space finite-difference scheme in which linear combination of Slater determinants are used as many-electron wavefunctions. The advantage of this method is the required number of Slater determinants for accurate calculations of the electron-electron correlation energy is less than that of configuration interaction (CI) method. This method is very interesting. I think I can try to apply this method to molecular system, not using real-space finite difference but the usual Gaussian type orbitals employed in quantum chemistry calculation.

Talk given by Tomoya Ono:

Ono-sensei mainly discussed about electron transport calculation on nanostructures using real-space finite-difference DFT and overbridging boundary method (OBM). Example of nanostructures discussed by Ono-sensei: sodium nanowire, Al nanowire, silicon oxide film, SiO_2/Si interface, C_{20} wires, C_{60} wires, helical gold nanowire, and Au nanowires.

Talk given by Soichiro Saito:

Saito-san discussed about his research about first-principles calculation on structure of GeO_2/Ge(001) interface. He found that sixfold GeO_2 reduces the lattice mismatch at the interface and is much more stable than the conventional fourfold interface. This means that interface stress between semiconductor and oxide can be reduced, hence minimizing interface defects. He also found that GeO_2/Ge is better than SiO_2/Si interface because Ge atoms are hardly emitted from the interface in the relaxation process. This opens up

possibility of using Ge instead of Si for advanced semiconductor devices, such as faster processor. Even though so the price of such device will be very expensive.

Talk given by Marcus Heide:

Marcus gave talk about implementation of spin-orbit coupling (SOC) and noncollinear magnetism in PAW (projector augmented wave) density functional calculations. In PAW we can access all-electron wave functions via transformation of smooth wavefunctions. SOC operator is not diagonal in spin so the wave functions have to be treated as two component spinors. Using this approach noncollinear magnetism also can be treated.

Research Progress

First-Principle Calculation on TiO_2 Anatase (101) Surface Sensitized by Cobalt-Phthalocyanine

TiO_2 is the most widely used photocatalyst material because it is very stable, cheap, non-toxic, and relatively easy to process. Even though so, the photocatalytic process using TiO_2 still have some shortcomings; the most noticeable of these is the fact that TiO_2 have band gap of about 3.2 eV which means that TiO_2 have to use ultraviolet spectrum (only about 5% of total sun energy radiation to Earth).

Many attempts have been made to in order to utilize the visible spectrum such as using doped TiO_2 and sensitized TiO_2.

Sensitization of TiO_2 surface has received special attention both theoretically and experimentally because of the development of dye-sentized solar cells (DSSC). DSSC is very promising because it has several advantages over conventional Si- or other semiconductor-based solar cells [1]:

- Low production cost ant thus low investment cost
- Design opportunities, such as transparency and multicolor options.
- Flexibility
- Lightweight
- Feedstock availability to reach terawatt scale
- Short energy payback time (< 1 year)
- Enhanced performance under real outdoor conditions; better than conventional solar cell at diffuse light and higher temperatures.
- Bifacial cell capture light from all angles
- Outperforms competitors for indoor applications

My main focus is to investigate the mechanism of sensitization of anatase phase of TiO_2. From literature[2], sensitization of TiO_2 surface is usually described by the following process:

1. Excitation of electrons from valence band of dye to conduction band of dye which utilize visible light radiation.

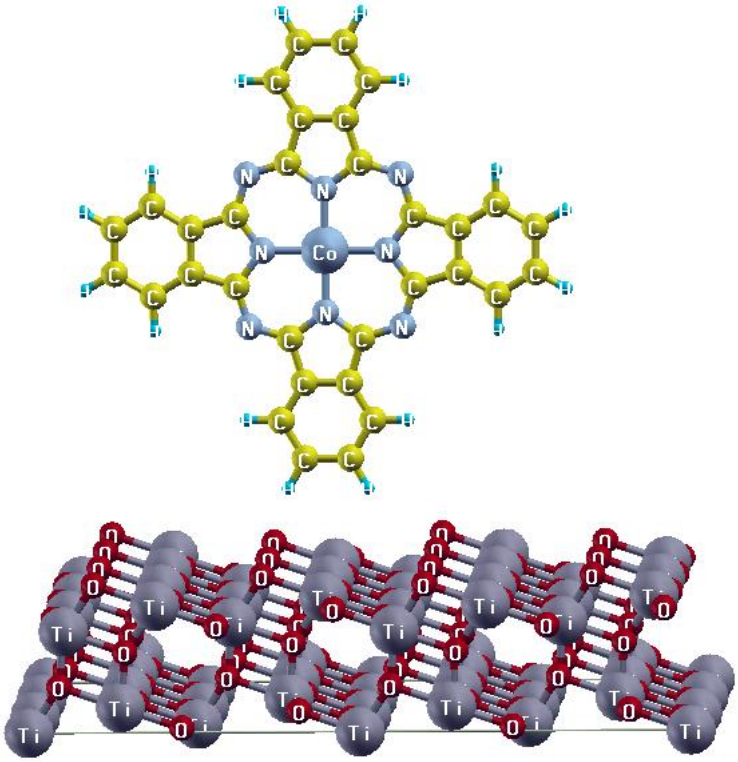
[1] A. Hagfeldt *et. al*. *Chem. Rev.* 2010, **110**, 6565-6663.
[2] E. Lee Tae *et. al*. *J. Phys. Chem. B.* 2005, **109**, 22513-22522.

2. Electron transfer from conduction band of dye to conduction band of TiO_2.

These mechanism is also referred as “two-step” electron injection mechanism. Dyes that bind to surface of TiO_2 using carboxylic acis groups have been known to inject electrons to TiO_2 according to this mechanism. Examples of such dyes are Ru(II)-complexes, coumarin derivatives, metal-porphyrin complexes, and others. Metal-phthalocyanine, including CoPc, belongs to the first group.

Another mechanism is direct, “one-step” electron injection from ground state of dye to conduction band of TiO_2 by photoexcited electrons. Examples of dye that belong to this group are cathecol and anthocyanine.

The main obstacle that I face is the size of the system is very large. To fit CoPc on TiO_2 anatase surface (101). I need more than 180 atoms which is very computationally demanding. The following picture is example of supercell that I will calculate.



Besides, the band structure calculation using standard DFT such as LDA or GGA suffers from underestimation of band gap. The simplest solution to this problem is maybe using DFT+U approach. GW approximation, which is more accurate than LDA+U, is very time consuming and the calculation is not trivial, even using developed standard package such as ABINIT.

Parallelization of Norm-Conserving Pseudopotential-based DFT Calculation on GPU using CUDA

Norm-conserving pseudopotential (NCPP) is regarded as standard method in DFT calculations. Many of the DFT-based first-principles calculations were done using this method. In this method, Kohn-Sham equations can be expressed as a simple eigenvalue problem. Even tough so, using the commonly used planewave bases, the size of matrix in the eigenvalue problem can be very large. Fully diagonalizing such matrix is very time consuming and require large computer memory. Because of that, iterative methods are

usually employed. Among popular ones used in first-principles calculations are Lanczos, Davidson, conjugate-gradient, residual-vector minimization, conjugate gradients, etc. My research interest is to parallelize these calculations on GPU, evaluate the performace and suitability of these kind of calculations on certain GPU. For this time, I only consider one GPU. Future research will include multi GPU.

GPUs (graphics processing units) are usually used for rendering computer graphics and recently have been used to speed up scientific and engineering calculations. Numerical intensive, parallel computations are sent and done on GPU which contains massively parallel processors that originally intended to renders graphics. The so called GP-GPU (general purpose computing on graphics processing units) paradigm is aimed at such applications. On the early development, the programmers must map computational task to graphics rendering problems which can be very hard for non-graphics programmer to understand. In order to cope with this problem, Nvidia, one of GPU vendors, offers an easier programming platform called CUDA (Compute Unified Device Architecture)[3]. Using this platform the programmer no longer needs to map his computational task to graphics rendering. Using some runtime API and minor extensions to standard C, writing GPGPU programs on Nvidia GPU can be relatively easier task. CUDA also offers several libraries that can be used conveniently for computational task such as CUBLAS (for BLAS operations), CUSPARSE (for sparse matrix operations), and CUFFT (for fast Fourier transform). There are also free third party library such as MAGMA[4] which offers some of LAPACK subroutines. There are also other alternatives to CUDA such as AMD Stream and OpenCL. OpenCL is standardized and thus can be applied not only to GPU but also other accelarators. OpenCL is harder to program because the programmer must think lower level abstraction and not as much developed as CUDA.

Traditional first-principles program packages traditionally use parallelization based on MPI for distributed memory computers and OpenMP for shared memory computers. Along with the advent of GPU computing, several first-principles softwares tried to take advantage of GPU, probably the most notable one is BigDFT [5], which uses wavelet basis set and HGH/GTH pseudopotentials.

In order to test the suitability of GPU for first-princples calculation, I have developed simple program in Fortran90 to implement NCPP plane wave DFT. This code is based on FHI98MD[6] package. I had made several modifications such as:

- Input file format is simpler (following the philosophy of ELK[7]).
- using pure plane wave basis, while in FHI98MD we also can use mixed basis set with local orbitals.

[3] http://www.nvidia.com/object/cuda_home_new.html
[4] http://icl.cs.utk.edu/magma/
[5] http://inac.cea.fr/L_Sim/BigDFT/
[6] M. Bockstedte *et. al*. *Comp. Phys. Comm.*, 1997, **107**, 187-222. www.fhi-berlin.mpg.de/th/**fhi98md**/
[7] http://elk.sourceforge.net/

- implement only electronic structure calculation; molecular dynamics and structure optimization are not implemented
- *k*-point generation is leaved to user, in FHI98MD user can generate *k*-point list using helper program. The feature to generate irreducible *k*-point by using symmetry will be implemented after the original purpose (i.e. parallelizing on GPU) is done.
- Hamiltonian matrix is not calculated explicitly. In FHI98MD the Hamiltonian matrix element is calculated explicitly. This allows my program to treat bigger system with higher cutoff energy.
- Using iterative diagonalization method: Arnoldi method and LOBPCG (locally optimal block preconditioned conjugate gradient) to solve eigenvalue problem. The smaller matrix eigenvalue problem is solved using LAPACK's ZHEEV. In FHI98MD the full Hamiltonian matrix is diagonalized using EISPACK subroutines.
- Several array variables have been deleted so that the memory requirement is much less than the original FHI98MD.

The most time consuming part of the electronic structure calculation is the diagonalization of Hamiltonian matrix and this part will be my main focus to be parallelized. Currently only Arnoldi method that worked quite well in my program. LOBPCG method needs more memory than Arnoldi so I will focus only on Arnoldi method.

The algorithm of Arnoldi method that I used in my program is as follows[8]. Suppose that we want to get *k* lowest eigenvalues and their corresponding eigenvectors of Hamiltonian *H*:

1. Guess input vector v_1 with unity norm.
2. Calculate $v_2 \leftarrow Hv_1$ (apply Hamiltonian).
3. Calculate $\alpha \leftarrow v_1^* v_2$. Assign: $h_{1,1} \leftarrow \alpha$
4. $v_2 \leftarrow v_2 - \alpha v_1$
5. Compute one step of iterative refinement:
   5.1. $\alpha \leftarrow v_1^* v_2$
   5.2. $v_2 \leftarrow v_2 - \alpha v_1$
   5.3. $h_{1,1} \leftarrow h_{1,1} + \alpha$
6. Compute *k*-steps of Arnoldi factorization: $AV_k = V_k h_k + f_k e_k^*$.
7. Do until convergence:
   7.1. Compute *p* additional steps of Arnoldi sequence, $p = \max(2k, N)$, *N* is number of basis set.
   7.2. Solve smaller eigenvalue problem: $h_k q = wq$
   7.3. Compute the converged Ritz value.
   7.4. Apply *p* implicit shifts if convergence is not happened. Otherwise continue.

[8] R. B. Lehoucq, D. C. Sorensen, and C. Yang. (1998). *ARPACK Users' Guide: Solution of Large-Scale Eigenvalue Problems with Implicitly Restarted Arnoldi Methods*. SIAM.

The most time consuming process in these steps are the Arnoldi factorization. The most strainghtforward strategy to parallelize this operation is using CUBLAS functions. Special attention must be given however, because transferring data from and to GPU is very expensive. I have done simple test to compare performance of MKL BLAS's against CUBLAS's ZGEMV[9] (using the provided Fortran90 interface in CUDA 4.0 SDK). From this test, MKL BLAS was generally faster than CUBLAS for 1 call of ZGEMV. CUBLAS may however gain better performace when the size of matrix is larger. My GPU only have 1 GB of memory so I can not test for bigger matrix size. Even tough so, for several calls of ZGEMV, without displaying the result or copy the result back to CPU, CUBLAS had better performance than MKL BLAS.
So, during the calculation, the operations that need to transfer data from and to GPU must be minimized. Right now, I am concentrating on creating a subroutine that apply Hamiltonian to arbitrary vectors. In order to minimize data transfer from and to GPU this operation must be done on GPU only. The data (arrays) that needed in this subroutine only copied once before the first iteration of Arnoldi. However, per-SCF iterations the Hamiltonian changes, so that these data need to be updated (copied to GPU). The standard Arnoldi algorithm must be modified in order to meet this need.

[9] Level 2 BLAS, double-precision complex matrix-vector multiplication

Carlo Antonio T. Ng

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I am Carlo Antonio T. Ng a second year masters student from De La Salle University – Manila in the Philippines. My thesis project is on the development of polymer electrolyte systems for dye-sensitized solar cells, improving on the current liquid electrolyte system by looking at possible solid-state electrolyte systems to improve the stability and performance of the solar cell. I was encouraged by our department head and my adviser to join this program to maybe get something out of the program for our research, since our research field is on materials chemistry.

In coming to the program, I had no background on computational design, or have performed any computational studies, since the researches I have been doing were all experimental. Upon looking at the scheduled itinerary of my stay, I was interested to learn more on a new field on computational materials design. We attended the 19th Computational Materials Design (CMD) Workshop in our first week stay and visited a professor's laboratory for three days and attended seminars presented by Professor Kasai's students in a day during our second week.

The CMD workshop was a very informative workshop, where the theoretical framework was presented and discussed in details for us with an accompanying hands-on exercise on the program, its basic features and basic operations. On this weeklong workshop, we were given an overview of computational materials design, why it is becoming a big research field and its importance to the development of real life materials to develop in various fields such as in the field of energy conversion and semiconductor materials. The main UNIX interface was also discussed since it was the main interface the used to run the computational programs. We were taught here the basic commands and the main interface on how to handle the system. These basic things were useful when the actual hands-on training using the programs were performed in the next days of the workshop.

The next few days of the workshop gave us a basic introduction on the computational design programs by the professors who developed them. They gave us an overview of the program, the theoretical concept and calculations involved in the operation of the program, and what important data could we get out of the calculations of the program. We were first introduced to the MACHIKANEYAMA2002 program by Professor Hisazumi Akai. The second program we were introduced to was the OSAKA2K program delivered by Professor Koun Shirai and the third calculation program was the ABCAP program introduced to us by Professor Hamada Noraiki.

In the MACHIKANEYAMA2002 program introduction lecture, the topics presented and discussed to us were very new to me, since I had no background in theoretical/computational chemistry and design programs and studies. The MACHIKANEYAMA2002 program discussed to us for the computational materials design course uses quantum simulation to determine the band structures of crystalline semiconductor materials. From what I learned in the lecture, the KKR method is based on the Density Functional Theory (DFT) which uses the Hohenberg-Khon theorem in calculations. The Kohn-Sham equations are also used to determine the Local Density Approximation (LDA) which the KKR method is based on. The DFT uses the ground-state electron density function of a particle, using the Hohenberg-Kohn theorem to be able to determine other observables/properties of the particle, e.g. band structure and band gap of the material.

The basic background of the program discussed to us was very useful in understanding the concept of the computational program and the various properties it could calculate, and the possible properties of certain

probable materials for future development and use. We were introduced to band structure calculations using the KKR Method, which is also called the "Green's Function Method" for crystals using partial differential equations. It uses scattering method and the muffin-tin potential model for calculation of scattering, it also takes into account impure scattering and scattering due to random potential in this particular model. Quantum mechanical scattering employed with the total probability amplitude equals to the sum of all indistinguishable processes in the scattering, where the probability is the square of the absolute value of the probability amplitude. This total scattering amplitude, which is the sum of each scattering amplitude is represented by a t-matrix. This describes the scattering by crystals.

In the KKR, normal band structure calculations can be performed with a solution to the scattering problem for system with deflections, impure systems, disordered systems and system with partial disorder. The KKR also deals with problems that require the Green's function to solve, including transport properties and many body systems.

After the short overview of the program, we then proceeded to the hands-on exercise in using the cpa2002v009c program to learn the basic functions of the program. We looked at some model systems to learn how to determine the density of states calculation, then included the effects of impurities and how to perform the calculations with these impurities, getting the CPA (coherent potential approximation), obtaining the Slater-Pauling curve, the hyperfine field calculation and the curie temperature of ferromagnets using MACHIKANEYAMA2002. This experience was very informative to me, being able to use programs to determine the properties of certain materials, and possibly to improve on the performance of materials theoretically, before performing experimental studies. This for me, was a good way to start materials design studies since it could make the development of better materials faster and more efficiently before proceeding to the actual experimental development of the material. This step could save time and resources, both money and raw materials, by surpassing the rigorous "trial and error" phase of studies in optimizing the performance of the material.

From the examples we did in the hands-on part of the workshop for this program, I was able to appreciate more the applicability of computational materials design. We were able to do a Slater-Pauling curve for alloys of transition metals, plotting their magnetic moments and we were able to determine that the results from the calculations were observed to behave similar to experimental results quite accurately, even with the branching patterns. The hyperfine field calculation was also taught to us in the case of a hydrogen atom in an infinite number of iron atoms; and the Curie temperature of ferromagnets determined for a hypothetical example. The temperature calculated and obtained was quite close to experimentally observed results. This slowed me that using computational materials design programs are indeed helpful in accurately determining properties of materials without having to actually go into the experimental development of the material, thereby saving time and resources.

Some of the real life applications of the MACHIKANEYAMA program presented to us includes the design of spintronics materials for half-metallic CrAs, design of zinc blend type half-metals, and the design of half-metallic, half-Heusler alloys.

The second program we were introduced to was the OSAKA2K program, discussed to us by Dr. Koun Shirai, based on 1st principle pseudopotential electronic structure calculations. The concept of the OSAKA2K program presented to us is based on self-consistent calculation to get the properties of the system, such as the total energy and charge density. From the properties, band density of state and the Hellmann-Feynman force stress can be calculated to determine structural optimization and get dynamical properties of crystals.

OSAKA2K theoretical concept is based on pseudopotential calculations to get the planewave expansion for the expression of the wavefunction. This results to the direct minimization of the total energy, forces and stress. The elements of the principle is to determine the ground state of the system by local density approximation, pseudopotential method, plane-wave expansion, minimization of total energy and special k-sampling method to lead to structural optimization by conjugated gradient method.

The idea of pseudopotential comes from the idea that chemical properties of a system are primarily determined by the valence electrons. These properties can be determined by simulation of only the valence charge. From this, smooth potentials can be constructed to represent the charge density of the system suitable for plane-wave expansion to easily evaluate the Hellmann-Feynman forces and stress for the dynamic property determination. This leads to suitable molecular dynamics applications.

The iterative minimization by conjugated-gradient method leads to efficient calculations. The total energy of a many electron system is simplified by the Kohn-Sham equation to a single electron problem. For the application of the program, it was discussed that the determination of the cohesive energy and formation energy is possible for systems. From atoms of 2 elements, through cohesive energy they form the solids and through formation energy, combine to form the alloy. From these calculations, comparison with experimental data resulted to accurate predictions; an example presented to us was for $B_{12}C_3$: the calculated cohesive energy for B was 6.841, for C was 8.390 and for BC 0.109 while experimentally, values of 5.77, 7.37 and 0.146 were obtained and by comparison, the calculated values obtained were satisfactory, since they were not very far from the experimental data but also not very close.

The lecturer also presented one of his studies on dynamics design using the program. From this program, they performed materials design utilizing atomic motion modifications of structures to specific applications to transform insulators to superconductors; and controlled atomic motions to control diffusion impurities on semiconductors by first principle calculations. After the discussion, hands-on exercises were also performed for the OSAKA2K program to familiarize us on the use of the materials design program. From the hand-on session, we were able to run calculations with silicon as the model system. After the initial calculations, optimization of the crystal construction was done and the effect of moving an atom in the crystal was also done.

The last program we were introduced to was the ABCAP (all electron band structure calculation package) which was discussed by Dr. Noraiki Hamada. The basic theories of the program were also briefly discussed to us before the hands-on sessions. The ABCAP program utilizes the density functional theory using the Kohn-Sham equations which is used to understand the behavior of many electron system in terms of a one electron state. It also uses the FLAPW (full-potential linearized augmented plane wave method) for the Muffin-Tin spheres, the Takeda-Kubler scheme for linearization and totally symmetric basis functions. Some of the properties that could be determined by the program includes determining the cut-off energy and the minimum value of l.

In the hands-on session, we were able to use the program to determine the band structures of sample systems through the TSPACE, utilizing translational symmetry (Bravais Lattice) and rotational symmetry (crystal point group) with nonprimitive translation. The translational symmetry uses the lattice translational vectors (T) whose operator obeys closure, associativity, has the identity element and has an inverse. The operator is also commutative and is Abelian. The space group meanwhile, is the group element represented in the Seitz notation. From this, we were able to get and draw the band structure of the sample systems and also determine its density of state. The irreducible representations of the k-group were also determined; and the crystal structure of the system also drawn.

After each programming lecture and hands-on sessions were over, special lectures and case studies were also presented. From these additional topics, I was able to see and appreciate more the importance and the applicability of these computational design techniques to actual materials development. We were given special lectures on quantum chemical calculations on proteins. This particular topic made me see the other areas of use in this method. Initially, I thought that the computational design techniques were only applicable to ordered crystal structures; but by seeing research on computational studies on bigger, more disordered systems such as proteins, I saw how broad this field could cover and could be used to develop materials for various uses.

Another special lecture was on the role of this method on industrial use. Due to the possible wide application of this method, it could be used by industries in developing materials. Due to the more uses of the programs, there are certain limitations now that have to be addresses to make this a better tool for commercial use. One of the current limitations of the method is on the computer. A lot of researches require very large numerical values in calculations. To be able to solve the problems and the verification process, very powerful computers should be available for these calculations.

Aside from the special lectures, other actual cases were presented to us by various researchers who specialize in this field. Studies using computational design were presented and discussed to us. One problem I encountered in the special lectures and the case study presentations was the language used in delivering the lecture. Almost all of the lectures and cases were given in Japanese which I did not understand. Even though the topics were very interesting, I was not able to understand them due to the language. From this, I just tried to study the lectures through the handouts given to us.

From the handouts, I saw more the actual application and uses of the computational design and have lead me to appreciate this method of research even more due to the vast applicability of the method and accuracy in determining actual properties of materials. From the cases, properties such as the electron transport ans electronic structure, metal surface properties and surface reaction design among others. From this, the development and design of new materials such as semiconductors, nanotubes and photovoltaic devices are some of the devices and materials which can be developed from this method.

In the second week of my stay, we were assigned to specific laboratories to stay for three days. I was assigned to visit Prof. Akai's lab. In my visit, I learned a lot n my first day with Prof. Akai, when he talked with us and introduced us to the researches his laboratory was doing. I, with a thesis in experimental chemistry, learned a lot of new things, some of them could even be applied in the material we are focusing our research on. In my stay, I also learned a lot from my fellow invited researchers, while discussing our thesis topics with each other. Three of us were assigned to Prof. Akai and all three of us had researches in different fields. One was in computational physics, another was in experimental physics and talking with each other about our research areas taught me a lot.

Also on the last day of our program, we were also given the chance to visit the Riken Institute which houses the super K computer. This computer system was the fastest in the world and is powerful enough to perform any calculations faster. This could lead to the rise of more researches in computational materials design due to the powerful ability of the computer system and how it could be used by a lot of researchers for studies in various areas.

This two week experience was a very informative and good experience for me. Overall, all of the lectures, workshop and activities we undertook the two weeks were very good and I have learned a lot from them. The CMD workshop and the visit to Prof. Akai's laboratory, along with being exposed to the researches

of other young researchers in other areas of interest have leaded me to realize the importance of computational design in materials design, aside from being a cheaper method for materials design, before performing actual experiments, which could save both time and resources. This step in researches is good since results obtained from computational studies yield values accurate with the experimentally determined values.

Also from the workshop and lectures, I see that computational design could be applied in the material we are currently studying. We are currently trying to improve dye-sensitized solar cells by studying polymer blends for application in the solar cell as electrolyte systems. Computational design could be performed on the polymer blend before experimentally testing this. The band structure and energy gap could be determined and an optimal blend determined before experimental study to be done, saving time and resources in dealing away with the currently performed "trial-and-error" method in materials design, while yielding possible predictions near to actual ones.

Another possible application in the material is on the nanocrystal TiO_2 semiconductor material for the solar cell. Dye-sensitized solar cells are composed of a nanoporous semiconductor oxide material, a dye sensitizer and an electrolyte system all sandwiched between conductive glasses connected to an external load. Another way to optimize the solar cell is to look for other possible materials as the semiconductor oxide material. From the lectures, the three programs we were introduced to involved the calculation of crystals including metal oxides. From this, I saw a lot of applications of the programs to the semiconductor oxide, to look at its band structure to look at how good of a material it could be.

The only downside to the CMD workshop for me was the language. Since most of the lectures on the programs and the hands-on sessions were delivered in both English and Japanese, I did not have a problem understanding them; but when it came to the cases and special lectures, they were delivered only in Japanese. The topics were interesting and I would like to learn more about them and the applications of computational design; but did not due to the language difference.

REASEARCH PROGRESS REPORT

Quantum engineering design research initiative (QEDRI) is composed of researchers in various fields (physics, chemistry, information and computer science). Its mission is to carry out researches that would effectively meet the ever-changing needs of society. The aims are to promote the design of novel material, highly sophisticated and functional devices, as well as, environment-friendly technology, through the development of novel theoretical routines and techniques. There is 3 core from QEDRI, 1st is creation of frontier mathematical methods, 2nd is elucidation of emergent material function, and 3rd is realization of new generation functional materials. Each core are connected each other.

Computational materials design (CMD) workshop is one of the QEDRI activities. In this workshop we are given lecture about software package for material simulations. I joined advance course and the special software package which is I chosen are ESOpt and HiLAPW.

ESOpt

ESOpt lecture is given by Koichi Kusakabe Sensei. ESOpt packagis a program package for the electronic structure calculation based on the density functional theory (DFT). The program adopting the planewave expansion method is originated from the package developed in the Institute for Solid State Physics (ISSP), University of Tokyo, which is called "opt". In this workshop was used a revised version of opt, was produced by choosing functions selectively and by applying the Fortran 95 scheme and also added another diagonalizing routine to the original version.

To understand practical calculation methods in the DFT simulation is define $R_I, Z_I, \hat{V}_I^{pseudo}(r - R_I)$ as the atomic coordinate, the ionic charge, and the pseudopotential of the I-th atom. The expression for the total energy of a crystal with the volume Ω is

$$E_{total} = E_{kin} + E_{el-el} + E_{xc} + E_{el-ion} + E_{ion-ion}$$

Here, E_{kin} is the kinetic energy of electrons, E_{el-el} represents a part of the electron-electron interaction called the Hartree energy, which is the classical Coulomb energy for the electron charge density. The exchange correlation energy E_{xc}, the static electron-ion Coulomb interaction E_{el-ion}, and the ion-ion repulsive Coulomb energy $E_{ion-ion}$, assuming that the ion core gives the spherical potential.

Each contribution has the next expression in the real space:

$$E_{kin} = \sum_{k,n,\sigma} \int_{\Omega} dr\, \phi^*_{k,n,\sigma}(r) \left(-\frac{1}{2}\nabla^2\right) \phi_{k,n,\sigma}(r),$$

$$E_{el-el} = \frac{1}{2} \iint_{\Omega} dr\, dr' \frac{n(r)n(r')}{|r - r'|},$$

$$E_{xc} = \int_{\Omega} dr\, \varepsilon_{xc}\big(n(r)\big) n(r),$$

$$E_{el-ion} = \sum_{k,n,\sigma} \sum_{I} \int_{\Omega} dr\, \phi^{*}_{k,n,\sigma}(r) \hat{V}_{I}^{pseudo}(r - R_I)\, \phi_{k,n,\sigma}(r),$$

$$E_{ion-ion} = \frac{1}{2} \sum_{I,J} \frac{Z_I Z_J}{|R_I - R_J|}.$$

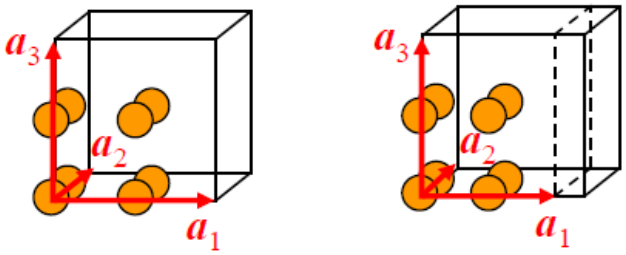
Here, $\mathrm{n}(r)$ is the single particle density given as,

$$\mathrm{n}(r) = \sum_{\sigma=\uparrow,\downarrow} n_{\sigma}(r),$$

$$n_{\sigma}(r) = \sum_{\varepsilon_{k,n,\sigma} \le E_F} |\phi_{k,n,\sigma}(r)|^2,$$

The Kohn-Sham orbital represented by a wave function, $\phi_{k,n,\sigma}(r)$, is given for the *n*-th band with the spin σ at the sampled *k* point, k. The energy of the orbital is given by $\varepsilon_{k,n,\sigma}$. The Fermi energy E_F is for the imaginative independent Fermion system.

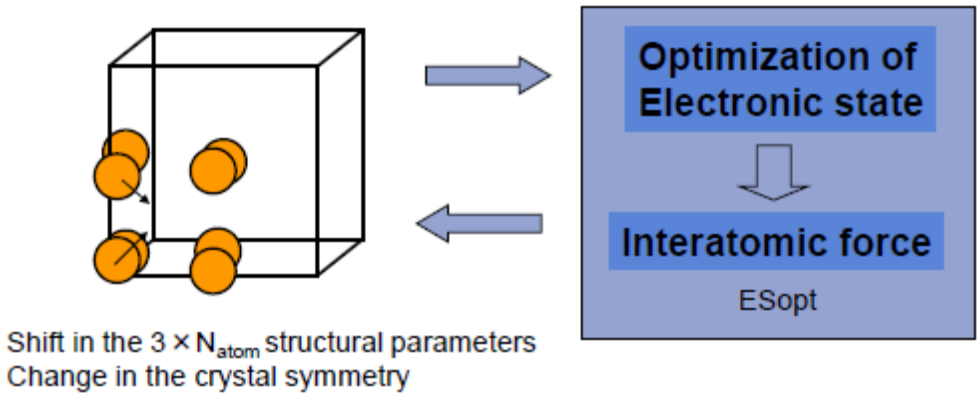
For multidimensional optimization problem, there are quantities as the variables determining of the system electronic state, atomic position, and unit cell (lattice parameters), restricted by the periodic boundary condition, various electronic states appear depending on atomic position in the variable unit cell. In the actual simulation, electronic state, atomic positions, and unit cell to be optimized in an order of the number. Structural change given by modification of lattice vectors induced by difference between internal stress and the external pressure.



There is 9-3=6 degrees of freedom after removing total rotation of the system.

1. Lattice constants ← optimization of all parameters
2. Elastic constants ← deformation of stable structure
3. Structural transformation ← molecular dynamics

Structural change and electronic structure of the structure obtained by shift in atomic position due to the interatomic force.



Thus, can be determined stable atomic configuration, intermediate state (transition state), and reaction energy. The explanation before are the theoretical method which is used in ESOpt package. In the ESOpt package, the input files should be prepared in the directory INPUT_DATA. Then, we have to do make in the main directory execution of the calculation is done in the working directory whose name is specified by a line of makefile. Procedure to perform computation using ESopt, are written as follow:

1. By creating INPUT_DATA/CORD, the user set the system parameters including atomic coordinates, atomic species, and the unit cell, as well as the essential conditions for the cutoff radius, and the *k*-sampling method.
2. The user should check and write destination, which determines the name of the working directory and is weitten in the line DESTDIR=*destination* at the head of makefile. In this instruction, we omit a description how to handle the machine dependence.
3. Do make.
4. Next, cd *destination*. Set the control files SOPT.CTNL, ALLOPT.CNTL, FILE_IO.CNTL for the execution properly.
5. Run the program by ./opt or by submitting job by qsub qsub using the job scheduling system, SGE. In the last action, the first qsub is the command, while the second qsub is a script prepared when you run make.

In the calculation, a sub-directory named by MONIT is created in the working directory, and in this directory there appears temporal information on the energy, etc. The total energy is in energy. The wavefunction may be given in intwf, if properly specified in the code. When the structural optimization is finished, wave999 for the wavefunction is given. The format of the wavefunction data is unformatted. The charge density is stored in another subdirectory CHARGE.

HiLAPW

HiLAPW lecture is given by Tamio Oguchi Sensei. HiLAPW is a first-principles calculation based on the density functional theory package originally developed by a theory group in Hiroshima University. The current developments of the package are being made in collaboration between Osaka University and Hiroshima

University. HiLAPW program package is composed of kernel executables such as xsets and xlapw, and some other optional ones. All the executables acan be made with use of makefile attached with the package and FORTRAN90 compiler on user's computer.

In this lecture we practiced to calculate Cu with fcc structure and we practice another material which is chosen by myself. I chose magnesium diboride (MgB_2). Under the directory hilapw3, new directory is created for calculations of MgB_2. By typing getdata on command promt, three database files atomdata, atomdens, and spgrdata are imported from the default database directory ~/hilapw/data.

cd hilapw3

mkdir MgB_2

cd MgB_2

getdata

To perform example calculations for MgB_2 extract eleven file from the directory ~/hilapw3/data

tar xvf ~/hilapw/data/ MgB_2.tar

For starting the SCF calculation, just type the shell-script as

#./JOB-SCF

After the execution xlapw, the tool command LAcopy is used for attaching a particular modifier (A1 or A2) to the output files.

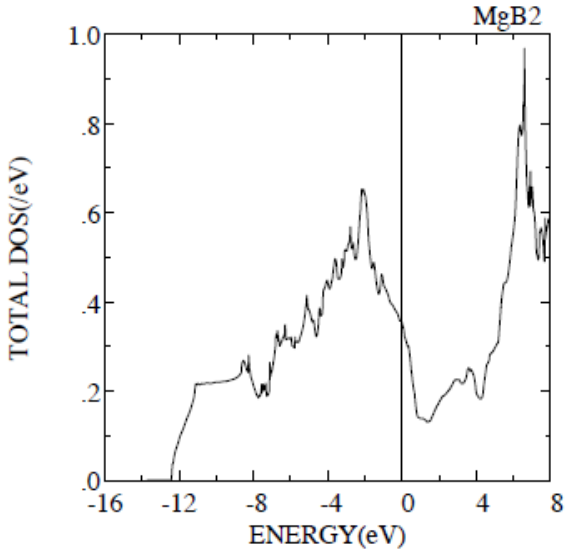
For the total density of states (DOS), type

xdoss

mv pdos pdosA2

getfermi outA2 > FermiA2

PSP < psp_tdos > tdos.ps



Then, it was obtained the plotting total DOS of MgB_2 on the figure above. It showed that MgB_2 is conductor material because there is overlap gap on the Fermi level. MgB_2 is a simple ionic binary compound that has proven to be an inexpensive and useful superconducting material. This material was first synthesized and its structure confirmed in 1953, but its superconducting properties were not discovered until 2001. Though generally believed to be a conventional (phonon-mediated) superconductor, it is a rather unusual one. Its electronic structure is such that there exist two types of electrons at the Fermi level with widely differing behaviour, one of them (σ -bonding) being much more strongly superconducting than the other (π -bonding). This is at odds with usual theories of phonon-mediated superconductivity which assume that all electrons behave in the same manner. Theoretical understanding of the properties of MgB_2 has almost been achieved with two energy gaps. In 2001 it was regarded as behaving more like a metallic than a superconductor.

The last lecture that I received was from Atsushi Yagi Sensei. His special topic is about mathematical methods for engineering, self-organization, mathematical model, mathematical analysis, and numerical computations. The point is how to make a model from the mathematical approaches. One of many mathematical approaches is fractal theory. Fractal theory is directly related to the measurement to biological structures at different magnifications. We can think of fractals in a simplistic, but still useful, way as geometric figures which repeat themselves at progressively smaller scales or exhibit progressively more complex structure when observed at larger and larger magnifications. With fractal there is often self-symmetry, or approximate self-symmetry. Yagi Sensei made a model for mangrove forest by using fractal method.

REPORT FOR JSPS INVITING YOUNG RESEARCHERS PROGRAM

RESEARCH

The Japan Society for the Promotion of Science is an "independent administrative institution". JSPS has, as a core agency promoting Japanese science, initiated and carried out a wide range of programs to advance scientific research, including research grants, researcher cultivation, and international exchange and cooperation. In 2008, the Japan Society for the Promotion of Science (JSPS) has launched the "Exchange Program for East Asian Young Researchers". Aimed at promoting researcher exchanges with East Asian countries, this program supports initiatives by Japanese universities and research institutions to invite young researchers (e.g. master's and doctoral students and postdoctoral researchers) from those countries. I was really happy when I was one of lucky students invited by Osaka University to attend this Exchange Program of JSPS. This is a good opportunity for me as well as other students to know about the life and scientific research in a developed country like Japan.

Our first activity in this exchange program was attending 19^{th} CMD® (COMPUTATIONAL MATERIALS DESIGN) workshop. CMD® workshop was established firstly in Philippines and then it was expanded in many other countries of Asian including Indonesia, Vietnam and Thailand. In this workshop, the computational approach which developes new materials with specified properties and functionalities has been shown. The basic technique is the use of quantum simulations to solve the materials science problems in order to design a material that suits this specification. CMD® has the high potentiality to impact the real industrial research and development. The purpose of these series of workshops is to provide the participants with a first-hand experience of how computational materials design CMD® is carried out, provide them with the basic knowledge and techniques, as well as to prepare them for the new paradigm in materials science research. This is also the main reason which encourages me to enter JSPS Exchange Program, because I have a small research on TiO_2 material base on ab-initio calculation. So I hoped the lectures in CMD® workshop would be useful for my research. At the 19^{th} CMD® workshop we attended Beginners Course and met many leading professors of computational materials design field in Osaka University. We also had a chance to meet many young researchers from other Asian countries and we have learned many interesting things about their religions and culture from them.

In Beginners Course we studied three calculation codes, Machikaneyama, OSAKA2K and ABCAP. The first is AkaiKKR (MACHIKANEYAMA) code. This is a software package used for first-principles

calculation of the electronic structures of metals, semiconductors and compounds, within the framework of the local density approximation or generalized gradient approximation (LDA/GGA) of density functional theory. Before this calculation code is introduced further more, we must clarify a terminology which is "first-principles". What we call nowadays first-principles calculations are also called in many ways, e.g., ab-initio calculation, parameterless calculation, etc. The naming is cynical. Which principle is the first one? The approach is not empirical, but heavy experiences are needed to master these skills of calculations. Parameterless is by no means no parameters in calculations. Although no parameter fitted to experiment is assumed, there are indeed a couple of controlling parameters of calculations, which may yield different answers by the input value. The statement that only atomic numbers are required as input is merely a slogan of first-principles researchers.

The AkaiKKR package, which features both high speed and high accuracy, uses the KKR–Green's function method. This is an all-electron method and does not suffer from any serious truncation errors such as those associated with plane-wave cutoffs. Moreover, the CPA (coherent potential approximation) is integrated into the package making it applicable not only to crystals but also to disordered systems such as impurity systems, random substitutional alloys and mixed crystals. Since the Green's function of the system is calculated, the package provides a good starting point for first-principles calculations of linear response theory, many-body effects, and so on. The package has been in continuous development since the late 1970s and this development is still continued today. It is written in Fortran 77 and is completely self-contained (no additional libraries are required). It runs equally well on a notebook PC and a supercomputer. It can be used on any platform (UNIX, Linux, Mac OS, Windows etc.) where a Fortran compiler is installed. The memory required depends on the physical system to be calculated. For instance, a spin-polarized calculation of a system with a single atom per unit cell requires no more than a megabyte of memory. However, a larger system with, say, 20 atoms per unit cell, may require 1GB of memory.

The second calculation code is Osaka2k or Osaka2002. This is a set of program codes which calculates electronic structures of materials by first-principles pseudopotential method. It covers a wide range of calculations from optimization of crystal structure to molecular dynamic simulations, in addition to standard self-consistent calculation and band calculations. Every component are the art-of-state calculations. As in many other calculation programs, Osaka2k is also not created by one person, A program atom which generates atomic pseudopotentials is created by Troullier and Martins, which itself has the long history. Osaka2k uses it as it were. Development of the core program of Osaka2k is dated back to 1987 at To-hoku University. There, under the direction of Prof. Katayama-Yoshida, Dr. N. Orita (Now, AIST) as the primary writer and Dr. T. Sasaki (NIRIM), and T. Nishimatsu (Tohoku Univ.) developed a first-principles molecular dynamic simulation program, named cpgs at that time, which based on Car-Parrinello method. The primal use of cpgs was study of impurities in semiconductors at that time, and for this purpose, cpgs had been completed. Therefore, they are really the parents of this program. cpgs had been developed there until 1995. However, the purpose of cpgs was

limited, several deficiencies were found, such as only Γ - point sampling, no use of symmetry, etc. After Prof. Katayama-Yoshida moved to Osaka Univ. in 1995, the present author began to rewrite it in order to use of crystal symmetry fully, and multi k sampling. In this process, the author reconstructed the code in order to make use of TSPACE created by Prof. A. Yanase. In addition, the core part of SCF calculation was replaced with the method of Teter-Payne-Allan, and functions of atomic optimization etc had been added. At the same time, band, DOS, phonon calculations were developed by the author. Until the fall of 2000, all the components had been integrated all together. This was the original form of Osaka2000, which was opened to public at 2000. After that, the whole codes were rewritten from beginning by new Fortran 90 under unified direction of programming design. This yielded a completely new version "Osaka2002 nano"

Finally is ABCAP package, this codename is abbreviation of phrase “All Electron Band Structure Calculation Package”. Similar to Osaka2k and Machikaneyama, ABCAP is based on density functional theory (DFT) with a full potential augmented plane wave (FLAPW) band - structure calculation in a local density approximation (LDA). ABCAP performs very good calculations of band – structure, Optical – constant and thermoelectric - power. The highlight point of this package is its interface and illustrations which help users to imagine input crystal structure and to obtain results easily.

In each code we were taught carefully by professors at Osaka University. Lectures were built from basic of density functional theory to how to use programs and read output results which give us a fundamentals of knowledge to understand basic theory building these codes. After each lectures we had a hand-on lesson, this is precious chance for us to practise what we have just studied. Finally, we were lectured about investigations using these calculation codes which help us to realize applications of these calculation packages in practice and also approach the first-principles calculation support for experiment research.

Our next activity was visiting laboratories. We were split into six groups and there were about three or four people in one group, each group had to visit a laboratory. There were three students in my group: one from Indonesia, one from Philipines and me - a Vietnamese student. This time, we visited Prof. Morikawa’s laboratory, in which we were lectured by Prof. Morikawa himself about main research and directions in the future of his laboratory. He also told us about the application of studies in practice with many areas including green power, environment and technology. This was the first introduction which showed us the general view of activities in laboratory. Next, we met members in the laboratory, they were very enthusiastic to show us their research not only making us understood their studies, but they also shared useful information in researching process, advantages, disadvantages and experiences during the time they study in the laboratory. During the time staying here, we received a lot of assistance from them. Although we just worked with them a short time, they really helped us to have a comprehensive view the academic life in laboratories of Osaka University. I think this is an extremely active environment for students who are looking for a place to study and research.

In conclusion, I think the lessons in this course are very helpful. The course provided best conditions for me to perform my research. I also prepared to use these calculation codes in my further investigation. The obtained results will be compared with my old research. And I strongly believe that they will be very interesting. Finally, I sincerely thank all professors at Osaka University who taught me with much love, and I also want to thank organizers of JSPS' Exchange Program for giving me such a wonderful time to work and study in Japan.

LIFE IN JAPAN

Osaka University is a major national university located in Osaka, Japan. It is the sixth oldest university in Japan as the Osaka Prefectural Medical College, and formerly one of the Imperial Universities of Japan. Numerous prominent scientists have worked or studied at the Osaka University such as the Nobel Laureate in Physics Hideki Yukawa.

Osaka University.

There are three campuses in Osaka University: Suita, Toyonaka and Minoh. Suita campus houses faculties of Human Sciences, Medicine, Dentistry, Pharmaceutical Sciences, and Engineering. And Toyonaka campus is home to faculties of Letters, Law, Economics, Science, and Engineering Science. It is also the academic base for Graduate Schools of International Public Policy, Language and Culture, Information Science, and the

Center for the Practice of Legal and Political Expertise. Finally Minoh campus is home to School of Foreign Studies, Research Institute for World Languages, and Center for Japanese Language and Culture. During 16 days living in Japan, we had chance to work at two campuses which are Suita Campus and Toyonaka Campus. This is precious time for us to know about life and working style in Japan.

The first thing I would like to talk about life in Japan is the friendliness of people here. It is presented by the way they greet, treat and help people around them. If you accidentally get lost in Japan you can ask any japanese men and he will guide you to your home. Japanese people also famous for their carefulness and discipline, especially when doing their work. People in this country always work on time. For example, public transports such as bus or train never depart or arrive late. Therefore, if you want to live here, you must study working on time first. Besides, products made by Japanese are unique and beautifully designed.

Some products made by Japanese artists.

Despite the fact that Oaska is one of the largest cities in Japan, the environment here is very airy and clean. Perhaps, this is a common characteristic of cities in Japan. And this is probably one of many reasons which help Japanese increase their average life-time.

A street in Osaka.

In Japan, public transports, for example, bus and train, are very well developed. They service most of Japanese travel demand. This is probably the main reason that help cities in Japan avoid the pollution. However, travel expenses in Japan is very expensive even for public transport. Therefore, I suggest that you should buy a bicycle and get used to long-distance walking if you want to stay here in a long time.

Finally, Japan is indeed a country of peace and prosperous. This is truly a great destination for students who want to live and study in a developed country.