QEDRI Meeting and workshop

2012/1/30(Mon)

		Presenter		Moderator
	10：20-10：30	Opening remark : Prof Hideaki Kasai		
1	10：30-10：50	Azizi Somayyeh	M1	Allan Abraham Bustria Padama
2	10：50-11：10	Zhang Wenlei	M1	
3	11：10-11：30	Alaydrus Musa	M1	
4	11：30-11：50	Ta Viet Ton	D1	
5	11：50-12：10	Nguyen Tien Quang	D2	
6	12：10-12：30	Ashim Kumar Saha	M2	
	12：30-13：30	Lunch		
	13:30-15：00	QEDRI Meeting		
7	15:00-15:20	Mary Clare Sison Escaño	D3	Joaquin Lorenzo Valmoria Moreno
8	15:20-15:40	Nghiem Thi Minh Hoa	D3	
9	15:40-16:00	Nguyen Duy Huy	D1	
10	16:00-16:20	Handoko Setyo Kuncoro	D3	
	16:20-16:40	Break		
11	16:40-17:00	Tran Linh Phan Thuy	D1	Nguyen Tien Quang
12	17:00-17:20	Chaunchaiyakul Songpol	M1	
13	17:20-17:40	Bui Pho Van	M1	

2012/1/31(Tues)

14	10:30-10:50	Ganes Shukri	M1	M Kemal Agusta
15	10:50-11:10	Ryan Lacdao Arevalo	M2	
16	11:10-11:30	Nguyen Hoang Linh	M2	
17	11:30-11:50	Chantaramolee Bhume	M1	
18	11:50-12:10	Joaquin Lorenzo Valmoria Moreno	M2	
	12:10-13:00	Lunch		
19	13:00-13:20	Saputro Adhitya Gandaryus	D1	Ryan Lacdao Arevalo
20	13:40-14:00	Li Xing Sheng	D2	
21	14:00-14:20	Febdian Rusydi	D2	
22	14:20-14:40	Allan Abraham Bustria Padama	D1	
	14:40-15:10	Break		
23	15:10-15:30	Doan Hai Duy	D3	Nghiem Thi Minh Hoa
24	15:30-15:50	Susan Meñez Aspera	D2	
25	15:50-16:00	Pan Jun	D3	
26	16:00-16:20	Ferensa Oemry	D2	
	16:20-16:30	Closing remark : Prof Yoji Shibutani		

Quantum Engineering Design Course Workshop

30 January 2012, 10:20-17:40
Room…
Suita Campus, Osaka University

PROGRAM

Opening Remarks by
PROF.　Hideaki Kasai
(10:20-10:30)

Workshop Proper
(Presentation: 15 minutes; Discussion: 5 minutes)

10:30 – 10:50	**AZIZI SOMAYYEH** **Genome rearrangement by DCJ operations** *Abstract:* First， I Would like to describe basic biology about genome and genome rearrangement especially sorting genome rearrangement by DCJ operations and types of DCJ operations． DCJ operation is first model for sorting genome rearrangement, although this is not the most natural model from the biological point of view ,and even not the first model from the historical point of view .however, mathematically it is the simplest to handle． Then， I will explain calculating the minimum number of DCJ operation that is necessary　to transform one genome into another.
10:50 – 11:10	**ZHANG WENLEI** **Design of Counter-Propagating Twin Photon Generation Devices** *Abstract:* Integrated nonlinear optical devices for the generation of twin photon beams are indispensable in the research of quantum information technologies. The major technique for generating twin photons is spontaneous parametric down-conversion (SPDC). In the TPG devices currently under development, the twin photons of signal and idler modes co-propagate in the same direction as the pump wave photon. Compared with co-propagating twin photon generation devices, counter-propagating twin photon generation (CPTPG) devices hold distinguished properties, such as direct generation of photons in quantum entangled states, and a narrow wavelength bandwidth suitable for fiber transmission. These properties leads to some unique functions and performances of the CPTPG device, which makes them easily compatible in quantum information systems. In my research, I am following the theoretical analysis for CPTPG devices using the SPDC technique in Ref. [1]. In the previous analysis, full description of the exact quantum states of the twin photon beams in the Heisenberg and Schrodinger pictures are given and mathematical expressions for device design and prediction of performances are deduced. Through the use of these mathematical expressions, I am building a mathematical

model with the MATLAB software. Using this model, different types of QPM waveguide structures are calculated and simulated, and their corresponding theoretical predictions of performance are examined. By comparison of the trade-off between different factors, practical device designs applying QPM $LiNbO_3$ waveguide structure (Fig. 1) can be obtained. The feasibility and method of fabrication for such devices will be explored. I am planning to achieve the goal of fabrication by considering the employment of third or fifth order QPM waveguide structures or ridge waveguide structures in thin film crystal.

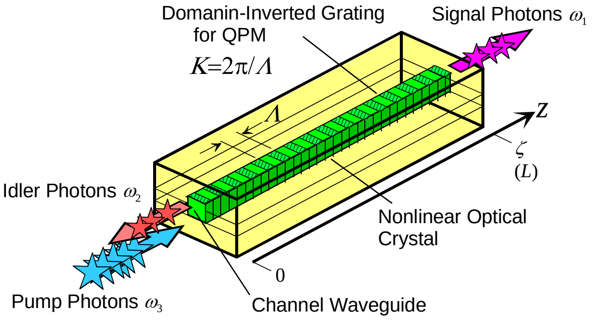

Fig. 1 Schematic diagram of CPTPG by SPDC in a QPM waveguide

References

[1] T. Suhara and M. Ohno, "Quantum Theory Analysis of Counterpropagating Twin Photon Generation by Parametric Downconversion," *IEEE Journal of Quantum Electronics*, vol. 46, no. 12, pp. 1739-1745, Dec. 2010.

11:10 – 11:30

ALAYDRUS MUSA

Platinum-Based Anticancer Drugs

Abstract: Platinum-based anticancer drugs are found to have strong impact on cancer chemotherapy. One of the well-known agents, cisplatin, has been used for more than three decades since its first discovery in 1960's by Barnett Rosenberg [1]. However, the efficacy of cisplatin has been greatly hampered by drug resistance and severe side effects [2]. Many cancers display inherent resistance to cisplatin while some others develop acquired resistance after initial treatment [3]. In addition, high systemic toxicities of cisplatin are reported to cause serious disorders and injuries [4-6].

To fix the imperfection of cisplatin, over the last 30 years, thousands of platinum compounds have been prepared and tested for potential anticancer drugs [7, 8]. However, only five among them, along with cisplatin, that have been approved for clinical treatment, that is, carboplatin, oxaliplatin, nedaplatin, lobaplatin, and heptaplatin (see Figure 1).

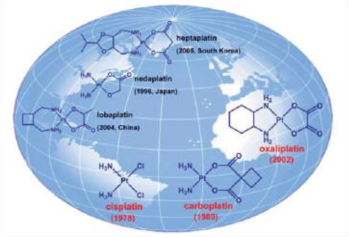

Figure 1 Platinum-Based anticancer drugs used globally (cisplatin, carboplatin, and oxalipaltin) and regionally (nedaplatin, lobaplatin, and heptaplatin) in chemotherapy [7].

This talk will be mainly discussed some reviews of platinum-based anticancer drugs and possible future improvement. Moreover, in our case, Density Functional Theory (DFT) related studies are specially emphasized, especially to unravel the physics of the drugs mechanism.

References

	[1] B. Rosenberg, L. Van Camp, and T. Krigas, "Inhibition of Cell Division in Escherichia coli by Electrolysis Products from a Platinum Electrode," *Nature*, vol. 205, pp. 698-699, 1965. [2] C. A. Rabik and M. E. Dolan, "Molecular mechanisms of resistance and toxicity associated with platinating agents," *Cancer treatment reviews*, vol. 33, pp. 9-23, 2007. [3] M. Galanski, M. A. Jakupec, and B. K. Keppler, "Update of the Preclinical Situation of Anticancer Platinum Complexes: Novel Design Strategies and Innovative Analytical Approaches," *Current Medicinal Chemistry,* vol. 12, pp. 2075-2094, 2005. [4] S. R. McWhinney, R. M. Goldberg, and H. L. McLeod, "Platinum neurotoxicity pharmacogenetics," *Molecular Cancer Therapeutics,* vol. 8, pp. 10-16, January 1, 2009 2009. [5] K. Barabas, R. Milner, D. Lurie, and C. Adin, "Cisplatin: a review of toxicities and therapeutic applications," *Veterinary and Comparative Oncology,* vol. 6, pp. 1-18, 2008. [6] A. A. Argyriou, P. Polychronopoulos, G. Iconomou, E. Chroni, and H. P. Kalofonos, "A review on oxaliplatin-induced peripheral nerve damage," *Cancer treatment reviews,* vol. 34, pp. 368-377, 2008. [7] X. Wang and Z. Guo, "New Trends and Future Developments of Platinum-Based Antitumor Drugs," in *Bioinorganic Medicinal Chemistry*, ed: Wiley-VCH Verlag GmbH & Co. KGaA, 2011, pp. 97-149. [8] C. X. Zhang and S. J. Lippard, "New metal complexes as potential therapeutics," *Current Opinion in Chemical Biology,* vol. 7, pp. 481-489, 2003.
11:30 – 11:50	**TA VIET TON** **Asymptotic behavior of solutions to a stochastic forest model** *Abstract:* A stochastic forest ecosystem of young and old age classes is studied. First, we prove the existence and uniqueness of the global positive solution and give upper bounds for both the young trees' class and the expectation of the old trees' class. Then, we show that the model is either asymptotically stable or sweeping with respect to compact sets. We also give some sufficient conditions under which the ecosystem falls into decay. Finally, numerical examples are presented to illustrate those results.
11:50 – 12:10	**NGUYEN TIEN QUANG** **The effect of substrate on the adsorption and dissociation of O_2 molecule on Pt_4/CeO_2 system** *Abstract:* We investigated the adsorption of Pt_4 cluster on CeO_2(111) surface and the adsorption and dissociation of O_2 on Pt_4 with and without the presence of CeO_2(111). We found that Pt_4 prefers to bind on CeO_2 at the three-fold Ce site and forms Pt-O-Ce bond. For O_2 adsorption on Pt_4, we found that O_2 molecule prefers to adsorb on isolated Pt_4 via top site. However, in the presence of CeO_2, the adsorption shifts from top to bridge site. Furthermore, the dissociation of the adsorbed O_2 molecule is easier on isolated Pt_4 than on Pt_4/CeO_2 and the dissociated O atom is more bound to the former. We attribute these changes in the reactivity of Pt4 to the CeO_2 support through the Pt-O interactions which promote Pt 5d hybridization with O 2p states (of CeO_2) leading to a decrease of Pt d states around the

Fermi level .

12:10 – 12:30

ASHIM KUMAR SAHA

Fabrication and Preliminary Experiment of Circular Grating Coupled Surface Emitting Laser

Abstract: Surface-emitting semiconductor lasers are attractive devices because of their salient features such as single-mode operation and wafer-scale 2-D integration. Objective of my work is to design and fabricate circular grating coupled surface emitting lasers (C-GCSEL) which can emit light in the nearly vertical direction of the laser plane. The C-GCSEL has many advantages such as *high output power* as compared to vertical cavity surface emitting laser (VCSEL), *beam shaping functionality* unfeasible in VCSEL and the conventional edge emitting lasers, *single mode operation* and *2-D array formation* which are difficult to accomplish in edge emitting and Fabry-Perot lasers.

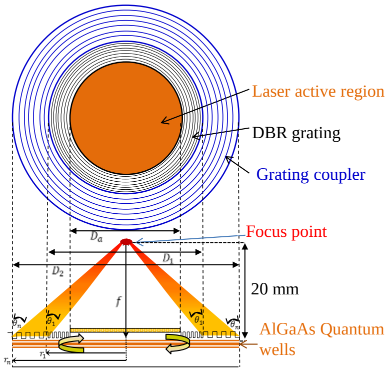

Fig. 1: Schematic representations of the top view (upper part) and the cross sectional view (lower part) of a C-GCSEL

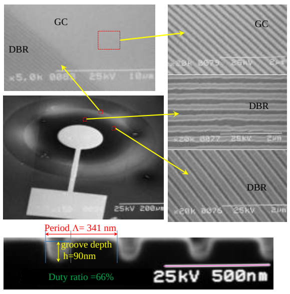

Fig. 2: Fig. 2: SEM micrograph of the complete C-GCSEL, DBR and Grating Coupler (GC) at different positions of the C-CGSEL and the cross sectional view of the DBR.

C-GCSEL emitting at 975 nm wavelength was reported by S. Kristjansson *et al.*[1]. I have fabricated AlGaAs based C-GCSELs which emit light at 780 nm wavelength. Schematic diagram of the C-GCSEL shown in Fig. 1 has three main regions (i) Laser active region (where light is generated), (ii) Distributed Bragg Reflector (DBR) grating (gives necessary optical feedback) and (iii) grating coupler (from where light comes out). On the basis of our previous works [2-3], I have designed DBR grating and theoretically calculated the coupling coefficient and reflectivity. Coupling coefficient (duty ratio) is 15mm^{-1}(85%) for third order DBR with groove depth of 70 nm. I also found that the length of DBR required to get 33% reflectivity is 120μm for third order DBR. First order grating coupler has also been fabricated to focus the output laser beam at a point on the axis which is normal to the laser plane. Other device parameters shown in fig. 1 were designed as D_a=185 μm, D_1=425 μm, D_2=650 μm and f=20mm.

I have completed the fabrication of the C-GCSEL. First I have written the circular active region on ZEP520A resist using electron beam writing system with circular scanning mode. After development, I have deposited 120 nm strontium fluoride (SrF_2) using vacuum deposition technique, and after lift-off the SrF_2 mask remains on the active region only. Using CH_4/H_2, CF_4/H_2 reactive ion etching (RIE) alternatively, ridge structure has been made. The polymer contamination layer deposited on the SrF_2 mask during RIE has been removed by O_2 plasma ashing. Then SrF_2 mask has been removed using 5% HCl.

To fabricate DBR and GC, at first 15 nm of SiO_2 intermediate layer has been deposited over the entire sample by plasma CVD using TEOS and O_2 gas. ZEP520A EB resist layer of 100nm thickness was deposited on the sample by spin coating. Then circular DBR and GC gratings have been written on the resist using electron beam writing system with circular scanning mode. After

	development, DBR and GC patterns have been transferred into the semiconductor epitaxial layer using two-step RIE. Then, 1.4 µm thick BCB layer has been made on the entire sample using spin coater. Top of the ridge is opened using RIE. Then, 1.0 µm thick resist mask was formed by EB writing to make top contact. Cr/Au top contact layer has been deposited using vacuum deposition technique. Then the unwanted Cr/Au layer was lifted-off. After reducing the thickness of the substrate appropriately by polishing, AuGe/Au bottom contact was deposited. I have performed preliminary test of the fabricated C-GCSEL. Thus far I have not yet accomplished the lasing but I have found out the reason for the insufficient electrical characteristics, and I am fabricating the device with improved process. I will test the performances such as output power vs. current characteristics, emission spectra, threshold current, spot size and external differential quantum efficiency of the laser. I will also compare the experimental results with the simulation results based on the semiconductor laser rate equations. **References** [1] S. Kristjansson, M. Li, N. Eriksson, M. Hagberg, K.-J. Killius, and A. Larsson, IEEE *Photon. Technol. Lett.*, vol. 9, pp. 416–418, 1997. [2] A. K. Saha and S. Islam,*The AIUB Journal of Science and Engineering (AJSE)*, vol. 8, no. 1, pp. 35-41, 2009. [3] S. Takushima, M. Uemukai and T. Suhara,*Jap. J. App. Phys*., vol. 48, no. 3, pp. 030206, 2009.
12:30 – 13:30	**LUNCH BREAK**
13: 30 – 15:00	**QEDRI Meeting**
15: 00 – 15:20	**MARY CLARE SISON ESCANO** **Theoretical Study on Oxygen and Borohydride Reaction on Metal Surfaces** *Abstract:* The reactivity of simple molecules on metal surfaces has been studied in light of the need to understand the interaction between these molecules and the metal for certain industrial applications. For instance, oxidation of metal surface is of outstanding practical importance in microelectronics, energy conversion systems and environmental devices. Borohydride reaction on metal catalyst, on the other hand, has been increasingly attracting researchers in field of hydrogen generation/evolution. An atomistic modeling of the interaction of these simple molecules with metals, focusing on the fundamental energetic, geometric and electronic properties, is sought to contribute to the understanding of the chemical reactivities. Generally, Pt catalysts are active and are widely used to study the reactivity of oxygen. The reaction of oxygen on paramagnetic Pt crystalline surfaces has been extensively investigated. The general consensus for its dissociative adsorption is that the reaction is activated. Several ways to tune the reaction energy profile of oxygen on Pt has been attempted. Fundamentally, by employing density functional theory and monte carlo simulations, we found that the reaction energy profile of oxygen on Pt drastically changes due to magnetic effects. In the Pt/M systems (where M = Fe(001) and Co(001)), the Pt layer is spin-polarized, herein denoted as ferromagnetic Pt, and the energetics of the dissociative adsorption exhibits decrease in both the dissociation barrier and the dissociated oxygen atom binding energy, with respect to that of the reference surface (Pt(001)). This phenomenon is termed as O2 activation. We also note an emergence of non-activated dissociative adsorption on Pt/Fe. The Fermi-level density of states was found to be

	an appropriate basis for the reactivity mechanism. Other important findings relate to the enhanced stability of Pt on M, which can be attributed to characteristic charge redistribution in Pt-M bond. The ferromagnetic property of Pt/M is found to be maintained at and beyond room temperature. The facile dissociation of O2 on Pt/Fe and Pt/Co has been observed experimentally. On the other hand, the hydrogen evolution from borohydride has been experimentally observed on Pt, while, such reaction is rarely observed on other metals such as Au and Ag. Density functional theory calculations on the interaction of borohydride with 4d and 5d transition metal surfaces, M(111), are conducted to draw the trends and the accompanying fundamental mechanistic insights. It was found that, adsorption structure is molecular on Au and Ag, while it is dissociated on Pt, yielding three H adatoms on the surface. While the binding energy of molecule correlates with the position of the d-band center of the metals, the adsorption structure does not. We note that the adsorption structure has orbital-specific dependence. The H2O co-adsorption is integrated to further investigate the role of water, which is known to enhance borohydride hydrolysis. It was found that the stable molecular structure on Os changed to dissociated structure in the presence of two H2O monomers. Moreover, this effect of H2O can be tuned by applying external electric field. These findings corroborates with the experimental observation variation of solvent and electric fields. Over all, the phenomena studied and the accompanying mechanistic and electronic explanations have benefitted several other experimentalists to further their research specifically in alternative power generation systems such as fuel cell. **References** 1. Mary Clare Sison Escaño, Hiroshi Nakanishi and Hideaki Kasai J. Phys. Chem. A, 113, 14302 (2009). 2. Mary Clare Sison Escaño, Hiroshi Nakanishi and Hideaki Kasai J. Phys.: Cond. Matt., 41, 492201 (2009). 3. Mary Clare Sison Escaño, Elod Gyenge, Ryan Arevalo, Hideaki Kasai J. Phys. Chem. C, 115, 19883 (2011) 4. Vincent Lam and Elod Gyenge J. Electrochem. Soc. 155, 1155 (2008). 5. M. Wakisaka, H. Suzuki, S. Mitsui, H. Uchida and M. Watanabe J. Phys. Chem. C 112 2750 (2008).
15:20 – 15:40	**NGHIEM THI MINH HOA** **Critical Crossover Between Yosida-Kondo Dominant Regime and Magnetic Frustration Dominant Regime in the System of a Magnetic Trimer on a Metal Surface** *Abstract:* Quantum Monte Carlo simulations were carried out for the system of a magnetic trimer on a metal surface. The magnetic trimer is arranged in two geometric configurations, viz., isosceles and equilateral triangles. The calculated spectral density and magnetic susceptibility show the existence of two regimes: Yosida-Kondo dominant regime and magnetic frustration dominant regime. Furthermore, a critical crossover between these two regimes can be induced by changing the configuration of the magnetic trimers from isosceles to equilateral triangle*. * N. T. M. Hoa, W. A. Diño, and H. Kasai: accepted to J. Phys. Soc. Jpn.
15:40 – 16:00	**NGUYEN DUY HUY** **First-principles study on the formation of carbon-contamined gold nanowires**

	Abstract: A nanowire of single gold atom width is an ultimate one-dimensional material. Its physical and chemical properties are of great interest from the view point of fundamental science. One of their remarkable properties is the quantized conductance, clearly seen even at room temperature [1]. A gold nanowire (GNW) has been confirmed to have a quantized unit of conductance quantum (G_0), using transmission electron microscopy combined with scanning tunneling microscopy, and the mechanical controllable breaking junction method [2]. In general, by detaching two gold (111) surfaces GNW is formed. However, in that process, the wire is usually contaminated by light elements such as carbon, leading to longer gold-gold atomic spacing as well as higher breaking force [3]. Recently, Oshima's group has observed GNWs with long atomic spacing of 0.5 nm, which might comes from the contamination of carbon. So it is my motivation to study the carbon-contaminated GNWs and propose the mechanism of the contamination process. Theoretical calculations were carried out within the framework of density functional theory using the real-space finite-difference method. Projector augmented-wave pseudopotentials were employed for interactions between ions and electrons, and the exchange-correlation term was approximated by the local density approximation formalism. Up to three carbon atoms were inserted between neighboring gold atoms and both freestanding GNWs and GNWs on the gold (111) surface were studied. Structural optimization was performed until all the remaining forces were less than 0.08 nN. The results show that, for the freestanding GNWs, the interatomic gold distances for pure GNW, one, two and three carbon contaminated GNWs (denoted Au-C, Au-C_2 and Au-C_3) are 0.27, 0.4, 0.5 and 0.64 nm, respectively. These are in good agreement with those reported. Thus, the observed GNW was determined to have the Au-C_2 structure, because the distance between two gold atoms was measured to be ~0.5 nm. When the GNWs were put on the gold (111) surface, gold atoms prefer the fcc hollow sites. I assume one-dimensional configurations were formed and calculate the formation energies of Au-C, Au-C_2 and Au-C_3 chains as a function of chemical potential of carbon atom which depends on the carbon initial binding state, ranging from one carbon atom of the surface to the isolated graphene. Within that range, the formation energy of Au-C_2 structure is the smallest indicating that its formation is favorable. This agrees well with the experiments and suggests that Au-C_2 nanowire may already be formed on the gold (111) surface before pulling. **References** 1. M. Brandbyge *et al. Phys. Rev. B* **52**, 8499 (1995). 2. H. Ohnishi *et al. Nature* **395**, 780 (1998). 3. G. Rubio-Bollinger et al. *Phys. Rev. Lett.* **87**, 026101 (2001).
16:00 – 16:20	**HANDOKO SETYO KUNCORO** **First-principle investigation on structure and ionization strength of triply-charged cationic water clusters formed around transition metal atoms** *Abstract:* The diverse application in biological processes and chemical reactions, a study on small cation-water interactions is taking important impact in recent bio-technology and industrial field. However, comprehensively understanding of the first water-cation layer interaction particularly for triply charged transition metal cations are arduous, for instance dealing with the

	sampling for experimental study. Fortunately, the structure of $[Cr(H_2O)_6]^{3+}$, $[Mn(H_2O)_6]^{3+}$ and $[Fe(H_2O)_6]^{3+}$ had been performed and reported by experiments[1-3], which they will be used for a verification matter in this study. Formerly, we had studied the behaviour of pure small water cluster system[4] and then advanced by the interactions with some cations addition[5] Na^+, Ca^{2+} and Fe^{2+}. In this studies, the structure and ionization strength of $[M(H_2O)_6]^{3+}$ nano-clusters for M = Cr, Mn, Fe, Co, and Ni have been investigated by density functional theory. An anisotropic nature of $[Mn(H_2O)_6]^{3+}$ and the rotational deviation of water molecular plane of $[Co(H_2O)_6]^{3+}$ have been found. They have been observed via some indirect quantities, such as electrostatic potential, atomic charged, and asymmetry parameter. We have also utilized donor-acceptor MOs and monomer dipole moment to get comprehensively understanding both the structure and ionization strength. **References** 1. D. T. Bowron and S. Daz-Moreno: *J. Phys. Chem. B* **113** (2009) 11858. 2. P. L. W. Tregenna-Piggott, H. Weihe, and A-L. Barra: *Inorg. Chem.* **42** (2003) 8504. 3. J. Lati and D. Meyerstein: *Inorg. Chem.* **11** (1972) 2393. 4. H.S. Kuncoro, R. Belkada, M. David, H. Nakanishi, H. Kasai, E.S. Dy and H. K. Dipojono: *e-J. Surf. Sci. & Nano Tech.* **07** (2009) 871. 5. H.S. Kuncoro, M. Sakaue, H. Nakanishi, H. Kasai, and H. K. Dipojono: *J. Phys. Soc. Jpn.*, in print.
16:20 – 16:40	**BREAK**
16:40 – 17:00	**TRAN PHAN THUY LINH** **La_2GeO_5 – based Oxide Solid Electrolyte** *Abstract:* Solid oxide fuel cells (SOFC) provide a highly efficient, pollution-free power generation technology. Much of the research carried out on SOFCs focus on optimising the ionic conductivity of the solid electrolyte. Almost all SOFC systems currently being developed employ an yttria-stabilised zirconia electrolyte which has operating temperature above 850 ^{0}C. However, in 2001, La_2GeO_5 was experimentally found by T. Ishihara et al. And La_2GeO_5 – based oxide pose a high oxide ion conductivity by increasing the amount of oxygen vacancy at low temperature. Therefore, La_2GeO_5-based solid electrolyte materials are chosen as a promising research object.
17:00 – 17:20	**CHAUNCHAIYAKUL SONGPOL** **Atomic and Electronic Configurations of Single-Walled Carbon Nanotubes Observed by Scanning Probe Microscopy** *Abstract:* Carbon nanotubes (CNTs), long thin carbon allotropes with interesting electronic and optical characteristics have been very attractive towards researchers due to its potential applications in nanodevices. To utilize its full potential, atomic and electronic configurations as well as optical properties of the individual CNT should be clarified. The purpose of my research is to investigate the electronic and optical properties of an individual single-walled carbon nanotube (SWNT) by utilizing scanning probe microscopy techniques. The sample used in this study was chiral-porphyrin-nanotweezer-extracted SWNTs on the highly oriented pyrolitic graphite substrate. For the sample preparation, the CNT solution was sonificated to obtain uniform distribution and isolation of CNTs when dropped onto the substrate. Topographic images

	of the isolated SWNTs were then obtained by Atomic Force Microscopy and Scanning Tunneling Microscopy, accompanied with photon detection measurement by a tunneling electron-induced light emission technique (STM-LE). The topographic image with its corresponding photon integration mapping will provide information on the nanoscale electronic and optical properties of SWNTs. I will seek further possibilities in its applications to nanodevices, especially optical switches and all-optical circuits which results in faster computational circuits and be of great benefit in the near future.
17:20 – 17:40	**BUI VAN PHO** **Study on Removal Mechanism of Catalyst-Referred Etching on 4H-SiC (0001) Surface** *Abstract:* Silicon carbide (SiC) is a promising new material for high-power, high-temperature, and high-frequency applications because of its excellent electrical, thermal, and mechanical properties. A crystallographically nondamaged SiC surface with good flatness and low micro roughness is a critical factor for such applications. However, such a surface is difficult to obtain because of the extremely high hardness and chemical inertness of SiC. For machining such a high-quality surface, we have already developed a new abrasive-free planarization method called “catalyst-referred etching (CARE)” [1-3] using the catalyst of platinum (Pt) in hydrofluoric (HF) acid solution. A flat, nondamaged surface with a root-mean-square (RMS) roughness of less than 0.1 nm can be obtained over a whole wafer by CARE. The alternating wide (FCC) and narrow (HCP) terraces, straight step edges, and a 0.25 nm single-bilayer step height have been clarified by high-resolution transmission electron microscopy (HRTEM) images. To understand removal mechanism of CARE, at first, we use X-ray photoelectron spectroscopy (XPS) and thermal desorption spectroscopy (TDS) to clarify surface termination species. XPS and TDS data show that the Si atoms at surface are terminated by both OH- and F- species. We are now clarifying the percentage of OH- or F- species. Additionally, with the aid of the experimental results, we study on the mechanism by Simulation Tool for Atom Technology (STATE) program package [4]. To understand the role of HF molecules, we applied a step-and-terrace 3C-SiC (111) model with HF and H2O molecules to investigate adsorption processes of HF molecules. We have performed total energy calculations and geometry optimizations based on the density functional theory (DFT) within a generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE). The results showed that the barrier height of a HF dissociative adsorption on a topmost Si atom at step edge is about 1.2 eV which is 0.6 eV smaller than that at terrace. The results suggest that the removal occurs only at the step edges, not at terraces, which coincides with experimental results of CARE. **References** [1] H. Hara, J. Electron. Mater.**35** (2006) L11. [2] K. Arima, Appl. Phys. Lett.**90** (2007) 202106. [3] T. Okamoto, Matter. Sci. Forum**600-603** (2009) 835. [4] Y. Morikawa, Phys. Rev. B **63** (2001) 033405.

Quantum Engineering Design Course Workshop

31 January 2012, 10:30-16:30
Room…
Suita Campus, Osaka University

PROGRAM

Workshop Proper

(Presentation: 15 minutes; Discussion: 5 minutes)

10:30 – 10:50	**GANES SHUKRI** **First-Principle Study on Electronic and Optical Properties of *anatase* TiO_2 Codoped With Nitrogen And *3d* Transition Metal Ions Under Visible Light Irradiation** *Abstract:* The necessity for environmental-friendly and renewable energy in the world nowadays has become more urgent due to rapid depletion of fossil fuel quantity and its hazardous waste emissions for living environment. An emerging alternative solutionto overcome this problem is the utilization of hydrogen-based energy devices. Various efforts have been performed in order to produce hydrogen efficiently. One of the most intriguing ways to produce hydrogen is to directly split water molecule into its constituents, Hydrogen and Oxygen. Among various techniques to split water directly, photocatalytic water splitting is an interesting way to achieve clean and renewable energy system. This hydrogen production technique is performed on the presence of photocatalyst and radiation from a certain level of energy source (e.g. sunlight). The photocatalytic water splitting involves the creation of photoinduced electron-hole pair when the photocatalyst is exposed to specific radiations. The generated electron-hole pair possibly dissociates water molecules into hydrogen and oxygen under certain circumstances. Since Honda and Fujishima reported the ability of TiO_2 to split water directly in 1969[1], TiO_2 has become the most widely used photocatalyst. Compared to other photocatalyst materials, TiO_2 has the most efficient photoactivity, the highest stability and lowest cost[2]. However, TiO_2 has a drawback on its efficiency since it can only be activated by UV irradiation. The UV irradiation only exists in a small amount of total solar energy (~5%), therefore in order to increase the photocatalytic efficiency, the absorbance range of TiO_2 needs to be broadened to visible light region (~45%). Various researches have been conducted to increase the absorbance range of TiO_2. One possible approach is to dope the TiO_2 by metal or non-metal elements. Numerous studies, both experimental[3-6] and theoretical[5,7-10], regarding this approach have been reported. Non-metal dopants such as N, C, S, I incorporated to TiO_2 have been shown to red-shift the absorbance spectrum of TiO_2 into visible light region[5,11-13]. Meanwhile several metal ion dopants (noble and transition metals) have also shown enhancement of photocatalytic activity of TiO_2[3,4]. Nonetheless most of those works focused only on the investigation of single dopant on TiO_2. There are still only few number of researches have been done on codoped TiO_2 by combination of both

non-metal and transition metal atoms [14-16].

This study aims to investigate systematically the effect of non-metal and transition metal ion dopants to TiO_2 electronic structures by means of first principles calculation using density functional theory. We have chosen Nitrogen (N) as the non-metal dopant and *3d* transition metal atoms as metal dopant. As for the TiO_2 polymorph, *anatase* phase has been chosen since several previous works have reported that *anatase* has higher catalytic activity compared to other TiO_2 phases[17,18]. The calculated electronic properties of doped and codoped bulk TiO_2 will become our references to further investigate TiO_2 surface modification via surface doping. Afterwards the interaction mechanism of water molecule and doped TiO_2 surfaces will be investigated.

References

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10:50 – 11:10

RYAN LACDAO AREVALO

Borohydride on transition metals and gold alloys

Abstract: The adsorption of borohydride (BH4ads) on the (111) facet of transition metals (Mn, Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Os, Ir, Pt, and Au) and gold alloys is studied using first principles calculations within the density functional theory. The adsorption energy is strongest on Fe and Mn and weakest on Ag and Au. For all these metals except Ir, Pt and Pd, borohydride adsorbs molecularly on the hollow site, characterized by the strong hybridization of the metal-dzz state

	with H-s state of the borohydride. The significantly elongated B-H bonds of borohydride can be easily dissociated by water molecules by inducing polarization along the B-H bond. For the case of Fe and Mn, there is a small preference (0.01eV) on the hollow site over the bridge site where borohydride dissociates resulting to BH2ads+2Hads which can be described by the competing dzz and dxz,yz states of the metal. For Pt, Pd and Ir, borohydride adsorbs dissociatively yielding BHads+3Hads. From these results, two criteria, on the surface science point of view, are proposed to guide the choice of anode catalyst for direct borohydride fuel cell. The interaction of borohydride with gold alloys is also discussed. For Au3Cr, Au3Mn and Au3Fe, the adsorption structure of borohydride is the same as that on pure gold but at higher adsorption energy. The adsorption of borohydride on Au3Fe monolayer on Fe is also studied to determine the effect of increasing the amount of alloying metal on the energetics and adsorption structure. It is found adsorption energy is increased compared to Au3Fe while the adsorption structure is retained.
11:10 – 11:30	**NGUYEN HOANG LINH** **Electronic Structure and Magnetic Properties of LaFeAsO** *Abstract:* Beside the well-know superconductivity, the electronic and magnetic properties of the parent material LaFeAsO have recently attracted more and more attentions in the field of materials science. Several electronic structure calculations on LaFeAsO have been performed so far [1, 2, 3]. However, their conclusions are somehow inconsistent with each other: the results seem to depend on the schemes of calculations and types of the exchange-correlation functional. More detailed calculations of this material are necessary for full understanding of its electronic and magnetic structures. In this paper, we have carefully studied LaFeAsO using the first-principles electronic structure calculation, Korringa–Kohn–Rostoker (KKR) Green's function method based on the generalized gradient approximation (GGA). The results show that the most stable magnetic state for LaFeAsO is the striped anti-ferromagnetic state with a Fe magnetic moment of 1.45 µB. In addition, we present our preliminary results obtained by the fixed local spin moment method that could partly explain the discrepancies between the experiments [4, 5] andthe calculations in the past [6]. **References** [1] H. Nakamura, N. Hayashi, N. Nakai, et al., **Physica C** 469, 908-911 (2009). [2] K. Haule, J. H. Shim, and G. Kotliar, **Phys. Rev. Lett.** 100, 226402 (2008). [3] S. Ishibashi, K. Terakura, and H. Hosono, **J. Phys. Soc. Jpn** 77, 053709 (2008). [4] C. de la Cruz, Q. Huang, J. W. Lynn, Jiying Li, et al., **Nature** 453, 899 (2008). [5] T. Nomura, S.W. Kim, et al., **Supercond. Sci. Technol.** 21, 125028 (2008). [6] I.I. Mazin, M.D. Johannes, L. Boeri, et al.,**Phys. Rev. B** 78, 085104 (2008).
11:30 – 11:50	**CHATARAMOLEE BHUME** **Comparison of adsorption and desorption mechanisms of H_2 on Cu and Si(100) surfaces: A preliminary study** *Abstract:* Surface chemical reactions have been studied for centuries. However, concepts those can be used to picture such reactions on surfaces in scale of intra- and inter- molecular interactions has been developed for only a few decades. Dissociative adsorption and associative desorption are among the most widely studied topic in the field of surface chemical reactions, and the Hydrogen/Cu system is served as an important model system in development of our

	understanding of these reactions [1]. After the successful of development of explanation for Hydrogen/Cu system, scientists extend their research to other systems, and one of the most interesting systems is the Hydrogen/Si system. The Hydrogen/Si system is the source of the problem so-called "barrier puzzle". This barrier puzzle, which is not occurring in Hydrogen/Cu system, seems to violate the principle of detailed balance that used to explain the Hydrogen/Cu system successfully. Barrier puzzle leads to a decade of intensive research on Hydrogen/Si system since 1994 [2]. After a decade and a half, the barrier puzzle has been solved.What are left are theories and concepts those reveal the nature of chemical reactions on Hydrogen/Si system, which is different to that of Hydrogen/Cu system. In this presentation, the principle of detailed balance, which is important to understand the adsorption and desorption mechanisms, will be presented [2-4]. Then the adsorption and desorption mechanisms on Si(100) and Cu will be compared. **References** [1] H.A. Michelsen, C.T. Rettner and D.J. Auerbach, in: R.J. Madix (Ed.), Surface Reactions, Springer Verlag, Berlin, 1994, pp. 185-237 [2] W. Brenig and E. Pehlke, Prog. in Surf. Sci. 83 (2008), pp. 263-336 [3] C. Kittel, Elementary Statistical Physics, Dover publication, 1986, pp. 169-170 [4] A. Namiki, Prog. in Surf. Sci. 81 (2006), pp. 337-366
11:50 – 12:10	**JOAQUIN LORENZO VALMORIA MORENO** **A DFT Study on the Interaction of Oxygen and Hydrogen Peroxide with Fe-filled Single-walled Carbon Nanotubes** *Abstract:* Carbon nanotubes (CNTs) filled with magnetic atoms have been receiving a great deal of attention since they demonstrate very high potential in providing modified magnetic properties, low dimensionality, and small volume that open possibilities for many applications. Recently, CNT research has focused on device applications such as field effect transistors and fuel cell technology – as catalyst support in the oxygen reduction reaction (ORR) in the cathode of the proton exchange membrane fuel cell (PEMFC). The main objective of the study is to investigate the adsorption of oxygen on Pristine and Fe-filled single-walled carbon nanotubes (SWNT). However, since the role of hydrogen peroxide formation must be considered in the characterization of novel cathode catalysts, hydrogen peroxide adsorption is also examined. Specifically, the adsorption energies and stable structures of the systems will be compared. The presence of activation energy barriers related to dissociation of O_2 and H_2O_2 will also be investigated. Finally, we aim to find a general trend for these adsorption reactions on SWNT based on the different properties of the cases investigated: (3,3), (5,5), and (5,0) pristine and Fe-filled SWNT. The results of the study could be useful in determining the stability, electronic, and magnetic properties of nanotubes in fabricating functional materials for fuel cell catalyst support and electronic devices.
12:10 – 13:00	**LUNCH**
13:00 – 13:20	**SAPUTRO ADHITYA GANDARYUS** **The Effect of Nitrogen Coordination Number on the O_2 Adsorption Properties on Co-N_x Clusters: Density Functional Theory Study** *Abstract:* Highly active non-precious metal-based materials have been intensively studied as

	alternative materials for oxygen reduction reaction (ORR) cathode catalyst in polymer electrolyte fuel cells (PEFCs).Many efforts have been conducted to improve its catalytic activity and stability. Among these non-precious metal-based materials, two families of catalysts have gained increasing attention due to its promising catalytic activity displayed towards the ORR: carbon-supported transition metals/nitrogen materials (M-N$_x$/C; M= Co, Fe, Ni, Mn, *etc*., and normally *x*= 2 or 4) and incorporating non-precious metal complexes into conductive polymer matrix (M-conductive polymer/C) 1). Applying high temperature heat treatment (~400-1000 ^{o}C) to both of catalyst families result in the improvement of its catalytic activity and stability. However, the active sites of the catalyst become unclear, since heat treatment will partially or completely decompose the atomic structure of the catalyst. Different active sites structure has been proposed in several studies including M-N$_4$, M-N$_3$, and M-N$_2$ species. These different reports can most likely be attributed to differences in the synthesis procedures. It is also reported that the N atoms which are bond to the transition metal center is in the form of pyrrolic or pyrridinic compound. Despite this finding, the details of the ORR mechanism and the catalytic nature of these active sites remain unclear. Elucidation of the interaction of these active sites with O$_2$ molecule in gas phase is the first step towards understanding the ORR mechanism in the systems. In this study we will discuss about the effect of nitrogen coordination number on the O$_2$ adsorption properties on Co-N$_x$ clusters (N$_x$ is in pyrrolic and pyridinic compound; x= 2,3,4) using density functional theory (DFT) calculations. We use cluster model to approach the active sites of the real system. We will explore two main conformations in each coordination number. First, Co atom coordinated by free monomers (Co-N$_x$; for x= 2,3,4). Second, Co atom coordinated by dimer or trimer (Co-N$_x$ with macrocyclic effect; for x=2,3). We will explain the stability of the Co center and the O$_2$ adsorption configurations in each cluster. **References** 1) Zhongwei Chen, Drew Higgins,Aiping Yu, Lei Zhang and Jiujun Zhang, *Energy Environ. Sci.*, 2011, **4**, 3167
13:40 – 14:00	**LI XING SHENG** **Design of the diaphragm in light touch switches used in telecommunication equipment by FEM** *Abstract:* A metal diaphragm, which is widely used for switching parts in electrical devices nowadays, is getting smaller in size, more light in weight, and more thinly. To design a diaphragm, the shape, the performance and durability need to be considered. It consumes much time and costs for evaluation by using experimental method. This study aims to propose a new approach for designing diaphragm. Diaphragm gives user a positive tactile feedback when depressed, allowing user to know that the switch has made contact without the aid of visual confirmation. However, there is no optimization for click characteristics, as the preference is different from people to people. Therefore, to provide required diaphragm, it is important to know the relationship between design parameter and click characteristics. In the previous study, the effect of the geometry of punch and die on click characteristics has been discussed, the design space of Φ4mm oval type diaphragm and round type diaphragm is constructed. In this study, firstly, the effect of material property is discussed. And then the reliability of proposed oval type diaphragm discussed in the

	previous study is evaluated combining with design space. The proposed approach consists of three procedures. Firstly, residual stress after press forming is evaluated by finite element method. And, the stress amplitude and the mean stress at dangerous point on the diaphragms can be calculated. Secondly, the experimental database about S-N curve and Goodman diagram considering the effect of anisotropy has been prepared. Finally, the fatigue lives considering failure probabilities on the diaphragm can be estimated by comparison of Goodman diaphragm with numerical results.
14:00 – 14:20	**FEBDIAN RUSYDI** **First principles study on the interaction between Zinc-porphyrin and Oxygen molecule** *Abstract:* Zinc-tetraphenylporphyrin (ZnTPP) is commonly employed in photooxygenation process [1]. Its interaction with oxygen molecule, which has triplet spin configuration in the ground state ($^3O_2$), has been known to generate singlet oxygen ($^1O_2$) [2]. Here we report our theoretical study on the behavior of Zinc-porphyrin (ZnP), the core of ZnTPP, toward oxygen based on density functional theory. In addition, we also investigate the effect of Zn atom and tetraphenyl (TP) ring ligand on the porphyrin system. The interaction between ZnP and oxygen molecule to form ZnP(O2) complex enables us to analyze the bond strength between Zn atom in the porphyrin and the nearest oxygen atom. The bond strength analysis points out that the most likely $^3O_2$ (ground state) quenching of ^3ZnP (excited state) is via singlet channel of ZnP(O2) complex and there is no charge transfer occurs during the quenching [3]. These results are in agreement with Gijzeman's scheme [4]. DFT calculations show that the presence of Zn atom and TP ring ligand stabilizes ZnTPP for different reasons: The former is due to the charge donation to the porphyrin ring and the latter is due to hybridization bonding between C atom from porphyrin ring and C atom from TP ring [3]. Zn atom and TP ring ligand significantly influence the molecular orbital energy level which can be explained by electronegativity perturbation: The former lowers the molecular orbital energy levels and the latter elevate them [3]. This study encourages us to investigate further on the $^3O_2$ quenching of ^3ZnP to approach singlet oxygen generation mechanism by ZnTTP. **References** [1] R. Bonnett, Chem. Soc. Rev. 24, 19, 1995 [2] C. Tanielian and C. Wolff, J. Phys. Chem. 99, 9825, 1995 [3] F. Rusydi, M. K. Agusta, A. G. Saputro, and H. Kasai, in preparation, 2012 [4] O. L. J. Gijzeman and F. Kaufman, J. Chem. Soc., Faraday Trans. 2, 69, 708, 1973.
14:20 – 14:40	**ALLAN ABRAHAM BUSTRIA PADAMA** **H atom diffusion on Pd(110) and Pd_3Ag(110) surfaces** *Abstract:* Biomass is considered as possible material for hydrogen production. It is a renewable source, and if processed efficiently, will supply large amount of hydrogen gas necessary for fuel cells [1]. Through the process of gasification, H2 and other gases are produced from biomass. However, it is necessary to extract H2 from the mixture of gases before utilizing it in fuel cell systems. The process of filtering H2 from the other gases is possible by using hydrogen permeable films such as Pd and Pd alloy membranes [2-5]. Realization and understanding the mechanism of H permeation on these systems will therefore give essential contribution for an

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<tr><td></td><td>efficient permeable film.
Experiments have shown that PdAg alloy is a promising material for H permeation [1, 5]. In this study, H atom permeation on Pd(110) and Pd3Ag(110) surfaces is investigated as it was previously identified that H atom diffuses better on the 110 facet [6]. Potential energy surface on the permeation of H on the surfaces is constructed and the reaction paths are compared. Electronic structures of the surfaces are analyzed in order to determine the effect of Ag on the Pd system. Details of the results will be presented in the workshop.
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<tr><td>14:40 – 15:10</td><td>BREAK</td></tr>
<tr><td>15:10 – 15:30</td><td>DOAN DUY HAI
An eRosERK temporal integration method for chemotaxis model
<i>Abstract:</i> Solving numerically a chemotaxis model consists of two steps. The first one is spatial discretization and then is temporal integration. The equation we obtain after the first step is a large ordinary differential system which contains both stiff and non-stiff terms. Two that terms generally require completely different numerical methods to deal with. In this talk we focus on that second step, introducing a new class of time stepping methods called eRosERK in order to solve the above system. Such methods are combination in some proper ways of a Rosenbrock method with explicit first stage and a strong stability preserving one. Some numerical demonstrations are given.</td></tr>
<tr><td>15:30 – 15:50</td><td>SUSAN MENEZ ASPERA
Density Functional Theory-based Analysis on O_2 Molecular Interaction with the Tri-<i>s</i>-triazine-based graphitic Carbon Nitride
<i>Abstract:</i> The structural and electronic properties of O_2 molecular adsorption on the Tri-<i>s</i>-triazine-based graphitic carbon nitride (g-C_3N_4) surface was investigated through first principles calculation based on density functional theory (DFT). We will show that the O_2 molecule is merely physisorbed on the surface of g-C_3N_4 through the interaction of its lowest unoccupied molecular orbital (LUMO) with the orbitals of the 2-coordinated nitrogen atoms of the surface. Though physisorbed, a stronger molecular adsorption was found as compared with its adsorption on pure graphene sheets. We also found that the O_2 molecule gains very small amount of electron charges from the surface, which, together with stronger adsorption energy, may attribute to a more effective oxygen reduction reaction (ORR) site as compared with pure graphene. These results would then be important for reactions with intermediate surface oxidation step in a carbon and nitrogen-based catalyst, and could lead to realization of an</td></tr>
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	effective materials design for surface application, e.g. towards a more efficient catalyst for the ORR on the cathode side of the proton exchange membrane fuel cell (PEMFC).
15:50 – 16:00	**PAN JUN** **Dislocation-inclusion interaction and prismatic loop formation using level set dislocation dynamics** *Abstract:* The interactions between dislocations and inclusions have been demonstrated using level set dislocation dynamics. Inclusions in crystal can highly effect the mechanism of the material by the way of disturbing dislocation from been gliding. Because of the complexities of the interactions of dislocation segments, the flexibility of the dislocation lines in three dimensions and topological changes, we present the results of full three-dimensional dislocation dynamics simulations, based on level set method. Using level set method, we also study the formation of prismatic loop which is a way of dislocation multiplication. Level set method (LSM) associated with Fast Marching Method (FMM) and Fast Sweeping Method (FSM) does not track individual dislocation line segments directly and thus can demonstrate various topological changes of interfaces observed in two or three dimensions naturally. Spatial internal stress distributions in the region containing the complex topological dislocation configuration can be easily calculated by the elastic field equations with dislocations in the infinite body. The internal stress field can be solved efficiently using FFT, assuming periodic boundary.
16:00 – 16:20	**FERENSA OEMRY** **Effects of Cluster Size on Pt-O Bonds Formation in Small Platinum Clusters** *Abstract:* We present the results of density functional theory calculation in oxygen dissociative adsorption process on two types of isolated platinum (Pt) clusters: Pt_4 and Pt_{10}, by taking into account the effect of cluster reconstruction during the process. The strength of Pt-Pt bonds in the clusters is mainly defined by d-d hybridization and interstitial bonding orbitals (IBO). Oxygen that adsorbed on the clusters is weakening the IBO and thus inducing geometry reconstruction as occurred in Pt_{10} cluster. However, cluster that could undergo apparent structural deformation such as Pt_{10} case is found to promote oxygen dissociation with no energy barrier. The details show that maintaining well-balanced of attractive and repulsive (Hellmann-Feynman) forces between atoms in the cluster during O-O bond elongation is considered to be the main key to avoid any considerable rise of energy barrier. Furthermore, a modest energy barrier that gained in Pt_4 cluster is presumed to be originate from inequality of intramolecular forces between atoms, not sourced from considerable work that exerted by oxygen atoms to overcome attractive force which holds the O-O bond together.

Closing Remarks by

PROF. Yoji Shibutani

Picture Taking