# Research Culture in an Academic Environment

H. Kasai Osaka University

# Overview

- 1. Internationalization Efforts in Developing a Culture of Research in Osaka University
- 2. Diversity and Mobility of Students and Academic Staff in Kasai Laboratory
- 3. Evidence of Research Outcomes
- 4. CMD: An Illustrative Case of Developing Research Culture in the Academe

Whenever I deliver my talk in conferences and workshops abroad, I share to the audience this popular haiku:

露の世は露の世ながらさりながら 一茶

Tsuyu no yo wa tsuyu no yo nagara Sarinagara Issa(1762-1826)

This dewdrop world – It maybe a dewdrop, And yet – and yet –

Trans. R. H. Blyth

#### 露の世は露の世ながらさりながら 一茶

Tsuyu no yo wa tsuyu no yo nagara Sarinagara Issa(1762-1826)

This dewdrop world –

It maybe a dewdrop,

And yet – and yet – Trans. R. H. Blyth

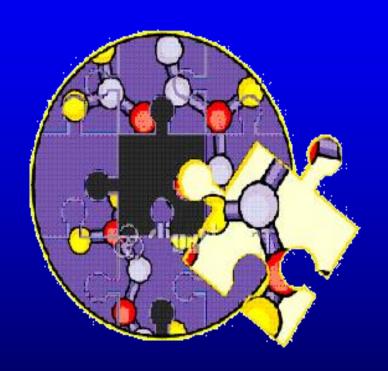
This has vividly portrayed the reality that life is fleeting and ephemeral as a dewdrop. And yet, by making the best of this short-lived and temporary dewdrop, life would be long enough to fulfill its profound purpose and meaning.

As a university professor, I have come to realize that one of my major purposes in life is the advancement of science and technology, not only in Japan, but also in other countries, especially those in the South East Asia.



# Motivation

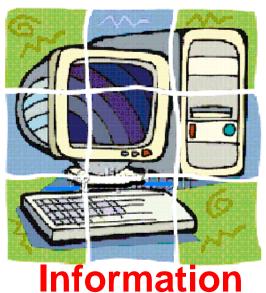
- Asians share the same problems
- We have different resources and competencies
- We are naturally an intricately-linked network



# Common Problems

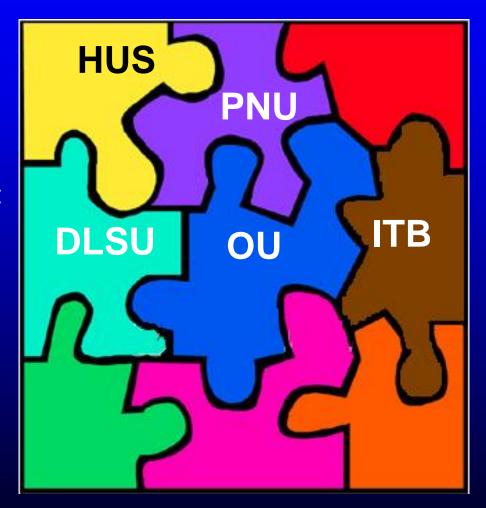






# An Asian Knowledge Network- *Our Vision*

- tolerant and open towards others
- people reach out to others and collectively share experiences
- no distinctions over what might be considered superior or inferior
- foster exchange and understanding between future government leaders, industrialists, tycoons, academic and scientific leaders (our students)



# Internationalization Efforts in Developing a **Culture of Research**



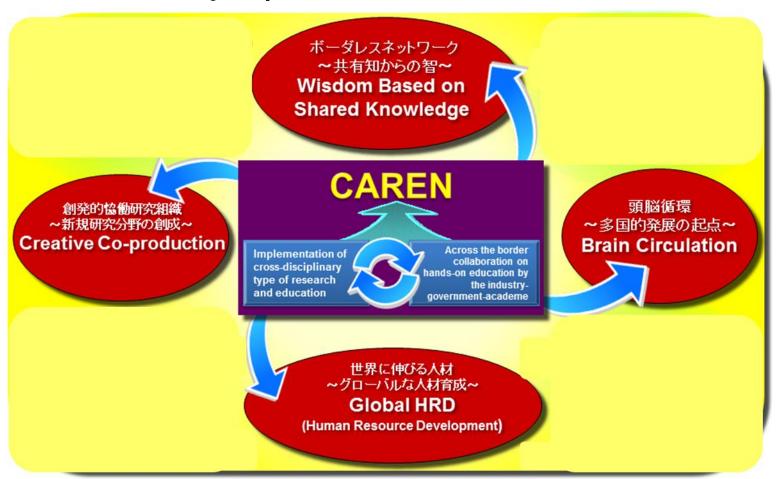
CAREN

**CAREN** 

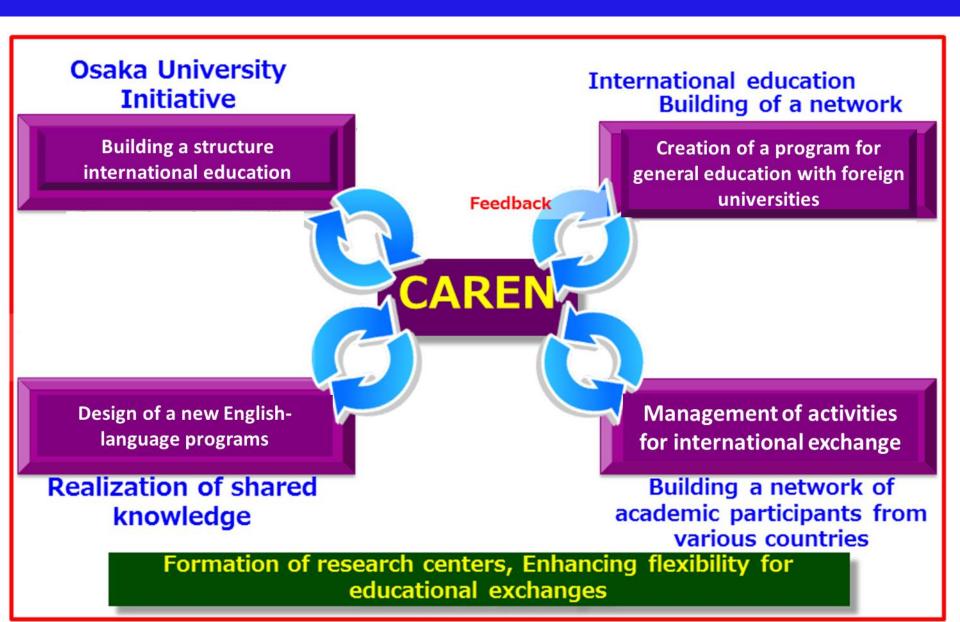
## **Concept of CAREN**

# Center of Asian Research & Education Network CAREN

Osaka University's promotion of international collaboration



### **Specific Aactivities of CAREN**



## General Idea of CAREN

# CAREN is a leader in global campus

Foreign students

Other country's bridge to Japan

Research and educational programs

A campus where foreign and Japanese students support each other







Japanese students

Plays active role in Japan



Assistant Professor, University of Fukui

# Ph.D. Graduates from Kasai Laboratory

36 Graduates as of Sept. 2014

Year	Name	Country of Origin	卒業年度	氏名	国籍
2014年度(H26)	Allan Abraham Padama	Philippines	2010年度(H22)	Do Ngoc Son	Vietnam
	Tran Phan Thuy Linh	Vietnam		窪田 善之	Japan
	Febdian Rusydi	Indonesia	2009年度(H21)	尾澤 伸樹	Japan
	Adhitya Gandaryus Saputro	Indonesia	2008年度(H20)	Melanie Yadao DAVID	Philippines
	Ferensa Oemry	Indonesia		Eben Sy Dy	Philippines
	三輪 邦之	Japan	2007年度(H19)	津田 宗幸	Japan
2013年度(H25)	Aspera Susan Meñez	Philippines		Md. Mahmudur Rahman	Malaysia
	Nguyen Tien Quang	Vietnam		Nelson B. Arboleda Jr.	Philippines
	Triati Dewi Kencana Wungu	Indonesia	2006年度(H18)	岸 智弥	Japan
	Abdulla Ali Abdulla Sarhan	Bahrain		Rifki Muhida	Indonesia
	Handoko Setyo Kuncoro	Indonesia	2005年度(H17)	松中 大介	Japan
	國貞 雄治	Japan	2004年度(H16)	信原 邦啓	Japan
2012年度(H24)	Nghiem Hoa Thi Minh	Vietnam	2002年度(H14)	三浦 良雄	Japan
	Escaño Mary Clare Sison	Philippines		長谷川 和彦	Japan
	Wahyu Tri Cahyanto	Indonesia	2001年度(H13)	福井 篤	Japan
	Mohammad Kemal Agusta	Indonesia	2000年度(H12)	坂上 護	Japan
	岸 浩史	Japan	1999年度(H11)	Wilson Agerico DIÑO	Philippines
2011年度(H23)	Roman Tanglaw Abat	Philippines			
	南谷 英美	Japan			

# Diversity of Students and Academic Staff

Doctoral Thesis:
Dynamics of
Hydrogen-Solid
Surface Reactions
(1998)



外国人客員研究員 ディニョ、ウィルソン アジェ リコ タン氏が日本物理学会論文賞を受賞





#### RIFKI MUHIDA, PH.D.

Design and Control of Dynamical Quantum Processes in Ortho-Para H<sub>2</sub> Conversion on Solid Surfaces and Clusters

**Application:** Hydrogen storage

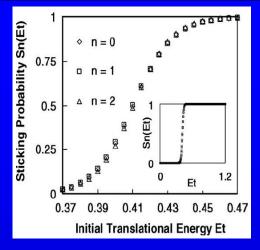
Graduated: 2005

Current:

Dean of Engineering Faculty, Surya University, Indonesia

(part of his work got two patents)





**Doctoral Thesis** 

Quantum Dynamics
Investigations and First
Principles Studies of
Vibrational Effects on
Hydrogen-Surface Reactions
(2006)

DLSU

固体表面反応における動的量 子過程に関する理論的研究

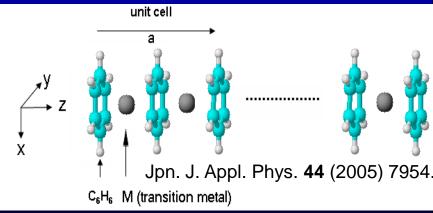
Dr. Nelson Arboleda



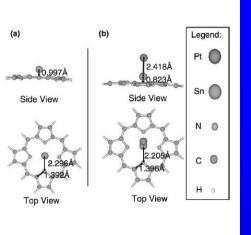


Dr.Rahman Md. Mahmudur
University Putra Malaysia
Doctoral Thesis
Theoretical study on the electric
and magnetic properties of
one-dimensional carbon
based nanomaterials with
transition metal atoms (2006)

遷移金属原子を含む一次元炭素系 ナノマテリアルの電気的・磁気的 性質の理論的研究



Benzene-transition metal sandwich chain



A theoretical analysis on the interaction between Sn (II) porphyrin & Pt and the electronic characteristics of their reaction product Chemical Physics Letters 422 (2006) 539–542

422 (2006) 539–542

Doctoral Thesis
Density Functional
Investigations on Heme- and
Hydrogenase-based Catalysts
for Potential Fuel Cell
Applications (2007)

Dr. Eben Dy

National Institute for FCA (Canada)





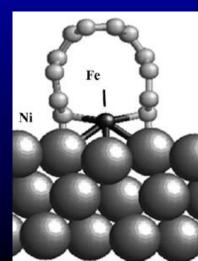
Dr. Melanie David
DLSU

Doctoral Thesis
Theoretical Investigations
on the Possible Nanoscale
Systems for Electronic and
Magnetic Devices (2007)

異種物質界面における反 応性の最適化に関する理 論的研究

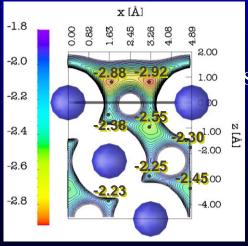
Carbon Nanoarch
Encapsulating Fe
Nanowire on Ni(111)

Japanese Journal of Applied Physics Vol. 45, No. 4A, 2006, pp. 2869–2871



# Dr. Nobuki Ozawa Tohoku University

Quantum states of hydrogen motion on the solid surface and in the subsurface of transition metals 遷移金属表面及び表面内部領域における水素原子の量子論的振る舞いに関する理論的研究(2008)



The contour plot of the adiabatic PES on a cross section, cutting thorough the top-fcc-hcp-top line, for the hydrogen atom motion on the Pd(111) surface and in the subsurface



博士論文

第一原理計算による二次電池と燃料電池の電極反応に

関する理論的研究 (2009) KEP Co.

Li-Graphite Intercalation Compounds Metallic L



Dr. Yoshiyuki Kubota



## Dr. Do Ngoc Son

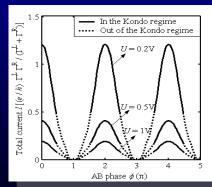
# VNU Ho Chi Minh Doctoral Thesis

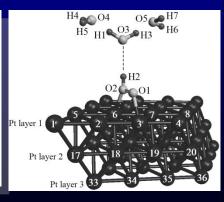
Dynamical behaviors of electrons in Aharonov-Bohm interferometer and protons in exchange membrane fuel cell (2009)

1. Electronic transport in the

Aharonov-Bohm interferometer

- 2. Proton transfer in aqueous Nafion membrane
- 3. Oxygen reduction reaction on catalytic surfaces



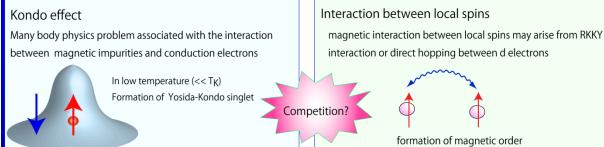




# Dr. Emi Minamitani

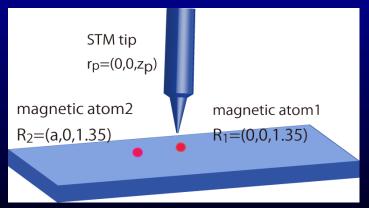
# **Tokyo University**

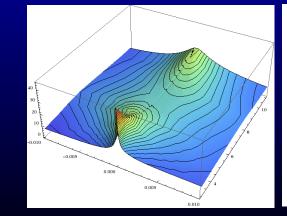
博士論文 磁性ダイマー吸着系に おける近藤効果と磁気的相互作用に関 する理論的研究(2009)

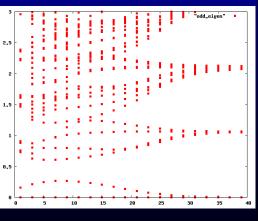


formation of magnetic order

Real space observation of Kondo Numerical Renormalization Group effect and RKKY interaction









Dr. Tanglaw Roman

**University Ulm** 

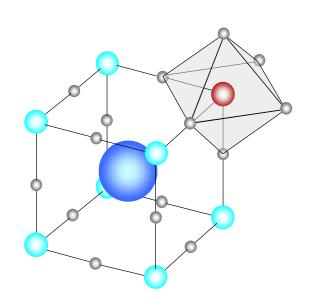
Doctoral Thesis Structural and dynamical properties of hydrogen in graphene and platinum surface systems (2009)

Hydrogen atom motion on a highly defective Pt surface, showing significant delocalization in regions outside a

vacancy.

# Self-forming nano-particle catalyst without precious metals





Dr. Hirofumi Kishi (2006)

**DAIHATSU** 



#### MOHAMMAD KEMAL AGUSTA, PH.D.

Theoretical Study of Hydrazine Adsorption on Metal Surfaces

**Application:** Direct hydrazine fuel cells

Graduated: 2012

Current:

Faculty at Engineering Physics Department, Institut Teknologi Bandung, Indonesia.

(part of his work is used by Daihatsu)





#### WAHYU TRI CAHYANTO, PH.D.

A DFT Study on the Interaction of Hydroperoxo(OOH) and Some Methanol Decomposition Species with Pt and Pt-alloy Surfaces

**Application:** Direct methanol fuel cells

Graduate: 2013

Current:

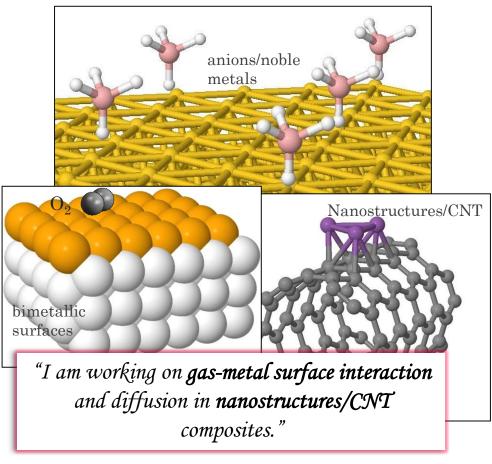
Faculty at Physics Department, Universitas Soedierman, Indonesia



## Quantum Simulation and Design of Novel Catalytic Materials for Energy Applications

新規高効率エネルギー技術開発のための量子シミューレション・マテリアル・デザイン





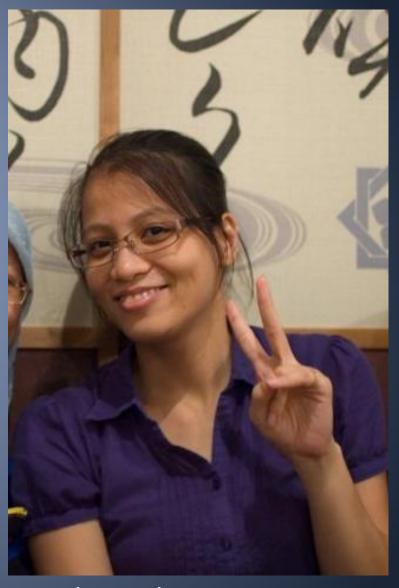
Dr. Mary Clare Escaño (2012) Fukui University

# Magnetic adatoms on a metal surface:

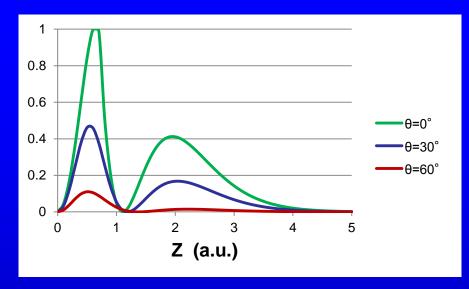
- Kondo effect at
  single adatoms
  +
- RKKY, and direct interaction between adatoms

1

Magnetic order? Frustration?



Dr. Nghiem Thi Minh Hoa (2012) Forschungszentrum Jülich GmbH



Intensity of Fermi contact

A theoretical study of Ortho-Para conversion of hydrogen molecules

水素分子の オルソ-パラ変換の理論的研究

> Dr. Yuji Kunisada (2013) Hokkaido University





#### HANDOKO SETYO KUNCORO, Ph.D.

Theoretical Study on Formation, Stability and Reaction of Small Water Clusters

**Application:** water treatment

Graduated: 2013

#### Current:

Faculty at the Center for Ceramics of Industrial Ministry, Indonesia

(part of his work is used by Otsuka Chemical Co. Ltd.)



# Dr. Abdulla Ali Abdulla Sarhan

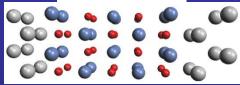
### (2013) Arabian Gulf University

Quantum Computation, Electronic Transport, and First Principles calculations

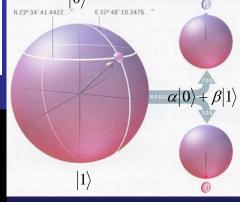
量子計算と電子輸送と第一原理計算

Resistance Random Access Memory

Pt /NiO/Pt

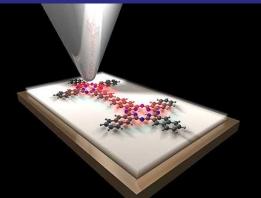


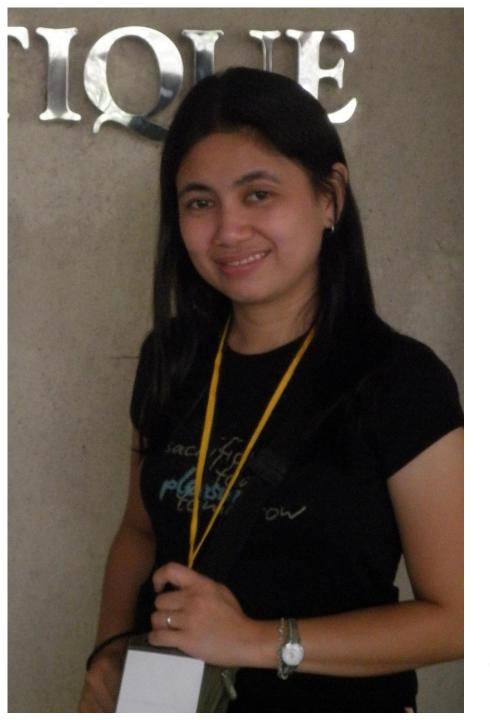
Molecular Switch



A qubit representation by Bloch sphere

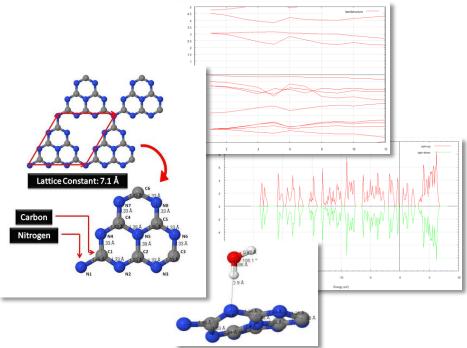






# Dr. Susan Meñez Aspera (2013) Osaka University

First Principles-Based Studies on the Potentials of Graphitic Carbon Nitride and other Non-Metal-Based Materials as Catalysts for Alternative Energy Sources





#### TRIATI DEWI KENCANA WUNGU, Ph.D.

Theoretical Study on Lithium-Montmorillonite

**Application:** Lithium-ion battery

Graduated: 2013

Current:

Faculty at Physics Department, Institut Teknologi Bandung, Indonesia

(part of her work is used by the Government under ALCA project)

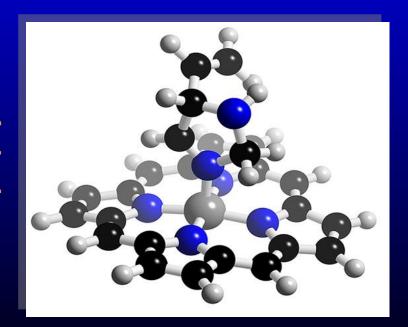


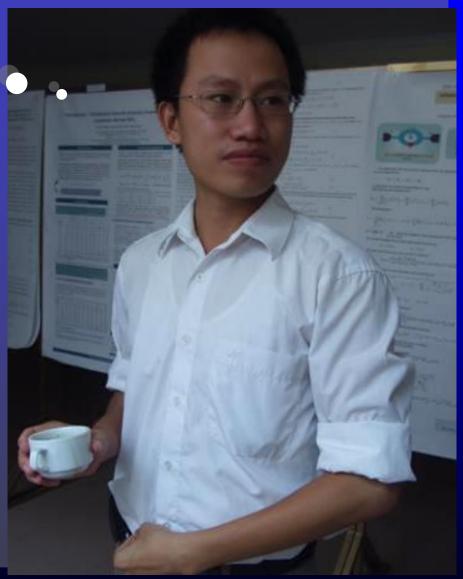
Fe porphyrin

**DFT** method? **Green's function**method?... hmm?
@\*#%&\$... ^\_^

Dr. Nguyen Tien Quang (2013) Osaka University

 Nano-scale Structure and Properties

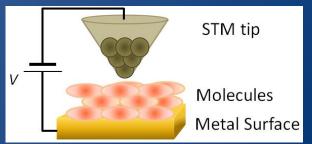


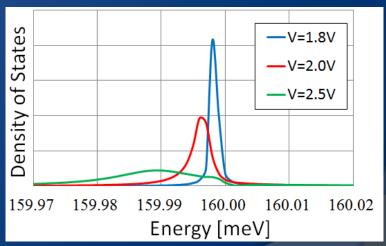


## Dr. Kuniyuki Miwa(2014)RIKEN



# Molecular Vibrational Dynamics Induced by Surface Plasmons





Vibrational DOS of admolecules in the presence of surface plasmon excited by STM current



#### FERENSA OEMRY, PH.D.

Theoretical Study of Geometry, Size and Alloying Effects on the Reactivity of Small Pt Clusters

**Application:** Diesel oxidation catalyst

Graduated: 2014

**Current:** 

Faculty at the Indonesian Institute of Science (LIPI), Indonesia

(part of his work is used by Isuzu)





#### FEBDIAN RUSYDI, PH.D.

Theoretical Study of Ligand and Solvent Effects on the Electronic Structure of Zinc Tetraphenylporphyrin

Applications: Photodynamic therapy and dye-

solar cell

Graduated: 2014

#### Current:

Specially-appointed Assistant Professor at Kasai Lab., Osaka University, Japan

Faculty at Department of Physics Universitas Airlangga, Indonesia (Permanent)

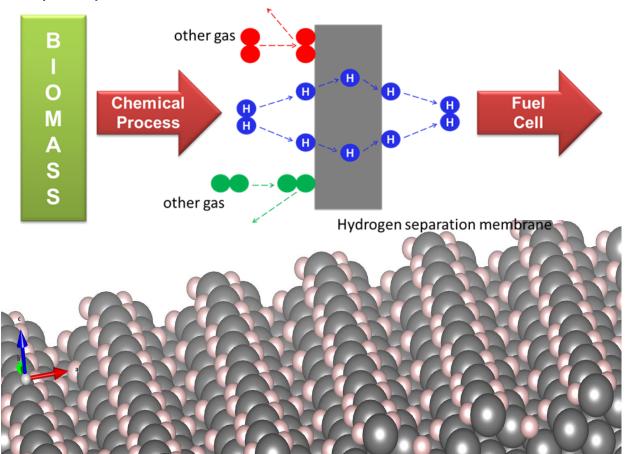
(part of his work is used by Panasonic)



### **Hydrogen Separation Membrane**

Understanding H absorption on (1X2) missing row reconstructed

Pd(110) surface





Dr. Allan Abraham Padama (2014) UP

A clear description on the behavior of H atoms on surfaces, especially its absorption process will be significant for various applications such as storage and hydrogenation or dehydrogenation of different molecules.



#### ADHITYA GANDARYUS SAPUTRO, PH.D.

Theoretical Study of Oxygen Reduction Reaction Mechanism on Transition-Metal-Nitrogen-Based (TM-Nx-based) Active Sites

**Application:** Direct Hydrogen Fuel Cells

Graduated: 2014

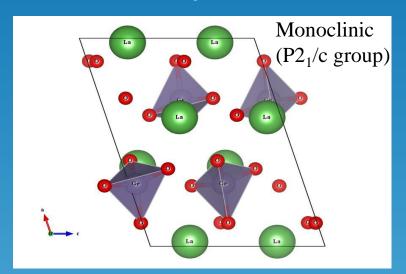
**Current:** 

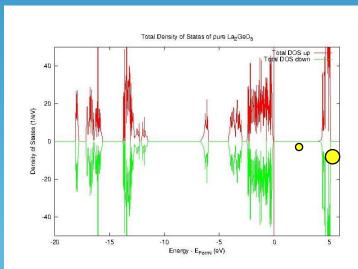
Specially-appointed Assistant Professor at Kasai Lab., Osaka University, Japan

(part of his work is used by Daihatsu)



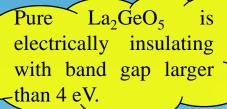
# Ph.D. Research Theme La<sub>2</sub>GeO<sub>5</sub> – based Oxide Solid Electrolyte





#### Dr. TRAN Phan Thuy Link Quantum Engineering Design Course (2014) Hue University













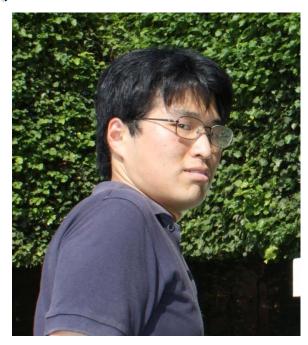


# Ph.D. Students who will graduate on March 25, 2015



Ryan L. Arevalo

Dissertation: Rational
Catalyst Design Approach
to Heterogeneous
Catalysis: Oxidation of
Borohydride and Nitric
Oxide



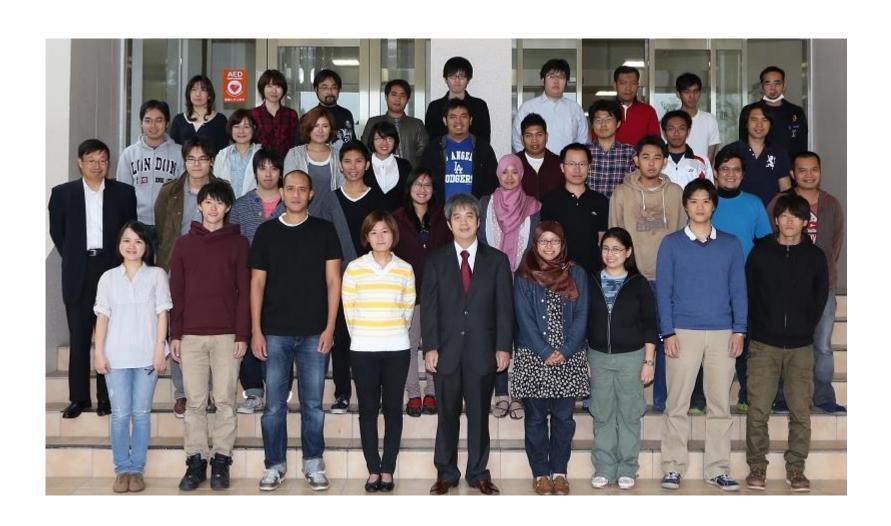
Kohei Oka

Dissertation: Profile of Segregation induced by Oxygen on Cu<sub>3</sub>Au with Protective Layers

#### **Current Members of Kasai Laboratory**



### Kasai Laboratory



# CURRENT PH.D. AND MASTER STUDENTS FROM INDONESIA





## FADJAR FATHURRAHMAN (PHD STUDENT D3)

"Theoretical study of  $N_2H_4$  decomposition reactions on transition metal surfaces"

Applications: Direct hydrazine fuel cell

(Part of his work is used by Daihatsu)





## Musa Alaydrus (PhD student D2)

"Ionic transport in ceria based solid electrolytes"

Applications: Solid oxide fuel cell

(Part of his work is used by the Government under ALCA project)





## GANES SHUKRI (PHD STUDENT D2)

"Unsaturated-small hydrocarbon molecules interaction with anatase  $TiO_2$  surfaces"

and

"Degradation pathways of polymer backbone and TMA of functionalized Fluorinated Poly(arylene ether)"

**Application:** Direct hydrazine fuel cells

(Part of his work is used by Daihatsu)





## LISTRA YEHEZKIEL GINTING (MASTER STUDENT M1)

"Photocatalytic Water-splitting Reaction for Hydrogen Production using GaN"

Applications: photocatalyst for water splinting

(Part of his work is used by Sumitomo electric)





## Paulus Himawan Lim (Master Student M1)

"Designing Pt-alloys as high performance electro catalysis in PEMFCs"

Application: Direct hydrogen fuel cells



#### SCIENTIFIC WORKS IN NUMBER

(up to January 2015) http://dyn.ap.eng.osaka-u.ac.jp

- 450 Scientific publication in various international journals
  - 36 Graduated Ph.D. students
  - Review articles in various international journals
  - 21 Patents
  - **Text books** in advanced physics



#### SCIENTIFIC AWARDS

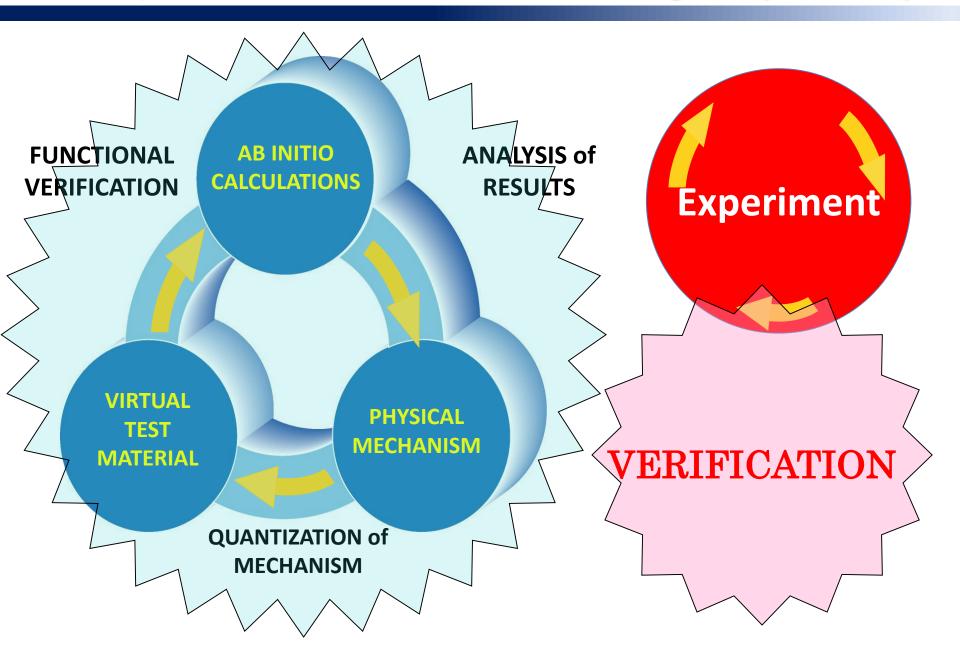
- 1. Ganesa Widya Jasa Adiutama from ITB Indonesia, 2014-July.
- 2. 総長顕彰 (Sōchō kenshō) award from Osaka University, Japan: This award is received who achieved outstanding performance in education, research or social and international contribution in order to further promote the development of Osaka University, 2014-August.
- 3. 文部科学大臣賞 (Monbukagaku daijin-shō) from Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan: Commendation prize for science and technology for his "Proposal of a Quantum Dynamics Theory and Pioneering Studies of Intelligent Materials Design Method", in 2012-April.
- 4. 5<sup>th</sup> Award for Academic Papers on Physics (日本物理学会第5回論文賞 (2000)), for "Rotational Alignment in the Associative Desorption Dynamics of Hydrogen Molecules from Metal Surfaces" from the Physical Society of Japan on September 24, 2000.
- 5. Other awards



# COMPUTATIONAL MATERIALS DESIGN (CMD®): an Outstanding Example of University-Government-Industry Collaboration

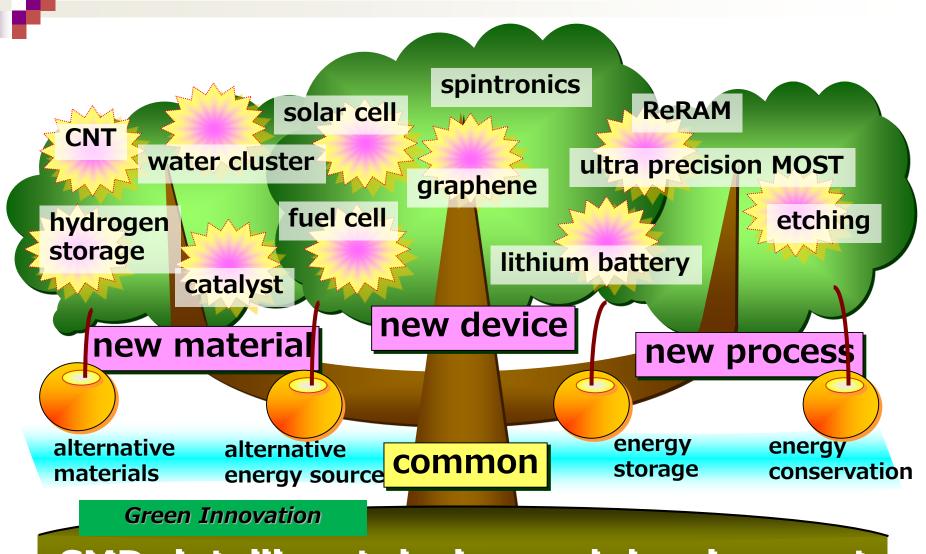


### Computational Materials Design® (CMD®)



#### Through CMD®

-creation of new technique and technology in the 21st century



CMD: intelligent design and development

### FIRST PATENT (2001):

### "METHOD OF PROMOTING HYDROGEN LIQUEFACTION"

• Inventors:

Hideaki KASAI, Hiroshi NAKANISHI, Wilson Agerico DIÑO, Rifki MUHIDA

- Patent No.: Japan 2001 274461
- Application: Liquid hydrogen storage
   Provides ortho-para conversion method for promoting and facilitating hydrogen liquefaction methods to high efficiency





Professor Hiroshi Nakanishi

## PROJECTS FROM THE GOVERNMENT AND INDUSTRIES

- After time goes, we got more patents and more publications.
- Our CMD® workshop (to be explained later) also became known to the public.
- CMD® has attracted the attention of the Industry and other Institutions.
- We got projects and grants from industries as well as from the Government.









#### Panasonic SHARP

















Japan Society for the Promotion of Science



Research and Development Program





#### SOME NOTABLE CUSTOMERS

Long term projects: involving graduate students (master and doctoral) and visiting researchers.

Some of our alumni are taken directly by these companies to work.

They continue to use CMD® in their professional career.





第10回コンピュテーショナル・マテリアルズ・デザイン(CMD)ワークショップ 於 国際高等研究所 平成19年3月10日出

# THE 10TH CMD® WORKSHOP KYOTO, 2007



### CMD® WORKSHOP

- The workshop became famous, attended not only by academicians (students, researchers, teachers), but also by people from industry.
- Right now the 23<sup>rd</sup> CMD<sup>®</sup> workshop is taking place in Osaka, from Feb-23 to Feb-27.
- In average, CMD® workshop is conducted twice a year, the summer session and the winter session.
- Since 2008, CMD<sup>®</sup> workshop begun to take place outside Japan. The name is Asia CMD<sup>®</sup> workshop.



# ASIA CMD® WORKSHOPS HELD IN THE PAST YEARS

2008	ITB (Indonesia) [credit to Prof. Hermawan K. Dipojono]
	De La Salle Univ. (The Philippines)
2009	ITB (Indonesia)
	De La Salle Univ. (The Philippines)
	Hanoi University of Science (Vietnam)
2010	ITB (Indonesia)
	De La Salle Univ. (The Philippines)
	Hue University (Vietnam)
2011	Univ. Riau (Indonesia)
	De La Salle Univ. (The Philippines)
	Saigon University (Vietnam)

2012	Mahidol Univ. (Thailand)
	De La Salle Univ. (The Philippines)
	Hanoi University of Science (Vietnam)
2013	ITB (Indonesia)
	Mahidol Univ. (Thailand)
	De La Salle Univ. (The Philippines)
	Hanoi University of Science (Vietnam)
2014	ITB (Indonesia)
	De La Salle Univ. (The Philippines)



# LONG STORY SHORT...

Computational methods become viable & improvements in computer performance.

We designed
a method
to engineer existing
materials to have new
functionalities.

We showed our concept to the Government and got support.

We established CMD®, we got our first patent by the help of CMD®.



## LONG STORY SHORT...

Computational methods become viable & improvements in computer performance.

We opened a program to educate international

students.

We got projects from the Government and industries using CMD®. Our students benefited from it

We designed
a method
to engineer existing
materials to have new
functionalities.

We showed our concept to the Government and got support.

We established CMD®, we got our first patent by the help of CMD®.

We provided our codes freely, we trained people freely.



## LONG STORY SHORT...

Computational methods become viable & improvements in computer performance.

We opened a program to educate international students.

We got projects from the Government and industries using CMD®. Our students benefited from it

Our students, lab., and CMD® grow together to become one of the top of its kind!

We provided our codes freely, we trained people freely.

We designed
a method
to engineer existing
materials to have new
functionalities.

We showed our concept to the Government and got support.

We established CMD®, we got our first patent by the help of CMD®.



# SO, WHAT WE CAN LEARN FROM OUR EXPERIENCE WITH CMD®?

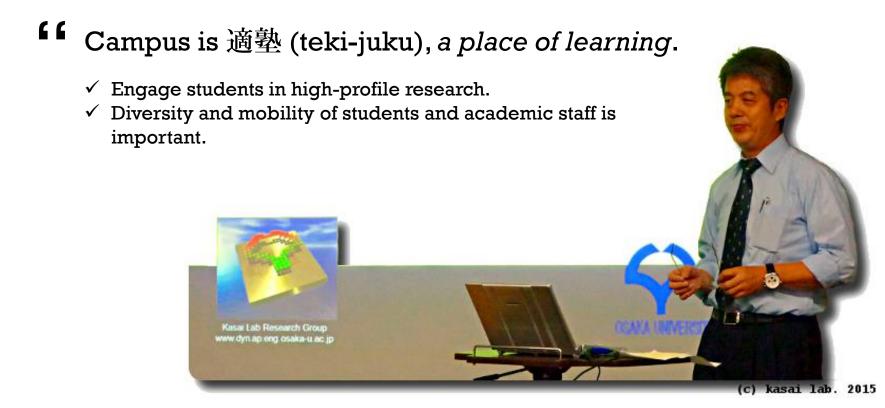


### 1. In Doing Research

Research is driven by the needs of our society and the academe. ✓ There should be a strong support from the Government √ The works of Social Sciences on the needs of society give insights for *Natural Sciences* to develop necessary technologies.

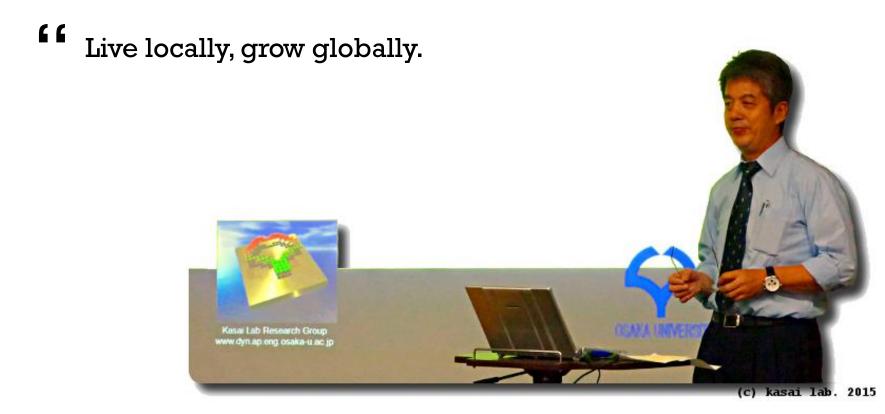


### 2. IN DOING EDUCATION





### 3. IN DOING COLLABORATION





### Overview

- 1. Internationalization Efforts in Developing a Culture of Research in Osaka University
- 2. Diversity and mobility of Students and Academic Staff in Kasai Laboratory
- 3. Evidence of Research Outcomes
- 4. CMD: An Illustrative Case of Developing Research Culture in the Academe

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### TERIMA KASIH ATAS PERHATIAN ANDA

