

International workshop on the Current Surface Science Trend

8 November 2012, 13:00-17:20

P1-212

Suita Campus, Osaka University



PROGRAM

13:00-13:10 Opening remarks and picture taking

Session1 Spatial session by the guests (moderator:Mr. Ferensa Oemry)

13:10-13:30 **Predrag Lazic** (Theoretical Physics Division Rudjer Boskovic Institute, Zagreb)

“Importance of non-local correlation effects in surface adsorption”

13:30-13:45 **Shun Sadakuni**(Department of Precision Science, Osaka University)

“Catalyst-referred Etching and an Investigation of Reaction Mechanism”

13:45-14:05 **Gerardo C. Janairo** (Dean of college of science, De La Salle University)

“Water Soluble Tetrathiafulvalene (TTF)”

Sesson2 Computational material design for membrane(moderator: Arguelles Elvis Flaviano)

14:05-14:20 **Triati Dewi Kencana Wungu**

“A First Principles Study on the Structural Stability and Electronic Structure of the
Montmorillonite-Based Organocray”

14:20-14:35 **Susan Meñez Aspera**

“Analysis of structural and electronic properties
of Pr_2NiO_4 oxide through first principles calculations”

14:35-14:50 **Tran Phan Thuy Linh**

“Activation barrier for oxygen atom migration in alkaline-earth doped monoclinic lanthanum germanate”

Coffee break

Session 3 Theoretical investigation for novel catalysts(moderator:Mr. Allan Abraham Bustria Padama)

15:00-15:15 **Mary Clare Sison Escaño**

“Spin effects in metal surface reaction: O_2 on ferromagnetic Pt/M”

15:15-15:30 **Ryan Lacdao Arevalo**

“Theoretical study of the structure and stability of borohydride on gold alloy”

15:30-15:45 **Nguyen Tien Quang**

“DFT+U investigation on the adsorption and desorption of oxygen on Pt-coated Ceria”

Session 4 Dynamics on Surface and Interface (moderator:Mr.Kohei Oka)

15:45-16:00 **Febdian Rusydi**

“A theoretical study on ZnP interaction
with O₂ via ZnP- O₂ complexes using density functional theory”

16:00-16:15 **Kuniyuki Miwa**

“Vibrational Dynamics of Molecules Induced by Surface Plasmons”

Session 5 A novel approach for surface science (moderator:Mr.Kuniyuki Miwa)

16:15-16:30 **Kohei Oka**

“The ferroelectrics and piezo-effect on PZT Thin film”

16:30-16:45 **Kazuki Kojima**

“Theoretical Study of Magnetic Anisotropy in Co/Ni Multi-Layers on W(110)”

16:45-17:00 **Allan Abraham Bustria Padama**

“Density functional theory investigation
on the behavior of H atom On Pd(110) surface”

17:00-17:15 **Saputro Adhitya Gandaryus**

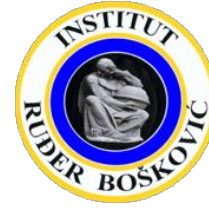
“A Density Functional Theory Study
on the Oxygen Reduction Reaction on Co-(6) Ppy Cluster”

17:15-17:20 Closing Greeting

November 27, 2012

16:00 - 17:40, P1-212, Suita Campus

Seminar in Quantum Simulation of Functional Materials



Prof. Hideaki Kasai

Opening Remarks

(16:00–16:10)

Insights in Thermoelectric Materials from First Principles

(16:10–16:40)

Dr. Predrag Lazic

Theoretical Physics Division, Rudjer Boskovic Institute, Zagreb

A Quantum Dynamics Investigation of Hydrogen Scattering on Graphite Edges: Revisited

(16:40–17:10)

Prof. Nelson Arboleda Jr.

Department of Physics, De La Salle University, Philippines

Indonesia–Japan Innovation Convention

(17:10–17:35)

Prof. Hideaki Kasai

Department of Applied Physics, Osaka University, Japan

Picture Taking

(17:35–17:40)

Dr. Mamoru Sakaue

Moderator

Snacks will follow at the lounge.

