

# International Symposium on Computational Science 2013

**Date:** February 18 – 21, 2013

**Venue:** Kanazawa University, Kakuma Campus, Kanazawa, Japan  
Building of Natural Science and Technology,  
Lecture rooms 105 and 108

**Organized by:**

Department of Computational Science,  
Faculty of Science, Kanazawa University



Faculty of Mathematics and Natural Sciences,  
Bandung Institute of Technology



Computational Material Science Initiative



**Organizing Committee:**

Kanazawa University (Japan)

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Muhamad A. Martoprawiro, Daryono Hadi Tjahjono, Acep Purqon, Suprijadi,

Gadjah Mada University (Indonesia)

Harno Dwi Pranowo

# Symposium Program

## Part 1

February 18<sup>th</sup> (Mon.) (Lecture Room 105)

*Special Session of International Symposium on Computational Science & Topical Meeting of CMSI, Spintronics: First-Principles Simulation & Measurement*

Morning session1 (chairperson: Tatsuki Oda)

- 9:30-9:35      Opening
- 9:35-10:15    **Ryo Maezono** (JAIST)  
*Non-additivity in metallic tri-wire binding*
- 10:15-10:55   **Masafumi Shirai** (Tohoku University)  
*Half-metallic Heusler alloys for magnetoresistive devices: An outlook based on ab initio calculations*
- 10:55-11:10   Coffee break

Morning session2 (chairperson: Masafumi Shirai)

- 11:10-11:50   **Hiroaki Sukegawa** (NIMS)  
*Giant tunnel magnetoresistance and coherent tunneling effect in epitaxial MgAl<sub>2</sub>O<sub>4</sub>-based tunnel junctions*
- 11:50-12:30   **Kohji Nakamura** (Mie University)  
*Perpendicular magnetocrystalline anisotropy in 3d transition-metal thin films*
- 12:30-13:40   Lunch Break

Afternoon session (chairperson: Tamio Oguchi)

- 13:40-14:20   **Akio Kimura** (Hiroshima University)  
*Spin resolved photoemission as a direct probe of spin textures for Rashba systems and topological insulators*
- 14:20-15:00   **Shuichi Murakami** (Tokyo Tech)  
*Spin-orbit Coupling in Topological Insulators*
- 15:00-15:20   Coffee Break

Evening session (chairperson: Kohji Nakamura)

15:20-16:00 **Tamio Oguchi** (Osaka University)

*First-Principles Study of X-ray Absorption Spectroscopy*

16:00-16:40 **Shigeki Onoda** (Riken)

*Topological magnetic insulators on the pyrochlore lattice: towards a first-principles design*

17:30- Banquet at Sumire-Tei (in Kanazawa university)

February 19<sup>th</sup> (Tue.) (Lecture Room 105)

Morning session1 (chairperson: Fumiyuki Ishii)

9:10-9:50 **Atsuo Kawasuso** (JAERI)

*Positron annihilation spectroscopy as a probe for spintronics-Hope to the first principles calculation-*

9:50-10:30 **Youhei Yamaji** (University of Tokyo)

*Mott Physics on Edge Transports of Topological Insulators Induced by Strong Spin-orbit Couplings*

10:30-10:40 Coffee Break

Morning session2 (chairperson: Mineo Saito)

10:40-11:20 **Koichiro Shimomura** (KEK)

*Muonium as an isolated hydrogen analog for the condensed matter science*

11:20-12:00 **Tomoya Ono** (Osaka University)

*First-principles study on electron transport property of nanoscale systems*

12:00-14:00 Lunch Break

## Part 2

February 19<sup>th</sup> (Tue.) (Lecture Room 105)

14:00 Opening of ISCS 2013

Afternoon session (chairperson: Tatsuki Oda)

14:10-14:40 **Teoh Teow Chong** (University of Malaya)

*Computational Science: A Biological Perspective*

- 14:40-15:10     **Acep Purqon** (Institut Teknologi Bandung)  
*The Geometrical Effects of Substitutional Impurities (Ga,N,As) on Electric and Magnetic Properties of by using Density Functional Theory (10,0) Carbon Nanotube*
- 15:10-15:40     **Kazutomo Kawaguchi** (Kanazawa University)  
*Molecular dynamics analyses of dissociation process of ADP from Hsp90*
- 15:40-15:50     Coffee Break

Evening session1 (chairperson: Karel Svadlenka)

- 15:50-16:20     **Khamron Mekchay** (Chulalongkorn University)  
*An Application of the LTDRM in Parameter Estimation of One-dimensional Ito Processes*
- 16:20-16:40     **Rhudaina Z. Mohammad** (Kanazawa University)  
*Multiphase Mean Curvature Flow: Signed Distance Vector Approach*

Evening session2 (chairperson: Kazutomo Kawaguchi)

- 16:40-17:00     **Muhamad Koyimatu** (Kanazawa University)  
*Theoretical Study of  $\pi$ -stacking Interaction in Carbonic Anhydrase*
- 17:00-17:20     **Micke Rusmerryani** (Kanazawa University)  
*Coarse-grained Simulation of Azurin Complex: Protein–protein Interactions*

**February 20<sup>th</sup> (Wed.) (Lecture Room 105)**

Morning session 1 (chairperson: Fumiyuki Ishii)

- 9:00-9:30       **Shinichi Miura** (Kanazawa University)  
*Development of the ab initio instanton method for tunneling processes in molecular systems*
- 9:30-10:00     **Tatsuki Oda** (Kanazawa University)  
*Development and application in fully relativistic pseudopotential first-principles molecular dynamics*
- 10:00-10:30     **Suprijadi** (Institut Teknologi Bandung)  
*3D simulation of dam break effect on a solid wall using Smoothed Particle Hydrodynamic*
- 10:30-10:40     Coffee Break

Morning session 2 (chairperson: Shinichi Miura)

- 10:40-11:10     **Daryono Hadi Tjahjono** (Bandung Institute of Technology)  
*DFT Calculation in Study of Porphyrins for Biological Application*
- 11:10-11:40     **Muhamad A. Martoprawiro** (Institut Teknologi Bandung)  
*Ab Initio Study of Initial Steps of Synthesis Reaction Mechanism of Alkylated Flavonoid*
- 11:40-13:15     Lunch Break

Afternoon session1

- 13:15-13:30     **Cometta Surya Guritno**, (Kanazawa University, ITB, chairperson: Shinichi Miura)  
*Structural fluctuation of a protonated water cluster*
- 13:30-13:45     **Meidy Triana Pakpahan**, (Kanazawa University, ITB, chairperson: Hidemi Nagao)  
*Binding Free Energy of Protein-Ligand by Combining Docking and MD Simulation: A Comparison of Calculation Methods*
- 13:45-14:00     **Isman Kurniawan** (Kanazawa University, ITB, chairperson: Hidemi Nagao)  
*Computational Study of Oxidation Potential Fluctuation of Ketone Molecule*
- 14:00-14:15     **Marhamni Syaputra** (Kanazawa University, ITB, chairperson: Mineo Saito)  
*First Principle Density Functional Theory Calculation of Water Adsorption on Graphene*
- 14:15-14:30     Coffee Break

Afternoon session2

- 14:30-14:45     **Sasfan Arman Wella**(Kanazawa University, ITB, chairperson: Tatsuki Oda)  
*Tight-Binding Molecular Dynamics with Fermi Operator Expansion: Application to Vacancy Defects in Silicon*
- 14:45-15:00     **Nurul Ikhsan** (Kanazawa University, ITB, , chairperson: Tatsuki Oda)  
*Magnetic, structural, and electronic properties of Co doped Fe/MgO interface*
- 15:00-15:15     **Indra Gunawan** (Kanazawa University, ITB, chairperson: Tatsuki Oda)  
*Implementation of Parallel Matrix Diagonalization for Ab-Initio Molecular Dynamics Program using ScaLAPACK*

15:15-15:30 Coffee Break

Evening session1

15:30-15:45 **Robbi Nur Rakhman** (Kanazawa University, ITB, chairperson: Hidekazu Ito)

*Qualitative Behavior of Solutions for Generalized Hénon-Heiles System*

15:45-16:00 **Ahmad Rio Adriansyah** (Kanazawa University, ITB, chairperson: Tatsuro Ito)

*On the Farthest Subconstituent of the  $q$ -Johnson Graph  $J_q(n; k)$*

16:00-16:15 **Rizal Dwi Prayogo** (Kanazawa University, ITB, chairperson: Seiro Omata)

*Three-Dimensional Smoothed Particle Hydrodynamics Method for Simulating Free Surface Flows*

16:15-16:30 Coffee Break

Evening session2

16:30-16:45 **Adil Aulia Akbar** (Kanazawa University, ITB, chairperson: Seiro Omata)

*Smoothed Particle Hydrodynamics (SPH) Using Riemann Solver on Three-Dimensional Dam Break Simulation*

16:45-17:00 **Raden Ahnaf Faqih Shaimy** (Kanazawa University, ITB, chairperson: Seiro Omata)

*Three-Dimensional Smoothed Particle Hydrodynamics Simulation for Solidification Process*

17:00-17:15 **Agra Barecasco** (Kanazawa University, ITB, chairperson: Seiro Omata)

*Free-surface detection on three-dimensional SPH solvers*

17:15-17:30 **Hanifa Terissa** (Kanazawa University, ITB, chairperson: Seiro Omata)

*Three-Dimensional Smoothed Particle Hydrodynamics Simulation for Liquid Droplet with Surface Tension*

**February 21<sup>st</sup>(Tue.) (Lecture Rooms 105 & 108)**

Morning session (Room 105, chairperson: Mineo Saito)

9:00-9:30 **Harno Dwi Pranowo** (Universitas Gadjah Mada)

*Selectivity of Some Crown Ether on Extraction of Strontium(II): Insights from Density Functional Calculation*

9:30-10:00     **Fumiyuki Ishii**     (Kanazawa University)  
*First-Principles Study of Spin Texture in the Graphene on Ni(111)*

10:00-12:00     Poster session (Lecture room 108)

12:00-13:00     Lunch Break

13:00-            **Muhamad A. Martoprawiro**  
*Closing (Lecture room 105)*

## List of Participants

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\* This Double-Degree program is an educational program based on the agreement of cooperation between Kanazawa University and Bandung Institute of Technology. Therefore, the affiliation of students participating in this program is as follows:

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