

International Workshop on Computational Science 2017

February 15–18, 2017

Kanazawa University, Japan

Date February 15–16, 2017 (Main Session)
February 17–18, 2017 (Special Session)

Venue Kanazawa University, Japan (Kakuma campus)
Kakuma-machi, Kanazawa 920-1192
Lecture hall: **203**, main building of Graduate school of natural science and technology, building S1.
<http://www.kanazawa-u.ac.jp/e/campuses/>

URL <http://polaris.s.kanazawa-u.ac.jp/iwcs2017/>

This workshop is supported by Kanazawa University SAKIGAKE Project.

The special session of IWCS2017: “Design of Novel Magnetic Materials for Device Applications: Simulation and Experiment” is co-organized by Post-K Priority Issue 7 - Creation of new functional devices and high-performance materials to support next-generation industries (“CDMSI”)

Program of the Main Session

February 15

13:30 – 13:40 Opening

Invited lectures (25min + 5min Q&A)

13:40 – 14:10 Edy Tri Baskoro (Institut Teknologi Bandung)
Ramsey number for graphs

14:10 – 14:40 Mirza Satriawan (Universitas Gadjah Mada)
Multicomponent Dark Matter in the Mirror Model with Massive Mirror Photon

14:40 – 15:10 Jiraphan Suntornchost (Chulalongkorn University)
Variable selection for a regression model when dependent variable is subject to measurement errors

15:10 – 15:40 Kazutomo Kawaguchi (Kanazawa University)
Theoretical Study of Intermolecular Interactions for protein systems

- 15:40 – 16:00 Break
- 16:00 – 17:00 Short presentations (3min)
- 17:00 – 18:00 Poster session (room **202**)

February 16

Invited lectures (25min + 5min Q&A)

- 09:30 – 10:00 Acep Purqon (Institut Teknologi Bandung)
Urban Physics and Its Implementation in Predicting Economic Growth Related to High Speed Train Development
- 10:00 – 10:30 Manabu Oura (Kanazawa University)
Ring of the weight enumerators of d_n^+
- 10:30 – 11:00 Fatimah A. Noor (Institut Teknologi Bandung)
Modeling of Tunneling Current in High-k-based MOS Capacitors by Considering the Effects of Coupling between Longitudinal and Transverse Motions
- 11:00 – 11:20 Break
- 11:20 – 11:50 Suprijadi (Institut Teknologi Bandung)
Experimental and Computational study on physical properties based on granular system
- 11:50 – 12:20 Triati Dewi Kencana Wungu (Institut Teknologi Bandung)
Natural Clay Mineral as Adsorbent for Health and Environment Applications: A Density Functional Theory Study
- 12:20 – 12:50 Tatsuki Oda (Kanazawa University)
Research and development of high performance material for voltage torque MRAM by means of first-principles calculation
- 12:50 – 13:00 Closing

Program of the Special Session “Design of Novel Magnetic Materials for Device Applications: Simulation and Experiment”

February 17

- 9:30 – 9:35 Opening
- 9:35 – 10:15 Y. Sakuraba (NIMS)
Exploration of ferromagnets with large anomalous Nernst effect for novel thermoelectric applications
- 10:15 – 10:40 Y. P. Mizuta (Kanazawa Univ.)
Skymion-driven thermoelectric conversion: An ab initio study
- 10:40 – 11:00 Break
- 11:00 – 1:40 T. Koretsune (RIKEN)
First-principles calculation of Dzyaloshinskii-Moriya interaction
- 11:40 – 12:05 M. Ohashi (Kanazawa Univ.)
Superconductivity of chromium thin film
- 12:05 – 13:35 Lunch
- 13:35 – 14:15 A. Kawasuso (QST)
Application of spin-polarized positron spectroscopy to some ferromagnetic systems
- 14:15 – 14:55 K. Hyodo (JST-CREST, Tohoku Univ.)
First-principles study on intrinsic and extrinsic anomalous Hall conductivity of transition metal alloys
- 14:55 – 15:20 Break
- 15:20 – 16:00 A. Edström (ETH Zürich)
Computational Design of Transition Metal Magnets with Large Magnetocrystalline Anisotropy
- 16:00 – 16:40 T. Nozaki (Tohoku Univ.)
Voltage control of magnetization using magnetoelectric antiferromagnet Cr_2O_3 sputtered thin film
- 16:40 – 17:05 M. Obata (Kanazawa Univ.)
Investigation of spin dependent van der Waals density functional approach
- 17:45 – Banquet (for special session participants, Sumire-Tei in Kanazawa university)

February 18

- 9:10 – 9:50 K. Ohishi (CROSS)
Chiral magnetism in CsCuCl₃ probed by polarized neutron scattering and muon spin rotation
- 9:50 – 10:30 H. Nakanishi (NIT, Akashi College)
Quantum simulation for the motion of positive-muon in materials and its application for Mu-SR spin state analysis
- 10:30 – 10:55 J. B. Lin (NIMS)
Linear-scaling DFT study on the structural optimization and electronic properties of real size Ge/Si core-shell nanowires
- 10:55 – 11:15 Break
- 11:15 – 11:55 Y. Onose (Univ.Tokyo)
Nonreciprocal propagation of elementary excitations in noncentrosymmetric magnets
- 11:55 – 12:35 Y. Ohnuma (JAEA)
Theory of spin current generation
- 12:35 – 12:40 Closing

List of posters

1. Yoshiho Akagawa (Kanazawa University)
Numerical simulation for dynamical elastic contact problem
2. Saeful Akhyar (Kanazawa University)
Smoothed particle hydrodynamic simulation of accretion disk in cataclysmic variable
3. Hasan Al Rasyid (Kanazawa University)
First-Principles Study of Electronic, Magnetic, and Optical Properties of Nickel Cobaltite: DFT and QSGW methods
4. Fadil Habibi Danufane (Kanazawa University)
Holonomic Gradient Method for the Distribution Function of the Largest Root of Complex Non-Central Wishart
5. Yosuke Funato (Kanazawa University)
First-principles study on θ -phase in solid oxygen
6. Kouta Futai (Kanazawa University)
Numerical study of an adaptive Lagrange-Galerkin scheme for pure convection problems
7. Nurul Ikhsan (Kanazawa University)
Theoretical study on multi-functional Fe/MgO interface: investigation of perpendicular magnetic anisotropy origin
8. Tomosato Kanagawa (Kanazawa University)
First principles calculation of magnetic anisotropy energy on double interfaces slab systems of X/Fe/MgO
9. Hiroyuki Kitano (Kanazawa University)
Numerical simulation of contact problem of an elastic body with friction
10. Susumu Minami (Kanazawa University)
Hyperfine structure of muonium in GaN
11. Masum Murshed (Kanazawa University + University of Rajshahi, Bangladesh)
On the prediction of storm surge along the coast of Bangladesh
12. Takumi Nakano (Kanazawa University)
3D simulation of crack propagation in an elastic body by a phase field model
13. Irma Palupi (Kanazawa University)
An Implicit Boundary Integral Method for Laplace Problem
14. Riska Wahyu Romadhonia (Kanazawa University)
Finite elements method of ergodic distribution function for Jaffe model
15. Ayu Shabrina (Kanazawa University)
Numerical method of nonlinear Black Scholes equation for American options pricing

16. Shogen Shioda (Kanazawa University)
Computation of an inverse free boundary problem for a shape optimization method
17. Hiroki Yamamoto (Kanazawa University)
A gradient flow structure of the Maxwell-type viscoelastic model and its finite element analysis
18. Yamaoka Ryohei (Kanazawa University)
4 way-hexagonal symmetric crystalline method and 2 dimensional snow crystal model allowing collision / splitting
19. Takuro Yoneda (Kanazawa University)
Development of a finite element method for a delamination model and its simulation
20. Yang Zhenxing (Kanazawa University)
Minimum energy state and gradient flow for interaction energy of particles