



JSPS International Meeting Series

The 3rd Hiroshima Workshop

— *Novel Functional Materials with Multinary Freedoms* —

Programme and Abstracts

November 16-19, 2005

Hiroshima University, Higashi-Hiroshima Campus



HIROSHIMA UNIVERSITY

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Foreward

The 3rd Hiroshima Workshop — *Novel Functional Materials with Multinary Freedoms* — takes place on the Higashi-Hiroshima campus of Hiroshima University, Japan, between Nov. 16 and 19, 2005. It follows the series of workshops “Transport and Thermal Properties of *f*-Electron Systems” held in 1992 and “Transport and Thermal Properties of Advanced Materials” in 2003. The scope of the 3rd Workshop is comprised of various fields: new functionalities with multinary degrees of freedom, superconductivity in layered and caged compounds, thermoelectric properties of novel compounds, hydrogen-related phenomena in nanostructured materials, and magnetic properties of *p*, *d*, and *f* electron systems. The subjects are related to the Center of Excellence (COE) Project “Novel Functional Materials with Multinary Freedoms” supported by the Ministry of Education, Culture, Sports, Science, and Technology of Japan.

This Workshop is attended by 110 scientists from 10 countries, who are involved in various research fields ranging from inorganic chemistry, nanostructured systems, solid state physics and photoemission spectroscopy, to theory and design of novel functional materials.

We wish to all participants a stimulating and fruitful meeting in a relaxed atmosphere.

Toshiro Takabatake, Chair
Shoji Yamanaka, Co-chair

Higashi-Hiroshima, Japan, November 2005

Wednesday, November 16

15:00 Registration
get-together-party

Thursday, November 17

Welcome and opening

8:40 Takabatake, T

Oral Session I Chair: Maple, M B

8:50 O01 Cava, R J The Structural Chemistry of Layered Sodium Cobalt Oxides
9:15 O02 Hiroi, Z Superconductivity and Rattling Behavior in the β -Pyrochlore Oxides
9:40 O03 Yamanaka, S High Pressure Synthesis and Structures of Three-Dimensional C₆₀ Polymers
10:05 O04 Bud'ko, S L Field-Induced Non-Fermi-Liquid Behavior in YbAgGe: Emerging Phase Diagram
10:25 O05 Takano, M Search for New Phases and new Functions in the 3d Transition Metal Oxide Family
10:45 Coffee

Oral Session II Chair: Pickett, W E

11:15 O06 Pachon, S Towards strongly correlated thermoelectrics
11:40 O07 Takabatake, T Carrier control of single-crystal thermoelectric clathrates A₈Ga₁₆X₃₀ (A=Sr, Ba, X=Ge, Sn)
12:05 O08 Alleno, E Double-filling in skutterudites: a promising path towards improved thermoelectric performances
12:25 O09 Terakura, K Variation in Electronic Properties in Novel Single-Component Organic Solids
12:45 O10 Terasaki, I Novel physics and functions in the layered cobalt oxides from thermoelectricity to ferromagnetism
13:30 Lunch

Oral Session III Chair: Majer, G

14:50 O11 Akimitsu, J Novel spin-Peierls compound TiOBr
15:15 O12 Chen, P Development of Metal-N-H Systems for Hydrogen Storage
15:40 O13 Fujii, H Composite Materials based on Light Elements for H-Storage
16:00 O14 Orimo, S Light element hydrides for solid-state hydrogen storage
16:20 O15 Hauback, B C Hydrogen storage in light complex hydrides — structures and effect of additives
16:40 Coffee

Oral Session IV Chair: Miyake, K

- 17:00 O16 Nolas, G S Structure and transport properties of silicon clathrates
17:25 O17 Goto, T Rattling and Tunneling of Off-Center Local Oscillator in Clathrate Compounds
17:45 O18 Udagawa, M Raman Scattering Study of Cage-trapped Mode in Cage-structured Compounds
18:15 Diner

Friday, November 18**Preliminary Session**

- 8:40 Jo, T Introduction to Hiroshima University

Oral Session V Chair: H. Sato

- 8:50 O19 Bauer, E REPt₃Si compounds: a new playground for extraordinary states of matter
9:15 O20 Maple, M B Strongly correlated electron phenomena in filled skutterudite lanthanide osmium antimonides
9:40 O21 Miyake, K Heavy Electrons due to Interstitial Degrees of Freedom
10:05 O22 Kuramoto, Y Response from ordered states of higher multipoles
10:25 O23 Tou, H Sb-NMR/NQR probe for novel paramagnetic and superconducting properties in the filled skutterudite superconductor PrOs₄Sb₁₂
10:45 Coffee

Oral Session VI Chair: Cava, R J

- 11:15 O24 Pickett, W E Non-cuprate Layered Transition Metal Oxide Superconductors
11:40 O25 Khomskii, D I Multiferroics: different ways to combine magnetism and ferroelectricity
12:05 O26 Oguchi, T Multiferroic Oxides: A First-Principles Study
12:25 O27 Katsufuji, T Magnetic-field switching of crystal structure in spinel MnV₂O₄
12:45 O28 Taguchi, Y Carrier Control and Superconducting Properties in Electron-doped ZrNiCl
13:30 Lunch

Oral Session VII Chair: Rogl, P

- 14:50 O29 Murakami, M Orbital Ordering and the Dilute Effect in Perovskites
15:15 O30 Tokura, Y Phase Competition and Gigantic Response in Correlated-Electron Oxides
15:40 O31 Huang, D J Spin, Charge, and Orbital Ordering of Transition-Metal Oxides

Poster Session Chair: Oguchi, T

- 16:00 P01–P54 Posters and Coffee

- 18:10 Banquet

Saturday, November 19

Oral Session VIII Chair: Bauer, E

- 8:50 O32 Rogl, P Constitution and Structural Chemistry of Rare Earth - Platinum Metal Group - Silicides related to Heavy Fermion Superconductor CePt₃Si
- 9:15 O33 Mignot, J M Neutron scattering study of spin dynamics in YbB₁₂
- 9:40 O34 Grin, Y Chemical Physics of intermetallic Chlathrates
- 10:05 O35 Leithe-Jasper, A Ferromagnetism, electronic and crystal structure of alkali-metal iron antimonides: NaFe₄Sb₁₂ and KFe₄Sb₁₂
- 10:25 O36 Jeong, Y H Orbital order, ferromagnetism, and ferroelectricity of BiMnO₃ and related compounds
- 10:45 Coffee

Oral Session IX Chair: Fujii, H

- 11:15 O37 Majer, G Proton NMR studies of the hydrogen dynamics in pure and Ti-doped complex chemical hydrides
- 11:40 O38 Akiba, E Defects Formation in the Lattice of Intermetallic Compound LaNi₅ with Hydrogenation
- 12:05 O39 Goll, G Andreev-Reflection Experiments on CeCoIn₅
- 12:25 O40 Shimada, K High-resolution photoemission study of Ce_{1-x}La_xRhAs: a collapse of the energy gap in the Kondo semiconductor

Closing Chair: Takabatake, T

- 12:45 Yamanaka, S
- 13:00 Lunch

Friday, November 18

16:00 – 18:00

Poster Session

- P01 Mori, T Thermoelectric Properties of Boron-Rich Cluster Compounds
- P02 Imai, M Lattice constants and electrical resistivity of C32-type $\text{LaAl}_{2-x}\text{Si}_x$ ($0.14 \leq x \leq 0.63$)
- P03 Sakurai, Y Optical Study on Clathrates $\text{Sr}_8\text{Ga}_{16}\text{Ge}_{30}$ and $\beta\text{-Eu}_8\text{Ga}_{16}\text{Ge}_{30}$
- P04 Tsutsui, S ^{149}Sm Nuclear Resonant Inelastic Scattering of Sm-based Filled-Skutterudite Compounds
- P05 Kwon, Y S Anomaly in magnetic properties of CePdGa_3
- P06 Umeo, K Effects of Rattling on the Thermal Conductivity and Specific Heat of Single-Crystalline Clathrates, $\text{Sr}_8\text{Ga}_{16}\text{Ge}_{30}$ and $\text{Ba}_8\text{Ga}_{16}\text{Ge}_{30}$
- P07 Mizumaki, M Determination of the Valence in Sm-based Filled-Skutterudite Compounds
- P08 Avila, M A Carrier-Tuning of Single-Crystalline Clathrate $\text{Ba}_8\text{Ga}_{16}\text{Ge}_{30}$
- P09 Cui, X Y High-resolution angle-resolved photoemission study on $\text{Fe}(110)$
- P10 Asahi, R First-principles studies of pseudogap formation and thermoelectric property in the $M_2\text{Zn}_{11}$ ($M = \text{Ni, Pd, Co, and Fe}$) γ brasses
- P11 Ribeiro, R A Tunneling spectroscopy of single-crystal clathrates $\text{Ba}_8\text{Ga}_{16}\text{X}_{30}$ ($X = \text{Ge, Sn}$)
- P12 Kume, T High Pressure Phase Transitions of Si Clathrates Studied by Raman Spectroscopy
- P13 Higashiguchi, M High-resolution angle resolved photoemission study on the self-energy of Ni, Cu and Pd single crystal
- P14 Miura, Y High-resolution angle-resolved photoemission study of kish graphite
- P15 Kanazawa, I A Broad Background of Optical Self-Energy and Quantized Massive Gauge Fields Mediating Cooper Pairing in High Tc Cuprates
- P16 Ito, M Specific heat of CuCrZrS_4
- P17 Koyama, K High Field X-ray Diffraction Measurements of Novel Ferromagnetic shape Memory Alloy $\text{Ni}_{50}\text{Mn}_{36}\text{Sn}_{14}$
- P18 Ogita, N Raman Scattering Investigation of Skutterudite Compounds
- P19 Higashitani, S Boundary Condition for Usadel Equation in Dirty Superconductor-contacts
- P20 Onoue, M Electronic structure and thermoelectronic properties of the half-Heusler compounds $M\text{NiSn}$ and $M\text{CoSb}$ ($M = \text{Ti, Zr and Hf}$)

- P21 Takasaki, T Tunneling spectroscopy of $A1B_2$ type superconductor $CaAlSi$
- P22 Ishii, I Elastic Properties of $Sr_8Ga_{16}Ge_{30}$
- P23 Ichikawa, Outlook for the metal-N-H Hydrogen Storage Systems
- P24 Hanada, N Catalytic Effect of Niobium Oxide on Hydrogen Storage Properties of Mechanically Ballmilled MgH_2
- P25 Miyaoka, Novel Metal-C-H Hydrogen Storage System
- P26 Miura, M Raman Spectra of Spin-triplet Superconductor Sr_2RuO_4
- P27 Inumaru, K Preparation and Structural Characterization of Transition Metal Nitride Epitaxial Thin Films
- P28 Ekino, T Electron tunnelling experiments on La-substituted Kondo-semiconductor $CeRhAs$
- P29 Matsuoka, E Magnetic and Thermoelectric properties of $Ba_yFe_{4-x}Co_xSb_{12}$
- P30 Yang, C H Large Positive Magnetoresistance in Fe doped $ZnO:Cu$ Thin Film
- P31 Takasu, Y Raman Scattering of type-I Clathrate Compounds
- P32 Kini, N S X-ray Structural Analysis and Molecular Dynamics Simulations of Three-Dimensional C_{60} Polymers
- P33 Lee, S H Ferroelectric Property in the $BiMn_{0.5}Fe_{0.5}O_3$ by the Piezoresponse Force Microscopy
- P34 Kawaguchi, M The Competition between Kondo Effect and Gap formed by Antiferromagnetic Order in $Ce_xNd_{1-x}B_6$
- P35 Kondo, A Nd-Doping Effect on Phase IV of $Ce_xLa_{1-x}B_6$
- P36 Tsugawa, N Angle-resolved 9Be NMR study of a heavy-Fermion superconductor UBe_{13}
- P37 Sera, M Pressure effect on the Long-range order in CeB_6
- P38 Kishimoto, S Coexistence of Antiferro-Quadrupole Order and Magnetic Order in $Ce_xPr_{1-x}B_6$
- P39 Sawada, M High Energy Photoelectron Spectroscopy of Pyrochlore Molybdenum Oxides $R_2Mo_2O_7$ ($R = Sm, Tb$)
- P40 Kimura, S Infrared study on electronic structure of SrT_4Sb_{12} ($T = Fe, Ru$)
- P41 Shigetoh, K Successive Magnetic Phase Transitions in the Heavy-Fermion System $Ce_4Ni_3Pb_4$
- P42 Uratani, Y First-principles exploration for double-perovskite multiferroics
- P43 Tsumuraya, T First-principles study on lithium hydrides for hydrogen storage

- P44 Sawada, Y A first-principles view of X-ray magnetic circular dichroism of uranium chalcogenide
- P45 Utsunomiya, K Josephson junction with tunable energy dissipation using quasi-particle injection
- P46 Sera, H Energy distribution of non-equilibrium quasiparticles in Superconductors
- P47 Kubota, T Fabrication of Cr/CrOx/Cr Single Electron Transistor using Plasma Oxidation
- P48 Tanaka, Y Incommensurate and commensurate quadrupole orders in $\text{Ce}_{0.7}\text{Pr}_{0.3}\text{B}_6$
- P49 Huo, D Low-temperature synthesis of CoSb_3
- P50 Mignot, J M Magnetic phase diagram of $\text{Ce}_{0.70}\text{Pr}_{0.30}\text{B}_6$
- P51 Negishi, S Photoemission study on electronic structure of TiSe_2
- P52 Michimura, S Magnetic Frustrations in the Shastry-Sutherland System ErB_4
- P53 Shishidou, T How is the 3d orbital ordering of LaMnO_3 reflected in x-ray linear dichroism?: A first-principles study
- P54 Shishidou, T First-principles study of multiferroic BiMnO_3
- P55 Hasegawa, T Lattice dynamics calculation of infrared active modes of cuprate superconductors