

1. Journals

Carbon Alloy Catalysts: Active Sites for Oxygen Reduction Reaction

IKEDA Takashi, BOERO Mauro, HUANG Sheng-Feng, TERAOKURA Kiyoyuki, OSHIMA Masaharu, and OZAKI Jun-ichi

J. Phys. Chem. C **112**, (2008) 14706-14709

Exact diagonalization study on nonmagnetic impurity effects in high-Tc superconductors

TSUTSUI Kenji, TOYAMA Atsushi, TOHYAMA Takami, MAEKAWA Sadamichi

J. Phys. Chem. Soli. 69 (2008) 3365-3368

Momentum-resolved charge excitations in high-Tc cuprates studied by resonant inelastic X-ray scattering

K. Ishii, M. Hoesch, T. Inami, K. Kuzushita, K. Ohwada, M. Tsubota, Y. Murakami, J. Mizuki, Y. Endoh, K. Tsutsui, T. Tohyama, S. Maekawa, K. Yamada, T. Masui, S. Tajima, H. Kawashima, J. Akimitsu

J. Phys. Chem. Soli. 69 (2008) 3118-3124

Possible Collective Spin Excitation in the Spin-Triplet Superconducting State of Sr_2RuO_4 : Multi-Band Theory

T. Nomura, D. S. Hirashima and K. Yamada

J. Phys. Soc. Jpn. 77, 024701 (2008)

Analysis of Incident-Photon-Energy and Polarization Dependent Resonant Inelastic X-ray Scattering from La_2CuO_4

M. Takahashi, J. Igarashi and T. Nomura

J. Phys. Soc. Jpn. 77, 034711 (2008)

Theory of magnetic properties in the spin-triplet superconducting state of Sr_2RuO_4

T. Nomura, H. Ikeda and D. S. Hirashima

J. Phys. Chem. Solids 69, 3352-3355 (2008)

Possibility of Unconventional Pairing Due to Coulomb Interaction in Fe-Based Pnictide

Superconductors: Perturbative Analysis of Multi-Band Hubbard Models

T. Nomura

J. Phys. Soc. Jpn. 77 Suppl. C, 123-124 (2008)

Possible Mechanism of Charge Stripe Formation Based on the Ring Exchange Interaction

T. Sakai

Physica C 468 , 1163-1165 (2008)

Quantum phase transitions of the asymmetric three-leg spin tube

T. Sakai, M. Sato, K. Okunishi, Y. Otsuka, K. Okamoto and C. Itoi

Phys. Rev. B 78 , 184415-1-11 (2008)

Numerical Diagonalization Study on a Phonon-assisted Hole Pairing Mechanism of an Extended t-J Holstein Model

T. Sakai

J. Phys.: Conf. Series. 108 , 012026-1-4 (2008)

X-ray absorption analysis of nitrogen contribution to oxygen reduction in carbon alloy cathode catalysts for polymer electrolyte fuel cells

NIWA Hideharu, HORIBA Koji, HARADA Yoshihisa, OSHIMA Masaharu, IKEDA Takashi, TERAKURA Kiyoyuki, OZAKI Jun-ichi, and MIYATA Seizo

J. Power Sources **187**, (2009) 93-97

First-principles calculation of the electronic properties of doped nitrogen and boron in a graphene cluster: analysis of catalytic activity for oxygen reduction reaction

HUANG Sheng-Feng, TERAKURA Kiyuyuki, OZAKI Taisuke, IKEDA Takashi, BOERO Mauro, OSHIMA Masaharu, OZAKI Jun-ichi, and MIYATA Seizo

Phys. Rev. B **80**, (2009) 235410

Exact Diagonalization Calculations of Hole Binding around Ni Impurities in Ni-substituted Cuprate Superconductors

TSUTSUI Kenji, TOYAMA Atsushi, TOHYAMA Takami, MAEKAWA Sadamichi

Phys. Rev. B 80 (2009) 224519-1~5

Perturbation Theory of High-Tc Superconductivity in Iron Pnictides

T. Nomura

J. Phys. Soc. Jpn. 78, 034716 (2009)

Field-Induced Incommensurate Order and Possible Supersolid in the $S=1/2$ Frustrated Diamond Chain

T. Sakai, K. Okamoto and T. Tonegawa

J. Phys.: Conf. Series. 145 , 012065-1-4 (2009)

Ground-State Phase Diagram of an $(S, S')=(1, 2)$ Spin-Alternating Chain with Competing Single-Ion Anisotropies

T. Tonegawa, T. Sakai, K. Okamoto and M. Kaburagi

J. Phys.: Conf. Series. 145 , 012066-1-4 (2009)

Two-step quantum spin flop transition in spin ladders

T. Sakai, T. Tonegawa and K. Okamoto

J. Phys.: Conf. Series. 150 , 042169-1-4 (2009)

Polarization Plateau in Atomic Fermi Gas Loaded on Triangular Optical Lattice

M. Okumura, S. Yamada, M. Machida and T. Sakai

Phys. Rev. A 79 ,061602(R)-1-4 (2009)

Dzyaloshinsky-Moriya Interaction in the $S=1/2$ Quasi-One-Dimensional Antiferromagnet $\text{Cu}_2\text{Cl}_4\text{H}_8\text{C}_4\text{S}_2\text{O}_2$ as Determined via High-Frequency ESR

M. Fujisawa, K. Shiraki, S. Okubo, H. Ohta, M. Yoshida, H. Tanaka and T. Sakai

Phys. Rev. B 80 ,012408-1-4 (2009)

Magnetic Field versus Temperature Phase Diagram of the Spin-1/2 Alternating-Bond Chain Compound F_5PNN

Y. Yoshida, T. Kawae, Y. Hosokoshi, K. Inoue, N. Maeshima, K. Okunishi, K. Okamoto and T. Sakai

J. Phys. Soc. Jpn. 78 ,74716-1-5 (2009)

Elementary excitations and spin dynamics in nanowire quantum magnets

T. Sakai, T. Tonegawa and K. Okamoto

Int. J. Mod. Phys. C 20 ,1467-1476 (2009)

Quantum Phase Transition of a Triangular Lattice Spin Tube and Edge Spin Effects

K. Okunishi, S. Yoshikawa, T. Sakai and S. Miyashita

Int. J. Mod. Phys. C 20 , 1423-143 (2009)

Structure of liquid water under high pressure up to 17 GPa

KATAYAMA Yoshinori, HATTORI Takanori, SAITOH Hiroyuki, IKEDA Takashi, AOKI Katsutoshi, FUKUI Hiroshi, and FUNAKOSHI Kenichi

Phys. Rev. B **81**, (2010) 014109

High-temperature water under pressure

IKEDA Takashi, KATAYAMA Yoshinori, SAITOH Hiroyuki, and AOKI Katsutoshi

J. Chem. Phys. **132**, (2010) 121102

Enhanced Catalytic Activity of Carbon Alloy Catalysts Codoped with Boron and Nitrogen for Oxygen Reduction Reaction

IKEDA Takashi, BOERO Mauro, HUANG Sheng-Feng, TERAOKURA Kiyuyuki, OSHIMA Masaharu, OZAKI Jun-ichi, and MIYATA Seizo

J. Phys. Chem. C **114**, (2010) 8933-8937

Field Induced Exotic Phenomena of the $S=1/2$ Three-Leg Quantum Spin Nanotube

T. Sakai, K. Okunishi, K. Okamoto, C. Itoi and M. Sato

J. Low Temperature Phys. 159 ,55-58 (2010)

Magnetization Process of the $S=1/2$ Distorted Diamond Spin Chain with the Dzyaloshinsky-Moriya interaction

T. Sakai, T. Tonegawa and K. Okamoto

J. Phys. Conf. Ser. 200 ,022052-1-4 (2010)

Half Magnetization Plateau of a Frustrated $S=1$ Antiferromagnetic Chain

T. Tonegawa, H. Nakano, T. Sakai, K. Okamoto, K. Okunishi and K. Nomura

J. Phys. Conf. Ser. 200 , 022065-1-4 (2010)

Field-Induced Nematic Phase in the Spin Ladder System with Easy-Axis Anisotropy

T. Sakai, T. Tonegawa and K. Okamoto

Physica Status Solidi B 247 , 583-585 (2010)

First-Order Phase Transition between One-Third Magnetization Plateau States in an Anisotropic (S, S') Spin Alternating Chain

T. Tonegawa, K. Okamoto and T. Sakai
Physica Status Solidi 247 , 688-690 (2010)

Magnetization Process of the Kagome Lattice Antiferromagnet
H. Nakano and T. Sakai
J. Phys. Soc. Jpn. (Letter) 79 ,053707-1-4 (2010)

2. Others

Hydration and Chemical Reactions of Metal Ions via First Principles Molecular Dynamics
Method
IKEDA Takashi
Ensemble **10** (2008) 3-8 (in Japanese)

Present Status and Future Subjects of First-Principles-Based Simulations for Chemical
Reactions
IKEDA Takashi, BOERO Mauro, and MORIKAWA Yoshitada
BUTSURI **64** (2009) 256-262 (in Japanese)

Electronic Structure and Catalytic Activity of Doped Graphene
IKEDA Takashi, HUANG Sheng-Feng, BOERO Mauro, and TERAKURA Kiyoyuki
Graphene: Functions and Applications, ed. SAIKI Koichiro and TOKUMOTO Hiroshi, Tokyo,
CMC-Books (2009) (in Japanese)

Mechanisms of Catalytic Activity for Carbon Alloy Catalysts
IKEDA Takashi, HUANG Sheng-Feng, BOERO Mauro, and TERAKURA Kiyoyuki
Platinum-Substitute Carbon Alloy Catalysts, ed. MIYATA Seizo, Tokyo, CMC-Books (2010) (in
Japanese)