ISAMMDoF2018

International Symposium on Advanced Materials Having Multi-Degrees-of-Freedom – Informatics in Advanced Measurements and Material Science –

November 1-2, 2018
Kumamoto University,
Kumamoto, JAPAN

SCOPE

The scope of the symposium covers comprehensive researches on material science and technology for advanced materials having multi-DoF. The following topics will be discussed in this symposium.

- Informatics in Advanced Measurements
- Materials Informatics
- Structure and Electronic states for optical functionalities
- Structural Imaging at active sites in advanced materials
- Multi-DoFin superionicconducting phenomena
- Hierarchical macro-structured materials
- Optical Properties of amorphous materials
- Dynamic processes under high temperature and high pressure
- Novel methods for Spectroscopy and analysis for advanced materials
- Control methods of multi-DoF by using extreme conditions

URL: http://phys.ipps.kumamoto-u.ac.jp/ISAMMDoF2018/

SESSIONS

Thu, 1st Nov, 2018		
Registration	9:00∼9:25	Entrance Hall
Opening (Prof. K. Hokamoto, Deputy Director, IPPS)	9:25∼9:30	C122
Session 1 (Chair: M. Aniya)	9:30∼11:00	C122
Coffee Break		
Session 2 (Char: S. Hosokawa)	11:15∼12:45	C122
Lunch Break		
Session 3 (Char: A. Koura)	13:50∼14:40	C122
Coffee Break		
Short presentation for poster	14:55∼15:30	C122
Photo	15:30∼15:35	C122
Poster presentation	15:40∼17:10	Entrance Hall
Fri, 2nd Nov, 2018		
Session 4 (Chair: F. Shimojo)	9:45∼10:30	C122
Coffee Break		
Session 5 (Chair: Y. Sakaguchi)	10:45∼12:00	C122
Lunch Break		
Session 6 (Chair: Y. Nakajima)	13:15∼14:45	C122
Closing (Prof. S. Hosokawa)	14:45∼14:50	C122

- Poster presentation accompanied with a short advertising oral talk (3 minutes)

VENUE

The technical sessions will be held at Kurokami South E1 Bldg. (Faculty of Science Bldg. 1) in Kumamoto University.

- Address:
  Kumamoto University,
  2-39-1 Kurokami Chuo-ku, Kumamoto 860-8555, Japan
  URL: `http://ewww.kumamoto-u.ac.jp/en/`
- Access: `http://ewww.kumamoto-u.ac.jp/en/about/access/access_map/`
- Campus map: `http://ewww.kumamoto-u.ac.jp/en/about/access/campus/`

INVITED SPEAKERS

- Dr. Marc de Boissieu

  "Icosahedral quasicrystals : atomic structure and lattice dynamics"

  SIMaP, Univ. Grenoble Alpes, France

- Prof. Matthieu Micoulaut

  "Characterizing structure and dynamcis of chalcogenides from coupled approaches : rigidity and molecular simulations"

  Sorbonne Universite, France

- Prof. Tomas Wagner

  "Metal doped chalcogenides for nanoscale memories"

  University of Pardubice, Czech Republic

- Prof. Laszlo Pusztai

  Understanding the structure of disordered materials via combinations of Molecular Dynamics Simulations and Reverse Monte Carlo modeling: handling information deficiency

  Hungarian Academy of Sciences, Hungary,
  IROAST, Kumamoto University, Japan

- Prof. Kouichi Hayashi

  "Element-selective structural analyses of disordered systems by X-ray fluorescence holography"

  Nagoya Institute of Technology, Japan

- Dr. Yasuhiko Igarashi

  "Sparse modeling of extended X-ray absorption fine structures"

  JST PRESTO, The University of Tokyo, NIMS, Japan

- Dr. Yoshifumi Sakaguchi

  "Kinetics study on silver photodiffusion into amorphous germanium sulfide using neutron reflectivity technique"

  Comprehensive Research Organization for Science and Society: CROSS, Japan

- Mr. Hiroyuki Kumazoe

  "Non-adiabatic ab initio molecular dynamics study of electric properties of layered transition metal dichalcogenides"

  GSST, Kumamoto University, Japan

- Prof. Koichi Shimakawa

  "Optical and Electronic Properties in Phase-Change Ge-Sb-Te System: Resonance bonds and metal-insulator transition"

  Gifu University, Japan

- Dr. Jens R. Stellhorn

  "A Model for the Fast Phase-Change Mechanism in Cu_2GeTe_3"

  Department of Physics, Kumamoto University, Japan

ORGANIZING COMMITTEE

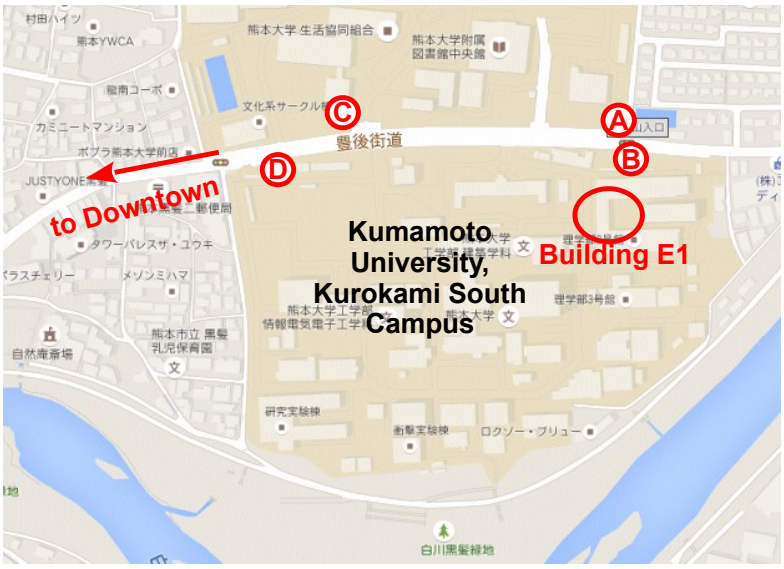
- Ichiro Akai (Chair), Institute of Pulsed Power Science, Kumamoto University, Japan
- Shinya Hosokawa (Chair), Faculty of Advanced Science and Technology, Kumamoto University, Japan
- Masaru Aniya, Faculty of Advanced Science and Technology, Kumamoto University, Japan
- Fuyuki Shimojo, Faculty of Advanced Science and Technology, Kumamoto University, Japan
- Yoichi Nakajima, Priority Organization for Innovation and Excellence, Kumamoto University, Japan

SPONSORS

- Kumamoto University
- Kumamoto University, Institute of Pulsed Power Science
- Kumamoto University, International Research Organization for Advanced Science and Technology Graduate School of Science

ACCESS MAP (DOWNTOWN ↔ KUMAMOTO UNIV.)

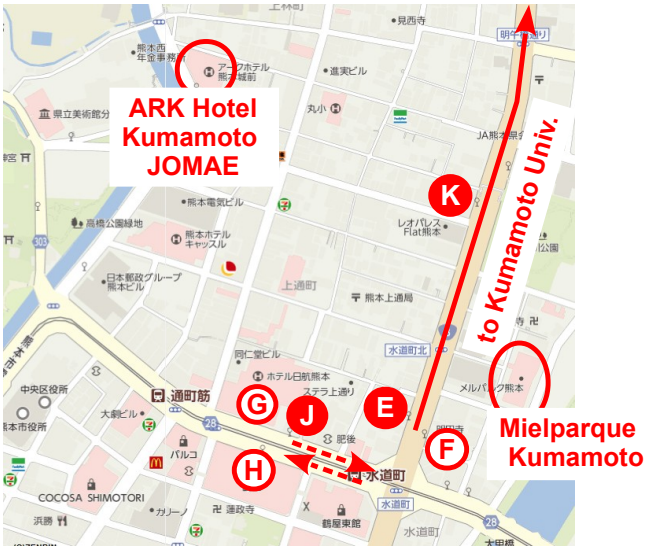
- Kumamoto University
  URL: `http://ewww.kumamoto-u.ac.jp/en/about/access/access_map/`



Kumamoto University is located 2.2 km from the downtown (Touricho-suji, Suido-cho). City bus services ($15 \sim 20$ minutes) connect the university with the downtown.

Ⓐ Bus stop (Tatsuta Shizen-Koen Iriguchi) from downtown
Ⓑ Bus stop (Tatsuta Shizen-Koen Iriguchi) to downtown
Ⓒ Bus stop (Kumamoto Digaku Mae) from downtown
Ⓓ Bus stop (Kumamoto Digaku Mae) to downtown

- Downtown (Touricho-suji, Suido-cho)



- Hotel Mielparque Kumamoto
  URL: `http://www.mielparque.jp/kumamoto/en/`

Ⓔ Bus stop (Suidou-cho): Departing bus station of the city bus services bound for Kumamoto University. Buses indicated with 子1, 子7, 子8, 子9, 子18 or 子20 go to Kumamoto University from this bus station. About 15~20 minutes for the University.

Ⓕ Bus stop (Suidou-cho): Arrival bus stop from Kumamoto University.

Ⓖ Bus stop (Touricho-suji):
Departing bus station of highway-buses bound for Fukuoka and Aso Kumamoto Airports.

Ⓗ Bus stop (Touricho-suji):
Arrival bus stop for the highway-buses from Fukuoka and Aso Kumamoto Airports and city bus services from Kumamoto university.

Ⓙ Bus stop (Touricho-suji)
Departing bus station of the city bus services bound for Kumamoto university.
Buses indicated with 子 1, 子 7, 子 8, 子 9, 子 18 or 子 20 go to Kumamoto university from this bus station. About 15∼20 minutes for the university.

Ⓚ Bus stop (Shirakawa-Kouen-mae)
Departing bus station of the city bus services bound for Kumamoto university.
Buses indicated with 子 1, 子 7, 子 8, 子 9, 子 18 or 子 20 go to Kumamoto university from this bus station. About 15∼20 minutes for the university.

INSTRUCTION FOR PRESENTERS

We will prepare a PC projector (SVGA: 1024x768). The presenters of invited talks and oral presentations should check if their own laptop PC could be correctly connected to the projector.

- Invited talks :

  Allotted time : 45 or 30 minutes (including the time for Q & A)

- Oral presentations ;

  Allotted time : 15 minutes (including the time for Q & A)

- Poster presentations :
  Short oral presentations are accompanied before the poster presentations.

  Poster boards : 180H x 120W
  Short oral presentations : Allotted time : 3 minutes (without Q & A)

  The posters must be fixed with pins. Posters should stay on display during the symposium.

Presenting authors should submit an extended abstract. The extended abstract is requested to have two or more pages of A4 size and should include a summary less than 50-words. The format of the summary is free.

ISAMMDoF2018

3rd International Symposium on Advanced Materials Having Multi-Degrees-of-Freedom — Informatics in Advanced Measurements and Material Science —

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1st ~ 2nd November, 2018,
Kurokami South E1 Bldg., Kumamoto University,
Kumamoto JAPAN

Thu, 1st Nov, 2018

- **Registration** — **9:00∼9:25** — **Entrance Hall**

- **Opening** (Prof. K. Hokamoto, Deputy Director, IPPS) — **9:25∼9:30** — **C122**
- **Session 1** (Chair: M. Aniya) — **9:30∼** — **C122**

9:30∼10:15 **I-1** 12

Metal doped chalcogenides for nanoscale memories

T. Wagner, B. Zhan, M. Fraenkl, M. Gottwald

Department of General & Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice and Centre for Nanomaterials & Nanotechnology (CEMNAT), Faculty of Chemical Technology, University of Pardubice, Cs. Legii Sq. 565, Pardubice 532 10, Czech Republic.

Metal-doped chalcogenide bulk glasses and their thin films have become attractive materials for fundamental research because of their structure, properties, and preparation. They have many current and potential applications in optics, optoelectronics, electronics, chemistry, and biology (optical elements, waveguides, bio- and chemical sensors, solid electrolytes, batteries, memories, light sources).

10:15∼11:00 **I-2** 15

Optical and Electronic Properties in Phase-Change Ge-Sb-Te System: Resonance bonds and metal-insulator transition

K. Shimakawa[1,2]

[1] *Faculty of Engineering, Gifu University, Gifu University, Gifu 501-1193, Japan*
[2] *Department of General and Inorganic Chemistry, University of Pardubice, Pardubice, Czech Republic*

Although a proposal of resonance bonds in crystalline phase-change Ge-Sb-Te (GST) materials has been provided, we do not find any clear evidence in favor of the proposal. The ellipsometry demonstrates that a change in the high frequency (optical) dielectric constant between the amorphous and crystalline states is only scaled by the average bandgap (the Penn gap rule). There is no special bond which may induce a significant change in the optical transition matrix element during the phase change, which is necessary to support the idea of resonance bonds. The electronic transport properties of GST are also not clearly understood. Negative temperature coefficient is found even in the metallic state (crystalline phase), when the carrier mean-free-path is short. It is shown that the concept of minimum metallic conductivity, often used in the metal-insulator transition, cannot be applied to electronic transport in GSTs.

- *Coffee Break* — **11:00∼11:15**

- **Session 2** (Chair: S. Hosokawa) — **11:15∼** — **C122**

11:15∼12:00 **I-3** ····· 18

Icosahedral quasicrystals : atomic structure and lattice dynamics

M. de Boissieu

Univ. Grenoble Alpes, CNRS, SIMaP, France

12:00∼12:45 **I-4** ····· 19

Element-selective structural analyses of disordered systems by X-ray fluorescence holography

K. Hayashi

Department of Physical Science and Engineering, Nagoya Institute of Technology, Japan

We observed heterogeneities in PMN and PZT by XFH. They provided clues to understand the mechanisms of high piezoelectric property of PMN and PZT.

○ *Lunch Break* **12:45∼13:50**

• Session 3 (Chair: A. Koura) **13:50∼** **C122**

13:50∼14:20 **I-5** ····· x.1

A Model for the Fast Phase-Change Mechanism in Cu_2GeTe_3

J. R. Stellhorn[1], S. Hosokawa[1], Y. Sutou[2]

[1] *Department of Physics, Kumamoto University, Japan,*
[2] *Department of Materials Science, Tohoku University, Japan.*

The structure of amorphous Cu_2GeTe_3 was investigated by a combination of anomalous x-ray scattering and extended x-ray absorption fine structure experiments. The experimental data were analyzed with a reverse Monte Carlo modeling, and interpreted in terms of the short- and intermediate-range order. Based on this information, a model for the phase transition in Cu_2GeTe_3 is proposed, in which atoms move toward the center of the sixfold rings of the crystal structure, leading to the formation of wrong bonds and a broader distribution of ring structure, but also preserving some structural motifs of the crystal.

14:20∼14:40 **O-1** ····· x.4

Temperature dependent local atomic structures in the traditional $Fe_{65}Ni_{35}$ Invar alloy by x-ray fluorescence holography

S. Hosokawa[1], J. R. Stellhorn[1], N. Happo[2], K. Hayashi[3], T. Matsushita[4], K. Yubuta[5]

[1] *Department of Physics, Kumamoto University, Japan,*
[2] *Graduate School of Information Sciences, Hiroshima City University, Japan,*
[3] *Department of Physical Science and Engineering, Nagoya Institute of Technology, Japan,*
[4] *Japan Synchrotron Radiation Research Institute (JASRI), Japan,*
[5] *Institute for Materials Research, Tohoku University, Japan.*

Fe and Ni $K\alpha$ x-ray fluorescence holography measurements were performed on a single crystal $Fe_{66}Ni_{34}$ Invar alloy at 100 and 300 K to investigate the temperature dependence of the three-dimensional local structures around the Fe and Ni atoms, respectively. Local structural information was obtained by detailed analyses using a L_1-regularized linear regression for the experimental data. At 100 K, the local atomic arrangements around both the elements show fcc structures as obtained by diffraction measurements. At 300 K, however, only the image around Fe shows a *bcc*-like image. We propose a model that with increasing temperature, an Fe atom with the low-spin state enters at the central position of the fcc lattice and is stabilized. Then, large angular positional fluctuations are induced for the atoms at the face-centered positions.

○ *Coffee Break* **14:40∼14:55**

• Short presentation for poster P-1∼P-9 **14:55∼** **C122**

• Photo **15:30∼15:35** **C122**

• Poster presentation-1 **15:40∼17:10** **Entrance Hall**

Bayesian spectroscopy on complicated excitonic photoluminescence spectra in a Cu_2O thin-crystal sandwiched by paired MgO substrates

K. Iwamitsu[1], S. Arishima[2], T. Yamashiro[2], M. Mizumaki[3], I. Akai[4]

[1] *Fac. Sci., Kumamoto Univ., Japan,*
[2] *GSST, Kumamoto Univ., Japan,*
[3] *JASRI, Japan,*
[4] *IPPS, Kumamoto University, Japan.*

Based on Bayesian spectroscopy, we studied polarization dependence of complicated excitonic photoluminescence (PL) spectra in a Cu_2O thin-crystal sandwiched MgO substrates. we decomposed to resonant weak PL bands of bifurcated ortho-excitons and their intense phonon sidebands and these polarization dependences can be understood by transition matrix elements of quadrupole transitions.

Sparse Modeling approach for EXAFS analyses

Y. Miyata[1], K. Iwamitsu[2], H. Setoyama[3], T. Okajima[3], Y. Igarashi[4], M. Okada[5], I. Akai[6,3]

[1] *GSST, Kumamoto Univ., Japan,*
[2] *Fac. Sci., Kumamoto Univ., Japan,*
[3] *SAGA-LS,*
[4] *JST PRESTO, The University of Tokyo, NIMS MADIS, Japan,*
[5] *The University of Tokyo, NIMS MADIS, Japan* [6] *IPPS, Kumamoto Univ., Japan.*

We propose a new analysis method of EXAFS data using sparse modeling. This method makes it possible to estimate the Debye-Waller factor without assuming the atomic scale local structure. We also succeeded in obtaining a radial structure function conforming to the sparsity of atomic coordination as a sparse solution.

Gas-phase grown single crystals of 1, 3, 5-triphenylbenzene

T. Yokota[1], T. Yamashiro[1], K. Iwamitsu[2], I. Akai[3]

[1] *GSST, Kumamoto Univ., Japan,*
[2] *Fac. Sci., Kumamoto Univ., Japan,*
[1] *IPPS, Kumamoto University, Japan.*

We have grown single crystals of 1, 3, 5-triphenylbenzene (tri-ph) by gas-phase growth method with argon exchange gas. The tri-ph molecule is one of important light-harvesting (LH) antenna molecules in LH-dendrimers, which show highly efficient energy transfer at room temperature. The grown crystals have needle-like shapes, and as the cooling duration being longer and the cooling-temperature gradient being gentle, many high-quality needle crystals have been obtained. Furthermore, the needle-like crystals show remarkable polarization characteristics which are owing to Davydov splitting.

Activation Energy of Ionic Conduction and Dielectric Constants in Superionic Conductors

H. Noda[1], M. Aniya[2]

[1] *Graduate School of Science and Technology, Kumamoto University, Japan,*
[2] *Faculty of Advanced Science and Technology, Kumamoto University, Japan.*

An attempt to correlate the activation energy of ion transport to the dielectric constants in ionic conductors is presented. Based on empirical grounds, an expression that permits to estimate the activation energy from optical dielectric constant is obtained. Preliminary result indicates that still crude, the found relationship could be a starting point to develop a predictive model.

Inelastic X-ray scattering measurements on liquid Fe-P alloy at high pressure

D. Kinoshita[1], Y. Nakajima[1,2], S. Kosugi[2], Y. Kuwayama[2,3], K. Hirose[3], D. Ishikawa[2,4], A. QR Baron[2]

[1] *Kumamoto Univ., Japan,*
[2] *RIKEN MDL, Japan,*
[3] *Tokyo Univ., Japan,*
[4] *JASRI, Japan.*

We determined the longitudinal sound wave velocity of liquid Fe-P alloy up to 60 GPa and 2800 K based on inelastic X-rays scattering measurements. We found that phosphorous has negligible effect on the sound velocity of liquid Fe under high pressures.

Effects of various substituents on dielectric constant of polyethylene based on first-principle calculations

S. Fukushima[1], H. Kumazoe[1], A. Misawa[2], S. Tiwari[3], F. Shimojo[1], A. Nakano[3], R. K. Kalia[3], P. Vashishta[3]

[1] *Dept. of Phys., Kumamoto Univ., Japan,*
[2] *Fac. of Sci. and Eng., Kyushu Sangyo Univ., Japan,*
[3] *Univ. of Southern California, USA.*

Dielectric polymers such as polyethylene (PE) have a wide range of energy and electronic applications. While recent studies have shown significant effects of chemical defects and substituents on the electronic structures of PE, those on the dielectric properties remains elusive. Here, first-principles quantum-mechanical calculations show anisotropic dielectric constants of PE, which are sensitive to the type of substituents. Addition of Iodine group increase the high frequency dielectric constant. While, addition of hydroxyl or carboxyl group does not change the high frequency dielectric constant significantly. However, a noticeable change is observed in static dielectric constant. The sensitivity of these substituents can be exploited to alter the behavior of PE.

First-principles molecular-dynamics study of static structure of liquid Fe-Si under pressure

S. Nakaguchi[1], A. Misawa[2], A. Koura[1], Y. Nakajima[3], F. Shimojo[4]

[1] *Dept. of Phys., Kumamoto Univ., Japan,*
[2] *Fac. of Sci. and Eng., Kyusyu Sangyo Univ., Japan,*
[3] *POIE, Kumamoto Univ., Japan,*
[4] *Fac. of Adv. Sci. and Tech., Kumamoto Univ., Japan.*

We performed first-principles molecular-dynamics simulations to investigate the structural and dynamical properties in liquid Fe, Fe-Si and Fe-S under the earth ' s outer-core conditions. It is found that Si atoms occupies atomic arrangement almost equivalent to Fe atoms in liquid iron structure and doesn ' t have effect on the transport properties of the earth ' s outer-core.

First principles study of the magnetic properties of Manganese Oxide nanosheets

R. Fukudome[1], M. Hara[1], A. Funatsu[2], F. Shimojo[1]

[1] *Dept. of Phys., Kumamoto Univ., Japan,*
[2] *Dept. of Chemistry, Kumamoto Univ., Japan.*

We have investigated the magnetic properties of manganese oxide nanosheets based on first principles simulations. The temperature dependence of the total magnetic moment of the system is discussed. The structural stability is also studied as a function of the direction of the magnetic moment.

Determination of Melting Temperature of Rb from Thermodynamic Integration based on First-principles Calculations

E. Ushijima, A. Koura, F. Shimojo

Dept. of Phys., Kumamoto Univ., Japan.

We have studied the melting temperature of Rb from thermodynamic integration (TI) based on first-principles molecular-dynamics (FPMD). In order to accelerate simulations, we constructed the potential based on an artificial neural network (ANN) from the result of FPMD, and performed TI using ANN potential. We also studied the system size dependence of the melting point.

Fri, 2nd Nov, 2018

• Session 4 (Chair: F. Shimojo) 9:45∼ C122

9:45∼10:30 **I-6** ····· 51

Kinetics study on silver photodiffusion into amorphous germanium sulfide using neutron reflectivity technique

Y. Sakaguchi[1] M. Mitkova[2]

[1] *Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society, Japan*
[2] *2Department of Electrical and Computer Engineering, Boise State University, U.S.A.*

Time-resolved neutron reflectivity measurement was carried out to investigate the kinetics of silver photodiffusion into amorphous germanium sulfide. It was found from the measurements that a metastable Ag-rich reaction layer was formed in the process of the silver photodiffusion for S-rich germanium sulfide, while such a metastable layer was not formed for Ge-rich germanium sulfide.

○ *Coffee Break* 10:30∼10:45

• Session 5 (Chair: Y. Sakaguchi) 10:45∼ C122

10:45∼11:15 **I-8** ····· 55

Sparse modeling of extended X-ray absorption fine structures

Y. Igarashi[1], K. Iwamitsu[2], T. Okajima[3], I. Akai[4,3], M. Okada[5]

[1] *JST PRESTO, The University of Tokyo, NIMS MADIS, Japan,*
[2] *Fac. Sci., Kumamoto Univ., Japan,*
[3] *Kyushy Synchrotron Light Research Center, Japan,*
[4] *IPPS, Japan, Kumamoto Univ., Japan,*
[5] *The University of Tokyo, NIMS MADIS, Japan*

In x-ray absorption spectra, fine structures appear due to interference between emitted photoelectron waves just above the absorption edge of a certain atom, which are called ex- tended x-ray absorption fine structures (EXAFS). We have applied sparse modeling (SpM) onto the EXAFS analysis on the basis of L1-regularization to obtain local structural informa- tions nearby the atom that absorbs x-rays. In this study, we introduce Bayesian LARS-OLS for EXAFS analysis, to optimize a parameter of L1-regularization and to extract the physical model appropriately.

11:15∼11:45 **I-9** ····· 57

Non-adiabatic *ab initio* molecular dynamics study of electric properties of layered transition metal dichalcogenides

H. Kumazoe[1], A. Krishnamoorthy[2], L. Bassman[2], S. Fukushima[1], S. Tiwari[2], R. K. Kalia[2], A. Nakano[2], F. Shimojo[1], P. Vashishta[2]

[1] *Department of Physics, Kumamoto University, Japan,*
[2] *Collaboratory for Advanced Computing and Simulations, University of Southern California, USA*

We have investigated the electric properties of layered transition metal dichalcogenides based on non-adiabatic ab initio molecular dynamics simulations. Our simulations promote an understanding for surface science on ultrafast time scales and open new opportunities for a direct characterization lattice structure at and across the interface of various materials.

11:45∼12:00 **O-2** ····· 60

Static structure of amorphous $Mg_{85}Zn_6Y_9$ alloy based on *ab initio* molecular dynamics simulations

A. Koura, F. Shimojo, S. Hosokawa

Department of Physics, Kumamoto University

We have investigated the static structure of amorphous $Mg_{85}Zn_6Y_9$ alloy based on *ab initio* molecular dynamics simulations. Correlations between impurity atoms, i.e., Zn-Zn, Zn-Y, and Y-Y bonds exist in the amorphous Mg alloy. This fact suggests the existence of fragments of Zn_6Y_8 $L1_2$-type clusters. These bonds are connected by metallic bonds.

○ *Lunch Break* **12:00∼13:15**

• Session 6 (Chair: Y. Nakajima) **13:15∼** **C122**

13:15∼14:00 **I-10** ····· x.7

Characterizing structure and dynamcis of chalcogenides from coupled approaches : rigidity and molecular simulations

M. Micoulaut

Sorbonne Université, Paris, France

The structure and dynamics of certain archetypal chalcogenides (As-Se, Ge-Se, GeTe, ...) is investigated from rigidity theory and molecular dynamics simulations. We first describe the ab initio framework that is necessary to accurately describe such materials and then connect ensemble averaged calculated properties to rigidity theory which is a popular approach used in glassy chalcogenides. Results show that a certain number of anomalies can be linked with the onset of molecular rigidity, and such methods also permit to clarify the question of geometrical motifs in more complex materials such as GeTe.

14:00∼14:45 **I-11** ····· x.8

Understanding the structure of disordered materials via combinations of Molecular Dynamics Simulations and Reverse Monte Carlo modeling: handling information deficiency

L. Pusztai

Wigner Research Centre for Physics, Hungarian Academy of Sciences, Hungary and International Research Organization for Advanced Science and Technology (IROAST), Kumamoto University, Japan

The problem of information deficiency, i.e., when the number of available diffraction (and/or EXAFS) experiments is (in many cases, much) lower than the number of partial radial distribution function in the system, is considered for disordered materials. Two approaches, both relying heavily on Reverse Monte Carlo (RMC) modeling [R.L. McGreevy, L. Pusztai, Molec. Simul. 1, 359 (1988)] are introduced: (1) molecular dynamics (MD) simulation, followed by RMC modeling (' RMCMD ' , see [L. Pusztai et al., Chem. Phys. Letts. 457, 96 (2008)]), and (2) RMC modeling that incorporates interatomic potential functions (' RMC_POT ' , see [O. Gereben & L. Pusztai, J. Comput. Chem. 33, 2285 (2012)]). We show that applying either method is useful. Although ' RMCMD ' is restricted to smaller molecules, it has a potentiality to play an important role when dealing with multicomponent glasses provided that direct simulations (either classical or ab initio) produce results with at least the same accuracy as they do for, e.g., alcohol-water mixtures (see [O. Gereben & L. Pusztai, J. Phys. Chem. B, 119, 3070 (2015); I. Bakó et al., Sci. Rep. 7, 1073 (2017)]). For molecular liquids containing larger molecules, the molecular structure begins to dominate the measurable total scattering structure factor and therefore, Reverse Monte Carlo is expected to play a more and more important role in conformational analyses in the liquid state.

• Closing (Prof. S. Hosokawa) **14:45∼14:50** **C122**

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