ISAM^4 2013

International Symposium on Atomistic Modeling for Mechanics and Multiphysics of Materials

ABSTRACT BOOK

July 22-24, 2013
Tokyo - Institute of Industrial Science, The University of Tokyo

SEIKEN SYMPOSIUM NO. 73

Welcome

It is a great pleasure to welcome all of you in Tokyo to the 2nd International Symposium on Atomistic Modelling for Mechanics and Multiphysics of Materials (ISAM4). This meeting started in 2011 with the aim to bring active scientists together in the field of computational materials science using atomistic modelling simulation and related methods to have intensive discussions about their new approaches and findings. For fruitful discussions we keep the door open to scientists in other fields such as experimentalists, theoreticians with macroscopic and mesoscopic simulations, etc.

Japan is still on the way of recovery from the Great East Japan Earthquake, which hit us just before our previous meeting. As the disaster brought about challenging issues including energy supply and scientific communication, Japanese scientists are strongly requested to meet the demand of society and address such problems. In other countries as well, investing money on scientific research may sometimes be questioned under the disrupted financial situation. Now is the time to broaden our horizons by exchanging ideas transcending the borders of nations, communities and fields. I hope that this meeting will provide the opportunity for promising scientists from many countries to meet new people and exchange excellent ideas to find breakthroughs.

Yoshitaka Umeno
Chairman of ISAM4
IIS, The University of Tokyo

Invited speakers

Prof. Erik Bitzek (Germany)
Prof. Dallas R. Trinkle (USA)
Dr. Martin Friák (Germany)
Dr. Matous Mrovec (Germany)
Prof. Miroslav Černý (Czech)
Prof. Sergey V. Dmitriev (Russia)
Prof. Takayuki Kitamura (Japan)
Prof. Yoji Shibutani (Japan)

Institute of Industrial Science, The University of Tokyo

Steering committee

Chair:
Prof. Yoshitaka Umeno (Univ. Tokyo)

Local steering committee members:
Dr. Masanori Kohyama (AIST)
Prof. Nobuhiro Yoshikawa (Univ. Tokyo)
Prof. Teruyasu Mizoguchi (Univ. Tokyo)
Dr. Yoshinori Shiihara (Univ. Tokyo)

General Information

Host Organization

Institute of Industrial Science, The University of Tokyo

SEIKEN SYMPOSIUM
No. 73

Co-host Organization

Center for Research on Innovative Simulation Software,
Institute of Industrial Science, The University of Tokyo

Supporting Organization

The Japan Society of Mechanical Engineers

Conference Secretary

Dr. Yoshinori Shiihara and Mrs. Chiharu Kadowaki
c/o Yoshikawa Lab., Institute of Industrial Science, The University of Tokyo, 4-6-1,
Komaba, Meguro-ku, Tokyo, Japan 153-8505
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Conference Homepage

www.young.iis.u-tokyo.ac.jp/isam4

Scope of this Symposium

Building of Conference Venue

Symposium topics include but are not limited to:
1. Atomistic modeling of materials
2. Quantum mechanics approach to various properties of materials
3. Numerical methods for materials science and engineering
4. Multiphysics analysis of materials

Oral presentation

The conference language is English. The scientific program of ISAM4 includes key lectures (30 min + 10min for discussion) and oral contributions (15 min + 5min for discussion).

Conference Fee

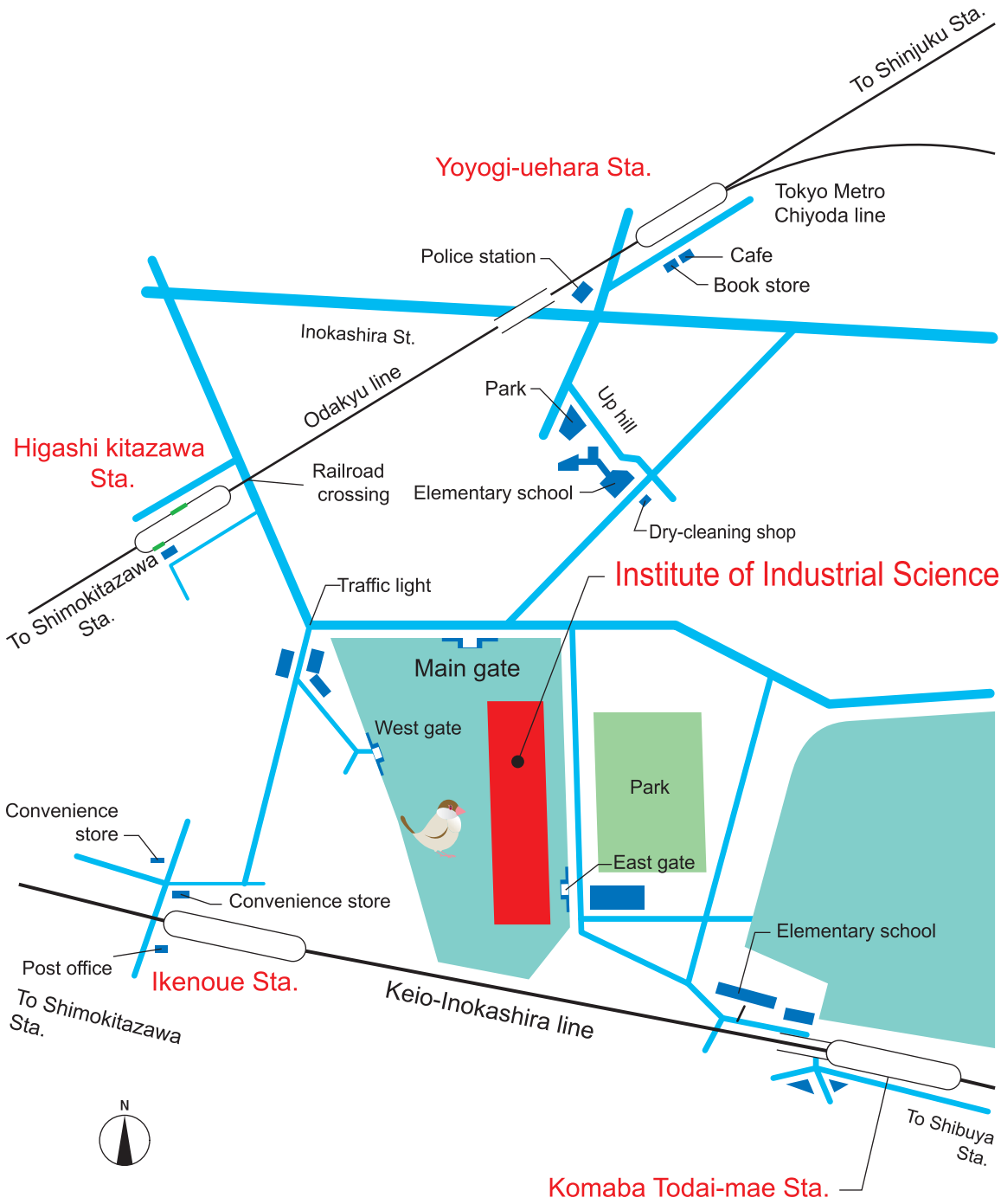
The conference fee is 30,000 JPY (20,000 JPY for student) per delegate.
(1USD=100 JPY, 1 EUR = 130 JPY as of July 1, 2013)

Internet connection

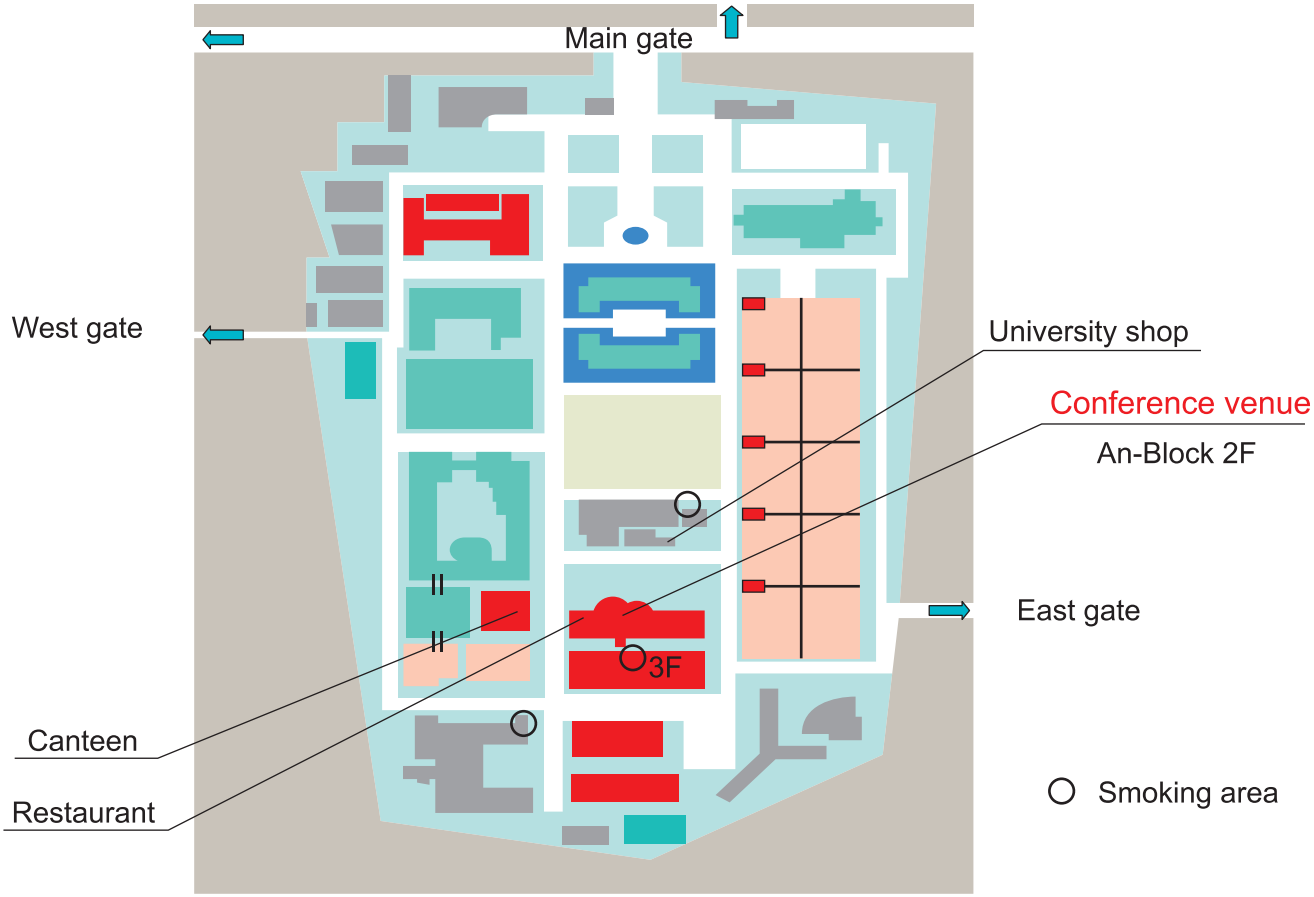
Free access to internet connection will be available in the conference venue.

Access Map

The ISAM4 conference will be held at the Institute of Industrial Science of the University of Tokyo located in west of Shibuya which is one of the major downtowns in Tokyo. The conference venue is easily reachable by public transportation.



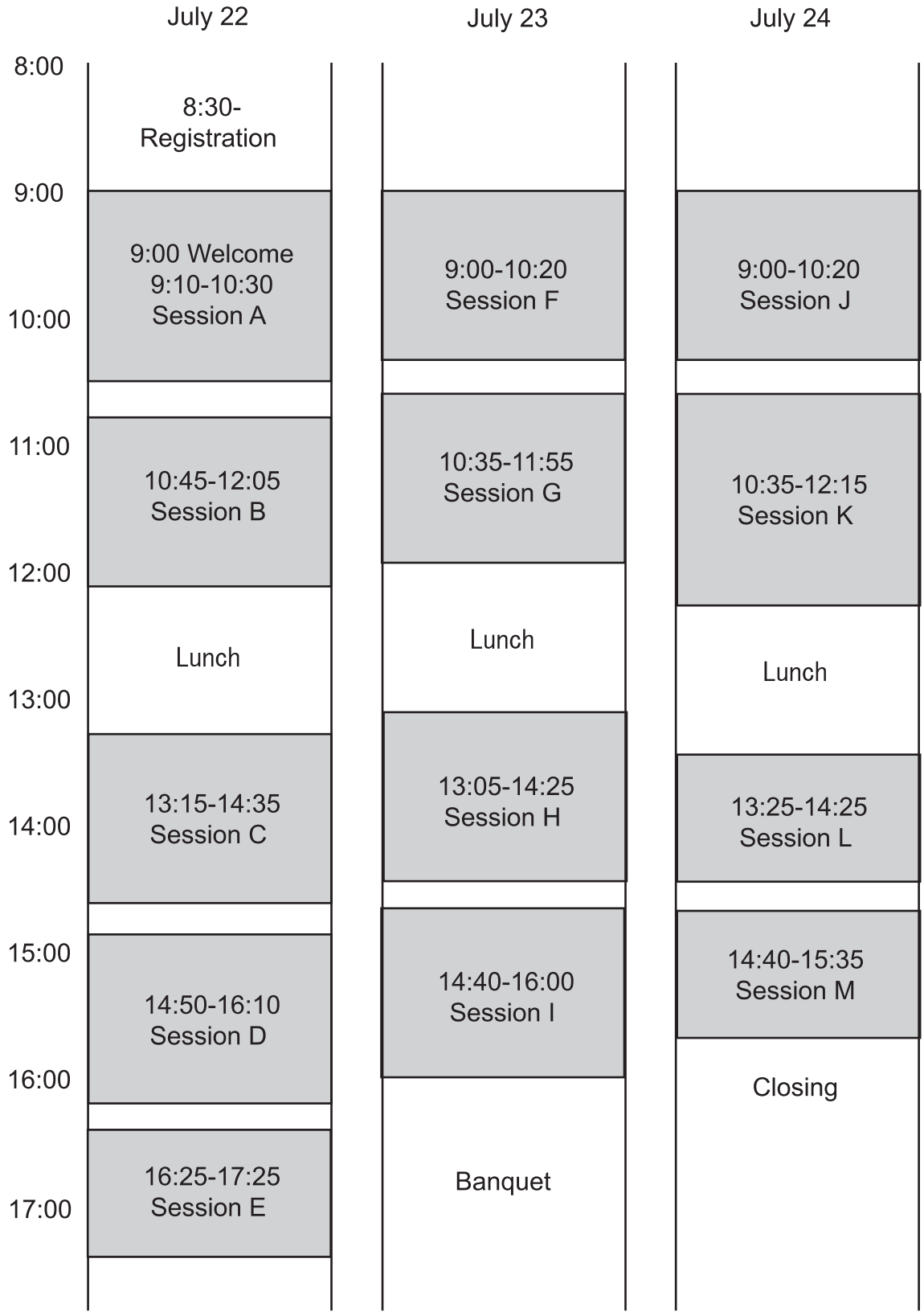
Campus Map



Canteen

University Shop

Time table


July 22
July 23
July 24
8:00
9:00
10:00
11:00
12:00
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14:00
15:00
16:00
17:00
8:30-
Registration
9:00 Welcome
9:10-10:30
Session A
10:45-12:05
Session B
Lunch
13:15-14:35
Session C
14:50-16:10
Session D
16:25-17:25
Session E
9:00-10:20
Session F
10:35-11:55
Session G
Lunch
13:05-14:25
Session H
14:40-16:00
Session I
Banquet
9:00-10:20
Session J
10:35-12:15
Session K
Lunch
13:25-14:25
Session L
14:40-15:35
Session M
Closing

Program

22 July (Mon)

9:00		Welcome
	Session	(Chair: Dr. Masanori Kohyama, AIST)
9:10	A-1	Multi-physics properties in nano-structured ferroelectrics from first-principles
Invited speaker		Takayuki Kitamura, and Takahiro Shimada
9:50	A-2	Origin of dilute ferromagnetism in deficient PbTiO3: A hybrid Hartree-Fock density-functional study
		Takahiro Shimada, Taku Ueda, Jie Wang and Takayuki Kitamura
10:10	A-3	Quantum chemical analysis of electromechanical properties in silicon carbide nanowires
		Koichi Nakamura
10:30		Coffee break
	Session	(Chair: Prof. Yoshitaka Umeno, The Univ. of Tokyo)
10:45	B-1	Theoretical strength under multiaxial loading
Invited speaker		Miroslav Černý
11:25	B-2	First-principles prediction of active slip systems in β-Sn
		Yusuke Kinoshita and Nobutada Ohno
11:45	B-3	Lattice constants and local lattice distortions in 55 Al-based solid solution alloys from first-principles calculations
		Tokuteru Uesugi and Kenji Higashi
12:05		Lunch
	Session	(Chair: Prof. Koichi Nakamura, Kyoto University)
13:15	C-1	Energy density method and Bader Integration for defect energies
Invited speaker		Dallas R. Trinkle, Min Yu, and Richard M. Martin
13:55	C-2	Development of *ab initio* local energy and local stress schemes
		Masanori Kohyama, Yoshinori Shiihara, Shingo Tanaka, and Shoji Ishibashi
14:15	C-3	*Ab initio* local surface eneregy and stress analysis on transition metals
		Yoshinori Shiihara and Masanori Kohyama
14:35		Coffee break
	Session	(Chair: Dr. Takahiro Shimada, Kyoto University)
14:50	D-1	Mechanical properties of Si-doped Fe grain boundaries : *ab initio* study
		Somesh Kr. Bhattacharya, Shingo Tanaka, Yoshinori Shiihara and Masanori Kohyama
15:10	D-2	*Ab initio* local energy and local stress calculations of grain boundaries in Al and Cu
		Hao Wang, Shingo Tanaka, Yoshinori Shiihara and Masanori Kohyama
15:30	D-3	Local stress and local energy distribution in iron/transition metal carbide interfaces using first-principles calculations
		Vikas Sharma, Shingo Tanaka, Yoshinori Shiihara and Masanori Kohyama
15:50	D-4	Local atomic and electronic structures of lithium titanate surface and interfaces
		Shingo Tanaka, Mitsunori Kitta, Tomoyuki Tamura, Yasushi Maeda, Tomoki Akita and Masanori Kohyama
16:10		Coffee break
	Session	(Chair: Prof. Nobuhiro Yoshikawa, The University of Tokyo)
16:25	E-1	Modeling of silica - peptide interactions based on the fragment molecular orbital (FMO) calculations
		Yuji Mochizuki, Kaori Fukuzawa, Yoshio Okiyama, Chiduru Watanabe
16:45	E-2	Application program designed to perform all-electron canonical molecular orbital calculation of macromolecule
		Toshiyuki Hirano, Fumitoshi Sato
17:05	E-3	Hydrogen-enhanced vacancy embrittlement of grain boundaries in iron: First-principles calculations
		Hiroyoshi Momida, Yusuke Asari, Yoshimichi Nakamura, Yoshitaka Tateyama, and Takahisa Ohno

23 July (Tue)		
	Session	(Chair: Prof. Yoshitaka Umeno, The University of Tokyo)
9:00	F-1	Combined theoretical and experimental studies of ductile Mg alloys
Invited talk		M. Friák, S. Sandlöbes, Z. Pei, L.-F. Zhu, A. Dick, J. von Pezold, S. Zaefferer, T. Hickel, S. Yi, D. Letzig, H. W. Sheng, C. P. Race, G. Leyson, B. Svendsen, J. Neugebauer, and D. Raabe
9:40	F-2	First-principles study of twin boundaries and solute atoms in Mg alloys
		Daisuke Matsunaka, Takayoshi Teramoto, and Yoji Shibutani
10:00	F-3	First-principles study of the anisotropic thermal expansion of Mg based on quasi-harmonic approximation
		Kazuki Matsubara, Hajime Kimizuka and Shigenobu Ogata
10:20		Coffee break
	Session	(Chair: Dr. Shingo Tanaka, AIST)
10:35	G-1	First-principles calculations on germanene multilayers under strain
		Florian Gimbert, Yukiko Yamada-Takamura and Taisuke Ozaki
10:55	G-2	The structure of calcium alginate: insights from the molecular modeling studies.
		Wojciech Plazinski and Mateusz Drach
11:15	G-3	Role of grain boundary on band gap in $CuInSe_2$
		H. Yamaguchi, H. Hiramatsu, H. Hosono, and T. Mizoguchi
11:35	G-4	First-principles investigation of possible clustering of noble gas atoms implanted in bcc W
		Tomoyuki Tamura, Ryo Kobayashi, and Shuji Ogata
11:55		Lunch
	Session	(Chair: Dr. Daisuke Matsunaka, Osaka University)
13:05	H-1	Bond order potentials for elements and compounds: The bridge between quantum mechanics of electrons and classical mechanics of atoms
Invited talk		Matous Mrovec, Christian Elsässer and Peter Gumbsch
13:45	H-2	Atomistic modeling of functional materials: Interatomic potential development for metals, oxides and magnetic materials
		Yoshitaka Umeno, Atsushi Kubo and Albert M. Iskandarov
14:05	H-3	Development of interatomic potential for molecular dynamics simulation of Ni/YSZ anode in solid oxide fuel cells
		Albert M. Iskandarov, Atsushi Kubo, and Yoshitaka Umeno
14:25		Coffee break
	Session	(Chair: Dr. Hideki Mori, College of Industrial Technology)
14:40	I-1	Development of interatomic potential for impurity-doped Sn and diffusion analysis
		Atsushi Kubo and Yoshitaka Umeno
15:00	I-2	Analyzing viscosity of refrigerant oil by molecular dynamics simulation
		Shigenori Matsumoto and Taisuke Sugii
15:20	I-3	Negative stiffness of intermetallic compound NiAl nanofilm
		K. A. Bukreeva, A. M. Iskandarov, S. V. Dmitriev, R. R. Mulyukov
15:40	I-4	Molecular mechanics study on the compressive Young's modulus and buckling stress of waved carbon nanotubes
		Masaki Kawachi, Yusuke Kinoshita, and Nobutada Ohno

24 July (Wed)		(Chair: Prof. Kisaragi Yashiro, Kobe University)
	Session	
9:00	J-1	Near-field defects interaction between dislocation and grain boundary
Invited talk		Yoji Shibutani, Tomohito Tsuru, and Tomoyuki Hirouchi
9:40	J-2	Entropic effect on the screw dislocation migration in BCC iron by using free energy gradient method
		Hideki Mori
10:00	J-3	Reaction pathway analysis for the dislocation mobility in 3C-SiC
		Satoshi Izumi, Ryota Muranaka, Jing Yang, Yu Sun, Shotaro Hara and Shinsuke Sakai
10:20		Coffee break
	Session	(Chair: Dr. Tomoyuki Tamura, Nagoya Institute of Technology)
10:35	K-1	Three-dimensional aspects of fracture: Atomistic simulations of crack ? microstructure interactions
Invited talk		Erik Bitzek and Johannes J. Möller
11:15	K-2	Molecular dynamics simulations on telescopic deformation of MWCNT
		Kisaragi Yashiro, Tomohiro Mouri and Yoshitada Isono
11:35	K-3	Atomistic modeling of high strength nanocomposite material
		Shin Yamamoto, Akio Ishii, Yunjiang Wang, and Shigenobu Ogata
11:55	K-4	Molecular dynamics study on atomic elastic stiffness and buckling behavior in carbon nanotubes
		Masaomi Nishimura, Yu Takagi and Masahiro Arai
12:15		Lunch
	Session	(Chair: Dr. Yusuke Kinoshita, Nagoya University)
13:25	L-1	Discrete breathers in crystals with NaCl structure
Invited talk		Sergey V. Dmitriev
14:05	L-2	Stability of nonlinear vibration modes in periodic structure of magnesium
		Yusuke Doi and Akihiro Nakatani
14:25		Coffee break
	Session	(Chair: Dr. Yusuke Doi, Osaka University)
14:40	M-1	Group-theoretical methods in studying discrete breathers in 2D and 3D lattice models
		George Chechin, Petr Goncharov and Stepan Shcherbinin
15:00	M-2	Numerical modeling of mobile discrete breathers in monoatomic 1D lattices
		G.M. Chechin and I. P. Lobzenko
15:15	M-3	Propagation of solitary waves in discrete systems free of the Peierls-Nabarro potential
		Yuri V. Bebikhov and Sergey V. Dmitriev
15:35		Closing