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