Oral Session

Keynote/Invited	Presentation NO	Presentation date	Time to start	Time to finish	Account: First name	Account: Middle name	Account: FAMILY NAME	Account: Affiliation	Abstract title
Chairperson: Yoshiyuki KAWAZOE (Tohoku Univ.)									
Invited	D-5-I24-001	9/24	10:30	11:00	Stefan		ADAMS	National University of Singapore	Ion Transport in Solid Electrolytes from Simulations with Bond-Valence Based Force-Fields
	D-5-O24-002	9/24	11:00	11:15	Ryo		KOBAYASHI	Nagoya Institute of Technology	Monte Carlo Study of Elastic Contribution to Li Migration in Graphite
	D-5-O24-003	9/24	11:15	11:30	Tomoyuki		TAMURA	Nagoya Institute of Technology	First-principles Study of Transition-metal K-edge XANES for Li-rich solid-solution layered cathode material
	D-5-O24-004	9/24	11:30	11:45	Shingo		TANAKA	National Institute of Advanced Industrial Science and Technology	Stoichiometry of (111) surfaces of LiTi2O4 and Li4Ti5O12
	D-5-O24-005	9/24	11:45	12:00	Craig	A. J.	FISHER	Japan Fine Ceramics Center	High-Coincidence Twin Boundaries in Thin Films of Lithium-Ion Battery Cathode Material LiCoO2
Lunch		9/24	12:00	13:30					
Chairperson: Masanori KOHYAMA (AIST)									
Keynote	D-5-K24-006	9/24	13:30	14:15	Jisoon		IHM	Seoul National University	Computational Design and Experimental Synthesis of Hydrogen-storage Nanomaterials
	D-5-O24-007	9/24	14:15	14:30	Yoshiyuki		KAWAZOE	Tohoku University	Predictable Materials Design with Certification
	D-5-O24-008	9/24	14:30	14:45	Koretaka		YUGE	Kyoto University	Modelling configurational energetics on multiple lattices
	D-5-O24-009	9/24	14:45	15:00	Wilfried		WUNDERLICH	Tokai University	Electron-Phonon-Coupling and Work function evaluated by data mining
Coffee Break		9/24	15:00	15:15					
Chairperson: Satoshi WATANABE (Univ. Tokyo)									
Invited	D-5-I24-010	9/24	15:15	15:45	Gour	Prasad	DAS	Indian Association for the Cultivation of Science	First-principles design and functionalization of Graphene-like 2D nanostructures
Invited	D-5-I24-011	9/24	15:45	16:15	Jer-Lai		KUO	Academia Sinica	Water on GaN Surfaces
Chairperson: Masato YOSHIYA (Osaka Univ.)									
Invited	D-5-I24-012	9/24	16:30	17:00	Sugino		OSAMU	The University of Tokyo	Development of a First-Principles Molecular Dynamics Simulation Scheme for Electrochemically Biased Solid-Liquid Interface
	D-5-O24-013	9/24	17:00	17:15	Shusuke		KASAMATSU	The University of Tokyo	Dielectric Response and Capacitance of Nanosized Capacitors
	D-5-O24-014	9/24	17:15	17:30	Tomofumi		TADA	The University of Tokyo	Multiscale investigation with kinetic Monte Carlo and density functional calculations on the Ni/YSZ anode cermet of solid oxide fuel cell
Chairperson: Masanori KOHYAMA (AIST)									
Invited	D-5-I25-001	9/25	10:30	11:00	Taisuke		OZAKI	Japan Advanced Institute of Science and Technology	Massively parallelized O(N) Krylov subspace method for large-scale density functional calculations
Invited	D-5-I25-002	9/25	11:00	11:30	Junichi		IWATA	The University of Tokyo	First-principles electronic structure calculations for 100,000-atom systems with real-space density functional theory code
	D-5-O25-003	9/25	11:30	11:45	Amrita		BHATTACHARYA	Indian Association for the Cultivation of Science	Substrate induced modulation in electronic properties of Silicene
	D-5-O25-004	9/25	11:45	12:00	Yunhao		LU	National University of Singapore	Half-Metallic Molecular Wire on Silicon Surface
Lunch		9/25	12:00	13:30					
Chairperson: Tomofumi TADA (Univ. Tokyo)									
Invited	D-5-I25-005	9/25	13:30	14:00	Seungwu		HAN	Seoul National University	Band structures and scattering mechanism of semiconducting oxides
	D-5-O25-006	9/25	14:00	14:15	Youngho		KANG	Seoul National University	Scattering mechanism in single-crystalline semiconducting oxides
	D-5-O25-007	9/25	14:15	14:30	Shih-kang		LIN	National Cheng Kung University	Ab initio energetics of charge compensating point defects
	D-5-O25-008	9/25	14:30	14:45	Sang Ho		JEON	Seoul National University	First-principles study on the influence of strain on the nature of oxygen vacancy in SnO2
	D-5-O25-009	9/25	14:45	15:00	Kazuaki		TOYOURA	Nagoya University	Proton diffusivity in lanthanum phosphates - A first principles study
Coffee Break		9/25	15:00	15:15					
Chairperson: Craig A.J. FISHER (JFCC)									
Invited	D-5-I25-010	9/25	15:15	15:45	Takeshi		NISHIMATSU	Tohoku University	Molecular dynamics simulations of bulk and thin-film ABO3 perovskite-type ferroelectrics
	D-5-O25-011	9/25	15:45	16:00	Masato		YOSHIYA	Osaka University	Surface Segregation of Point Defects and Resultant Change in Surface Energy of Y2O3 by Ab-Initio Calculations
	D-5-O25-012	9/25	16:00	16:15	Takashi		YAMAMOTO	the University of Tokyo	Defect Formation and Migration in LaAlO3 : A First Principles Study
Chairperson: Shingo TANAKA (AIST)									
Invited	D-5-I25-013	9/25	16:30	17:00	Claude		EDERER	ETH Zurich	Combining first principles electronic structure calculations for transition metal oxides with model approaches
	D-5-O25-014	9/25	17:00	17:15	Hannes		RAEBIGER	Yokohama National University	Spin multiplicity of octahedral cobalt complexes
	D-5-O25-015	9/25	17:15	17:30	Takeshi		FUJITA	Yokohama National University	Tuning of d-d interactions in transition metal (TM) compounds
Chairperson: Fumiyasu OBA (Kyoto Univ.)									
Invited	D-5-I26-001	9/26	9:00	9:30	Shoji		ISHIBASHI	AIST	Electronic structure calculation with two-component relativistic formalism
	D-5-O26-002	9/26	9:30	9:45	Takahiro		SHIMADA	Kyoto University	First-principles Study of Vacancy-induced Ferromagnetism at Non-magnetic Ferroelectric PbTiO3 (001) surfaces
	D-5-O26-003	9/26	9:45	10:00	Bora		LEE	Seoul National University	Hybrid functional studies on d0 and d1 titanates
	D-5-O26-004	9/26	10:00	10:15	Joohwi		LEE	Korea Institute of Science and Technology	Point Defects in Inverse Spinel Zinc Tin Oxide Using DFT+U and Screened Hybrid Functional Approach
Coffee Break		9/26	10:20	10:30					
Chairperson: Shoji ISHIBASHI (AIST)									
Keynote	D-5-K26-005	9/26	10:30	11:15	Georg		KRESSE	University Vienna	The many electron Schroedinger equation: improved descriptions and applications to materials science
	D-5-O26-006	9/26	11:15	11:30	Fumiyasu		OBA	Kyoto Univ.	Doping of Hexagonal and Cubic Boron Nitride
	D-5-O26-007	9/26	11:30	11:45	Kye Yeop		KIM	Department of Materials Science and Engineering, Seoul National University	Local order competition depending on exchange-correlation functional in disordered phases of Ge2Sb2Te5
	D-5-O26-008	9/26	11:45	12:00	Yoshiki		MATSUI	Institute of Industrial Science, the University of Tokyo	Theoretical calculation of carbon-K edge electron energy loss spectrum (EELS) of liquid methanol
Lunch		9/26	12:00	13:30					
Chairperson: Abhijit CHATTERJEE (Accelrys K.K.)									
Invited	D-5-I26-009	9/26	13:30	14:00	Sheng		MENG	Chinese Academy of Sciences	Electron dynamics for renewable energy: applications to organic photovoltaics and water photosplitting
	D-5-O26-010	9/26	14:00	14:15	Marco		CALIFANO	University of Leeds	Efficient Hole Surface Trapping Via Inverse Auger Cooling in CdSe Nanocrystal Quantum Dots
	D-5-O26-011	9/26	14:15	14:30	Masataka		MIZUNO	Osaka University	First-principles Study of Vacancy Formation in Metal Hydrides
Invited	D-5-I26-012	9/26	14:30	15:00	Karsten		REUTER	TU Munich	Beat the heat: Watching phonons getting all excited during O2 dissociation at metal surfaces
Coffee Break		9/26	15:00	15:15					
Chairperson: Takahiro SHIMADA (Kyoto Univ.)									
	D-5-O26-013	9/26	15:15	15:30	Harald		OBERHOFER	Technical University Munich	How do metal clusters split water? Towards a theoretical understanding of co-catalysts for water oxidation.
	D-5-O26-014	9/26	15:30	15:45	Keju		SUN	National Institute of Advanced Industrial Science and Technology	Application of Huckel theory to locate the active sites for O2 activation on gold/oxide catalysts
	D-5-O26-015	9/26	15:45	16:00	Ming		YANG	Department of Physics, National University of Singapore	Graphene oxide: An ideal support for gold cluster based nanocatalysts
	D-5-O26-016	9/26	16:00	16:15	Abhijit		CHATTERJEE	ACCELRYS	ELECTRONIC STRUCTURE PROPERTY CORRELATION FOR ZEOLITE ACIDITY FOR NANO-REACTORS-A QM/MM STUDY
Chairperson: Yuan Ping FENG (Natl Univ. Singapore)									
Invited	D-5-I27-001	9/27	10:30	11:00	Mads		BRANDBYGE	Tech. Univ. of Denmark (DTU)	Transport properties and atomic dynamics of nanoconductors from first principles calculations
	D-5-O27-002	9/27	11:00	11:15	Daisuke		HIRAI	The University of Tokyo	Influence of Defects on AC Response of Metallic Carbon Nanotubes
	D-5-O27-003	9/27	11:15	11:30	Kenji		SASAOKA	The University of Tokyo	Non-Linear AC Response of a Quantum Dot: Non-Equilibrium Green's Function Approach
	D-5-O27-004	9/27	11:30	11:45	Yukihiro		TAKADA	Tokyo University of Science	Multi-Electron Wave Packet Dynamics for Electron Transport in Classical-Quantum Crossover Regions
	D-5-O27-005	9/27	11:45	12:00	Asako		TERASAWA	Queen's University Belfast	Multi-terminal Atomic Waterwheel
Lunch		9/27	12:00	13:30					
Chairperson: Mads BRANDBYGE (Tech. Univ. Denmark)									
Invited	D-5-I27-006	9/27	13:30	14:00	Yuan Ping		FENG	National University of Singapore	Materials and Devices for Spintronics: First Principles Investigations
	D-5-O27-007	9/27	14:00	14:15	Lei		SHEN	Department of physics, National Universit of Singapore, Singapore 117542	Electron Transmission Modes in Electrically Biased Graphene Nanoribbons
Invited	D-5-I27-008	9/27	14:15	14:45	Takahiro		YAMAMOTO	Tokyo University of Science	Heat Transport in Carbon Nanotubes: Non-Equilibrium Green's Function Simulation
	D-5-O27-009	9/27	14:45	15:00	Derek	Ashley	THOMAS	University of Tokyo	Non-equilibrium thermal transport simulation of carbon nano fiber nanostructures
Coffee Break		9/27	15:00	15:15					
Chairperson: Shigenobu OGATA (Osaka Univ.)									
	D-5-O27-010	9/27	15:15	15:30	Atsushi		TOGO	Kyoto University	First-principles Calculations of Phonon linewidths for Rock-salt Type Crystals
	D-5-O27-011	9/27	15:30	15:45	Yohei		MIYAUCHI	Osaka University	Mechanisms behind low lattice thermal conduction of high density of planar defects containing TiO2-x by atomistic simulations
	D-5-O27-012	9/27	15:45	16:00	Tomohiro		KABASHIMA	ITOCHU Techno-Solutions Corporation	Phonon Dynamics at Si/Ge Interface by Molecular Dynamics Simulation
	D-5-O27-013	9/27	16:00	16:15	Yuki		YAKUSHIGAWA	Okayama University	Controlling Acoustic Wave Propagation on Semiconductor Surface : Large-Scale Molecular Dynamics Simulation
Chairperson: Atsushi TOGO (Kyoto Univ.)									
Invited	D-5-O27-014	9/27	16:30	17:00	Shigenobu		OGATA	Osaka University	Modeling and simulation of atomic diffusion and creep deformation
	D-5-O27-015	9/27	17:00	17:15	Akio		ISHII	Graduate School of Engineering Science, Osaka University	Molecular dynamics calculation and geometric analysis reveal the carbon diffusion mechanism in BCC iron dislocation core
	D-5-O27-016	9/27	17:15	17:30	Kazuaki		TAKATA	Okayama University	Stability of Screw Dislocation in Alumina: A Large-scale Molecular Dynamics Study
Chairperson: Tokuteru UESUGI (Osaka Pref. Univ.)									
	D-5-O28-001	9/28	9:00	9:15	Nobufumi		UESHIMA	Osaka University	Role and effectiveness of external magnetic field on variant selection of L10-type ferromagnetic materials: A numerical study by Phase-Field Modeling
	D-5-O28-002	9/28	9:15	9:30	Wolfram	Georg	NOEHRING	Friedrich-Alexander Universitaet Erlangen-Nuernberg	Deformation mechanisms of twinned Au-nanoparticles under uniaxial compression
Invited	D-5-I28-003	9/28	9:30	10:00	Zhongchang		WANG	Tohoku University	Atom-by-Atom Structural and Electronic Analysis of Interfaces and Grain Boundaries in Electronic Ceramics
	D-5-O28-004	9/28	10:00	10:15	Bin		FENG	The University of Tokyo	Atomic structure analysis of CeO2 grain boundary: a combined atomic resolution STEM and ab initio study
Coffee Break		9/28	10:20	10:30					
Chairperson: Zhongchang WANG (Tohoku Univ.)									
	D-5-O28-005	9/28	10:30	10:45	Tatsuya		YOKOI	Osaka University	Atomistic analysis of relationship with dopant and oxygen vacancy grain boundary segregation and ionic conductivity in M2O3-doped ZrO2
	D-5-O28-006	9/28	10:45	11:00	Hideaki		SAWADA	Nippon Steel Corporation	First-principles study of interface structure and energy of Fe/NbC
	D-5-O28-007	9/28	11:00	11:15	Tokuteru		UESUGI	Osaka Prefecture University	Origin of Grain Boundary Energy from First-Principles Calculations
	D-5-O28-008	9/28	11:15	11:30	Masanori		KOHYAMA	National Institute of Advanced Industrial Science and Technology	First-Principles Local-Energy and Local-Stress Calculations by the PAW Method: Applications to Metallic Grain Boundaries
Lunch		9/28	12:00	13:30					

Poster Session

Presentation NO	Presentation date	Time to start	Time to finish	Account: First name	Account: Middle name	Account: FAMILY NAME	Account: Affiliation	Abstract title
D-5-P24-001	9/24	18:00	20:00	Chung-Yuan		REN	National Kaohsiung Normal Univeisty	First-principles study of S=1/2 Kagome antiferromagnet
D-5-P24-002	9/24	18:00	20:00	Takahiro		SHIMADA	Kyoto University	Noncollinear Magnetic Spin-spiral Wave Excitation in Epitaxial Fe(110) Monolayer from First-principles
D-5-P24-003	9/24	18:00	20:00	Bo		XIAO	The University of Tokyo	First-Principle study on the Switching Mechanism of Ta2O5 Atomic Switch
D-5-P24-004	9/24	18:00	20:00	Hikaru		NAKAYAMA	Yokohama National University	Several quasi 1-dimensional Cr atomic chains embedded in (Zn,Cr)Te
D-5-P24-005	9/24	18:00	20:00	Shota		ONO	Yokohama National University	A systematic investigation of electron capture decay rate of 7Be encapsulated in carbon nanostructures
D-5-P24-006	9/24	18:00	20:00	Aron		WALSH	University of Bath	Design and Optimisation of Electronic and Optical Energy Materials
D-5-P24-007	9/24	18:00	20:00	Masahiko		ITAMI	Okayama University	Ab-initio Study of Doping Effect on Optical Response of Graphite Nanotube
D-5-P24-008	9/24	18:00	20:00	Hong		GUANG	Gifu University	First-principles Prediction on Adsorption of Oxygen Molecule onto Defect in Single-layer Graphene
D-5-P24-009	9/24	18:00	20:00	Taishi		KAWANO	The University of Tokyo	Calculation of the electronic structure of graphene on a SiO2 substrate
D-5-P24-010	9/24	18:00	20:00	Masahiko		HIGUCHI	Shinshu University	Relativistic tight-binding approximation method for materials applied by an external magnetic field and its application to silicon with vacancies
D-5-P24-011	9/24	18:00	20:00	Atsushi		KUBO	The University of Tokyo	Development of polarizable interatomic potential for solid oxides
D-5-P24-012	9/24	18:00	20:00	Yasushi		SASAJIMA	Ibaraki University	Computer Simulation of High-Energy-Beam Irradiation of Ceria and Uranium Dioxide
D-5-P24-013	9/24	18:00	20:00	Joohee		LEE	Seoul National University, Seoul 151-744, Korea	DFT+U Calculations on the Point Defects in alpha-Fe2O3
D-5-P24-014	9/24	18:00	20:00	Tsuyoshi		YOSHIOKA	Waseda University	Charge Compensation Mechanism in Pr1-xAxCoO3-d (A=Ca, Sr)
D-5-P24-015	9/24	18:00	20:00	Daisuke		YAMADA	waseda university	Substitution Mechanism of Mn Ions in CaTiO3
D-5-P24-016	9/24	18:00	20:00	Yuta		INABA	Waseda University	Electronic structure analysis of RE1-xAxMnO3-d (RE = La, Pr, A = Ca, Sr, Ba)
D-5-P24-017	9/24	18:00	20:00	Toshiya		KAGAWA	Yokohama National University	First principles calculation of the Schottky barrier height at the GdN:GaN interface
D-5-P24-018	9/24	18:00	20:00	Rachid		BELKADA	Unitee de Developpment des Techniques du Silicium	First-Principles Calculations of Novel Materials for PV Applications
D-5-P24-019	9/24	18:00	20:00	Craig	A. J.	FISHER	Japan Fine Ceramics Center	Surface Structures of Three Polymorphs of Lithium Ion Battery Cathode Material Li2MnSiO4
D-5-P24-020	9/24	18:00	20:00	Renbo		ZHAO	Yonsei University	Surface carbidic structures on Nickel nanocrystals
D-5-P25-021	9/25	18:00	20:00	Masahiro		TADA	Osaka University	Impact of interlayer bonding on lattice thermal conduction in NaxCoO2
D-5-P25-022	9/25	18:00	20:00	Tomohito		TSURU	Japan Atomic Energy Agency	Multiscale computational approach of grain size effect on plastic deformation
D-5-P25-023	9/25	18:00	20:00	Yuito		WATANABE	The University of Tokyo	Vacancy Formation and Diffusion Behaviors in alpha-Al2O3 Grain Boundary: First-Principles and Molecular Dynamics Calculations
D-5-P25-024	9/25	18:00	20:00	Shuhui		LV	Tohoku University	Atomic and Electronic Structure of La2CoMnO6/SrTiO3 Interface from First-principles Calculations
D-5-P25-025	9/25	18:00	20:00	Takafumi		OGAWA	Japan Fine Ceramics Center	Density functional calculations of oxygen-vacancy formation at a sigma13 grain boundary in Y-doped alpha-alumina
D-5-P25-026	9/25	18:00	20:00	Yoshinori		SHIIHARA	The University of Tokyo	Ab initio local stress analysis on GaAs/AlAs interface
D-5-P25-027	9/25	18:00	20:00	Adil	Pozilovich	MUKHTAROV	Institute of Nuclear Physics of Uzbekistan Academy of Sciences	Influence of the Surface Passivation by Hydrogen on Structure and Electronic Properties of Silicon Clusters
D-5-P25-028	9/25	18:00	20:00	Wolfram	Georg	NOEHRING	Friedrich-Alexander Universitaet Erlangen-Nuernberg	Atomic scale analysis of structural instability in nanostructures
D-5-P25-029	9/25	18:00	20:00	Naoya		KIYOKANE	Graduate School of Engineering, Hokkaido University	Modeling of a displacive transformation by four-body approximation within Continuous Displacement Cluster Variation Method
D-5-P25-030	9/25	18:00	20:00	Shotaro		HARA	The University of Tokyo	Atomistic Study on Cation Diffusion of Electrolyte in Solid Oxide Fuel Cell
D-5-P25-031	9/25	18:00	20:00	Kouta		IMAIZUMI	Nagoya University	Theoretical analyses on interstitial oxygen sites in apatite-type oxide-ion conductors
D-5-P25-032	9/25	18:00	20:00	Narumasa		MIYAZAKI	Osaka University	An energy approach of the viscosity and fragility of amourphous alloys
D-5-P25-033	9/25	18:00	20:00	Shuji		OBATA	Tokyo Denki University	Electronic State Calculations of Methane using CI-LCVB Method
D-5-P25-034	9/25	18:00	20:00	Kenji		ISEYA	Graduate School of Engineering, Hokkaido University	A quantitative evaluation of Phase Field microstructure based on the variational principle within the pair approximation of the CVM
D-5-P25-035	9/25	18:00	20:00	Yosuke		YAMAMOTO	Kwansei Gakuin University	Temperature dependency of phase stability for SiC polytypes
D-5-P25-036	9/25	18:00	20:00	Hideki		MORI	College of Industrial Technology	Temperature Dependence of Mobility of Screw Dislocation in BCC Iron
D-5-P25-037	9/25	18:00	20:00	Shigeki		MATSUNAGA	Nagaoka National College of Technology	Dynamical Behavior of Ag+ and Cu+ in Super Ionic AgBr-CuBr
D-5-P25-038	9/25	18:00	20:00	Shigeki		MATSUNAGA	Nagaoka National College of Technology	Molecular Dynamics Simulation in Molten RbAg4I5
D-5-P25-039	9/25	18:00	20:00	Nu	Thi	PHAM	Graduate School of Engineering, Yokohama National University	Adiabatic and non-adiabatic quantum molecular dynamics approaches to chemical reactions
D-5-P25-040	9/25	18:00	20:00	Katsuhiko		HIGUCHI	Hiroshima University	Density functional scheme for superconductors applied by an external magnetic field
D-5-P25-041	9/25	18:00	20:00	Sergio		MEJIA-ROSALES	UANL Fac. de C. Fisico-Matematicas	Molecular Dynamics study of the tensile strain and compression of gold nanowires