Oral Session

Yokohama Port Opening Plaza, Room 1

Entry No	Invited	Presentation	Date	Time to start	Time to finish	Presenter_J (Family)	Presenter_J (First)	Presenter_E (Family)	Presenter_E (First)	Affiliation	Paper Title(E)
座長:クレイグ・フィッシャー/JFCC Chair: Craig A. J. Fisher/JFCC											
10136	**Invited**	**R-O9-001**	**12月9日**	**9:30**	**10:10**	**小林**	**亮**	**KOBAYASHI**	**Ryo**	**NITECH**	**Multiscale simulation of defects in solids**
10474		R-O9-002	12月9日	10:10	10:30	池田	裕治	IKEDA	Yuji	Kyoto University	Calculations of Phonon Dispersions for Paramagnetic Crystals Based on the Spin Space Averaged Method
10065		R-O9-003	12月9日	10:30	10:50	西松	毅	NISHIMATSU	Takeshi	Tohoku University	Fast Molecular-Dynamics Simulations of Dipolar Magnetic Nanoparticles
Break											
座長:チャタジャー・アビジット/Accelrys Chair: Abhijit Chatterjee/Accelrys											
10805		R-O9-004	12月9日	11:00	11:20	福島	鉄也	FUKUSHIMA	Tetsuya	Osaka University	First Principles Calculations of Hubbard U Parameters in Dilute Magnetic Semiconductors
10193		R-O9-005	12月9日	11:20	11:40	竹内	一仁	TAKEUCHI	Kazuhito	Kyoto University	Direct evaluation of free energy for large system through structure integration approach
Break											
座長:大場史康/京都大学 Chair: Fumiyasu Oba/Kyoto University											
10133	**Invited**	**R-O9-006**	**12月9日**	**14:10**	**14:50**	**田中**	**真悟**	**TANAKA**	**Shingo**	**AIST**	**First-Principles Study of Atomic and Electronic Structures and Chemical States of LTO Surfaces and Interfaces**
10015		R-O9-007	12月9日	14:50	15:10	渡邉	学	WATANABE	Manabu	Osaka University	Effect of Interface Energy on γ-Fe Nucleation upon δ/γ Phase Transition of Carbon Steel
10134		R-O9-008	12月9日	14:50	15:10	王	昊	WANG	Hao	AIST	First-Principles Local-Energy and Local-Stress Calculations of Grain Boundaries in Al and Cu: Effects of Impurities
Break											

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座長:田中真悟/AIST **Chair: Shingo TANAKA/AIST**											
10457	**Invited**	**R-O9-009**	**12月9日**	**15:40**	**16:20**	**笠松**	**秀輔**	**KASAMATSU**	**Shusuke**	**University of Tokyo**	**First principles analysis of materials properties modification at metal/oxide interfaces**
10423		R-O9-010	12月9日	16:20	16:40	浦長瀬	正幸	URANAGASE	Masanori	Kyoto University	Thermal Activation Process of Nucleation of a Dislocation Loop in a Magnesium Single Crystal
10451		R-O9-011	12月9日	16:40	17:00	横井	達矢	YOKOI	Tatsuya	Osaka University	Modification of Local oxygen conductivity by Grain Boundary Segregation in Impurity doped ZrO2
Break											
座長:田村友幸/NITECH **Chair: Tomoyuki TAMURA/NITECH**											
10067		R-O9-012	12月9日	17:10	17:30			Sharma	Vikas	AIST	Local Mechanical Properties of Iron-Precipitate Coherent Interfaces Using First-Principles Calculations
10464		R-O9-013	12月9日	17:30	17:50	藤田	武士	FUJITA	Takeshi	Yokohama National University	Transition metal-cluster formation in transition metal doped semiconductors or insulators for n- or p- type doping conditions
10227		R-O9-014	12月9日	17:50	18:10	日沼	洋陽	NINUMA	Yoyo	Kyoto University	Obtaining ionization potentials and band offsets in chalcopyrite and zincblende semiconductors using first principles calculations
座長:笠松 秀輔/東京大学 **Chair: Shunsuke KASAMATSU/University of Tokyo**											
10284		R-O9-015	12月9日	18:10	18:30	藤井	進	FUJII	Susumu	Osaka University	Analysis of Correlation between Interlayer Interaction and Phonon Thermal Conduction in a Layered Cobalt Oxide $Ca_3Co_4O_9$
10076		R-O9-016	12月9日	18:30	18:50	祐村	渥人	YUMURA	Akuto	Osaka University	Systematic Study on the Stability and Property of 2.5-D Layered Oxides by *ab initio* Calculations
10417		R-O9-017	12月9日	18:50	19:10	森	英喜	MORI	Hideki	College of Industrial Technology	Analysis of Mobility of Screw Dislocation in BCC Iron by using Magnetic Bond Order Potential
座長:小林亮/NITECH **Chair: Ryo Kobayashi/NITECH**											
10028	**Invited**	**R-O10-001**	**12月10日**	**9:30**	**10:10**	**中山**	**将伸**	**NAKAYAMA**	**Masanobu**	**Nagoya University**	**Analysis of Charge-Discharge Reactions in Li-Ion Battery Cathode Materials Using First-Principles Calculations and Electrochemical Measurements**

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10488		R-O10-002	12月10日	10:10	10:30	稲吉	輝	INAYOSHI	Akira	NITECH	Li-ion migration in a Li-rich layered cathode material: a first-principles study
10738		R-O10-003	12月10日	10:30	10:50	屋山	巴	YAYAMA	Tomoe	Kyushu University	The dopant effect on hydrogen storage of binary Pd alloy
10481		R-O10-004	12月10日	10:50	11:10	横山	智康	YOKOYAMA	Tomoyasu	Kyoto University	Photovoltaic Conversion Efficiency Simulations of Impurity Doped Cu_2O with an Intermediate Band
10482		R-O10-005	12月10日	11:10	11:30			Chatterjee	Abhijit	Accelrys	Surface reaction over Pt-Ru catalyst for methanol fuel cell – a first principle rationalization
Break											
座長:世古 敦人/京都大学 **Chair: Atsuto Seko/ Kyoto University**											
10408	**Invited**	**R-O10-006**	**12月10日**	**13:00**	**13:40**			**RAEBIGER**	**Hannes**	**Yokohama National University**	**3d transition metal atoms in small molecules and insulators**
10411		R-O10-007	12月10日	13:40	14:00	小谷	岳生	KOTANI	Takao	Tottori University	Quasitparitcle self-consistent GW method implemented in the linearized APW+MTO method
10551		R-O10-008	12月10日	14:00	14:20	服部	達徳	HATTORI	Tatsunori	NITECH	A MD study on helium-induced defect-formation mechanism in tungsten
Break											
座長:レービガー ・ハンネス/横浜国立大学 **Chair: Hannes Raebiger/Yokohama National University**											
10318	**Invited**	**R-O10-009**	**12月10日**	**14:30**	**15:10**	**世古**	**敦人**	**SEKO**	**Atsuto**	**Kyoto University**	**Efficient material exploration based on systematic density-functional calculations and machine learning techniques**
10386		R-O10-010	12月10日	15:10	15:30	東後	篤史	TOGO	Atsushi	Kyoto University	Development of materials-simulation software from an automation viewpoint
10467		R-O10-011	12月10日	15:30	15:50	高橋	亮	TAKAHASHI	Akira	Kyoto University	Accurate Interatomic Potential for Aluminum based on First Principle Calculation and Neural network regression
Break											

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座長:中山将伸/ 名古屋大学 Chair: Masanobu NAKAYAMA/Nagoya Univesity											
10205		R-O10-012	12月10日	16:00	16:20	大脇	創	OHWAKI	Tsukuru	Nissan Motors	An Orbital-Analysis Method for O(N)-DFT Calculation Schemes
10355		R-O10-013	12月10日	16:20	16:40	上杉	徳照	UESUGI	Tokuteru	Osaka Pref. University	Design of Solid Solution Strengthening Based on First-Principles Calculations of Misfit Strain in Aluminum Alloys
10084		R-O10-014	12月10日	16:40	17:00			Bhattacharya	Somesh	AIST	Mechanical properties of FeSi alloys : from the viewpoint of ab initio local energy and local stress
10344		R-O10-015	12月10日	17:00	17:20	田村	友幸	TAMURA	Tomoyuki	NITECH	First-principles investigation of possible clustering of noble gas atoms implanted in bcc W