

MI²I全体会議 ポスターセッション / All researchers meeting Poster session

1月18日 (金) 13:00–15:00 第一会議室 / Jan.18th 13:00–15:00 Meeting Room No.1

Session A 13:00–14:00, Session B 14:00–15:00

Time	No.	Title	Author
Battery Materials Group / 蓄電池材料グループ			
A	BMG01	Battery Materials Group: Activity Report 2018	M. Nakayama, Y. Tateyama, K. Sodeyama
A	BMG02	Efficient Bayes Optimization of Li-ion-conductive Fluorides	M. Nakayama, I. Takeuchi
B	BMG03	DFT fitted Force Field Calculations for Li-ion Diffusion	R. Ward, K. Nakano, Y. Miyaji, R. Kobayashi, M. Nakayama
A	BMG04	Exploration of Possible High Potential Ilmenite Type Na ₁ TMO ₃ (TM=3d, 4d Transition Metals) Cathodes Based on Oxygen Redox Reaction	M. H. N. Assadi, Yoshitaka Tateyama
B	BMG05	Possible high-capacity Si anodes in solid-state batteries	Narumi Ohta and Kazunori Takada
A	BMG06	Descriptors and Machine Learning Techniques for Computational Solid Electrolyte Screening	Randy Jalem, Ichiro Takeuchi, Yoshitaka Tateyama, Masanobu Nakayama
B	BMG07	Investigation of Interface between LiCoO ₂ and Sulfide Electrolyte in Solid-State Battery by CALYPSO Method	Bo Gao, Randy Jalem, Yoshitaka Tateyama
A	BMG08	Machine Learning based Efficient Exploration of Grain Boundary Structures	M. Karasuyama, T. Yonezu, T. Tamura, R. Kobayashi, R. Arakawa, Y. Shiihara, and I. Takeuchi
B	BMG09	Combination of first-principles MD and XANES simulations for LiCoO ₂ -electrolyte interfacial reactions in a LIB	Tomoyuki Tamura
A	BMG10	A machine learning approach for characterizing atomic transport by using Gaussian process and dynamic programming	Kenta Kanamori, Kazuaki Toyoura, Ichiro Takeuchi
B	BMG11	Automatic determination of descriptors for machine-learning force-fields	Ryo KOBAYASHI
A	BMG12	Machine-Learning Prediction for Coordination Energies of Alkali Group Elements to Electrolyte Solvents of Batteries	Atsushi Ishikawa, Keitaro Sodeyama, Yasuhiko Igarashi, Tomofumi Nakayama, Yoshitaka Tateyama, Masato Okada
Magnet Materials Group / 磁石材料グループ			
B	MMG01	Report from Magnet Materials Group	Takashi Miyake and Hiori Kino
A	MMG02	Quantitative estimation of importance of descriptors on Curie temperatures of rare-earth transition metal binary systems	Hiori Kino
Thermal Management Materials Group / 伝熱制御材料グループ			
B	TMMG01	MI Data Strategy for Thermal Management Materials	Yibn XU
A	TMMG02	Reproducibility Evaluation of Thermoelectric Materials	Y. Shinohara, Y. Okamoto

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B	TMMG03	Computational Materials Design Based on Materials Simulations and Informatics	Kenta Hongo
A	TMMG04	Machine-learning-assisted synthesis of Al-Fe-Si thermoelectric materials	Yoshiki Takagiwa, Zhufeng Hou, Yoshikazu Shinohara, Yibin Xu, Koji Tsuda
B	TMMG05	Thermophysical property database of solids for materials informatics	Tetsuya Baba, Erina Fujita, Yibin Xu
A	TMMG06	The novel measurement method of thermal diffusivity from infrared thermal movie	Yoichi Okamoto
B	TMMG07	Interface Design of Thermal Insulating Thin Film by Machine Learning	Yen-Ju Wu, Michiko Sasaki, Masahiro Goto, Lei Fang, Yibin Xu
A	TMMG08	Designing Thermal Functional Materials via Materials Informatics	Shenghong Ju, Atsushi Sakurai, Ryo Yoshida, Koji Tsuda, and Junichiro Shiomi
Data Science Group／データ科学グループ			
B	DSG01	Overview of Data Science Group	Koji Tsuda, Ryo Tamura
A	DSG02	Machine learning-based quantitative odor analysis	Ryo Tamura and Kota Shiba
B	DSG03	Machine Learning Interface/Surface Roughness optimization for Thermal Transport	Shenghong Ju, Thaer M. Dieb, Koji Tsuda Junichiro Shiomi
A	DSG04	Structure determination of catalytic nanomaterials based on genetic algorithm	Toshiaki Taniike
B	DSG05	Roadmap to design functional materials & catalysts for oxidative coupling of methane via data science	Keisuke Takahashi
A	DSG06	Reforming materials database construction and infrastructure via ontology and first-order logic	Lauren Takahashi, Keisuke Takahashi
B	DSG07	Development of unexplored materials by combining DFT calculation, machine learning and experiment	Isao Ohkubo, Zhufeng Hou, Koji Tsuda
A	DSG08	Crystal Structure Prediction by Data Assimilation	Synge Todo
B	DSG09	Development and Application of Computational Methods for Data-Driven Exploration of Electronic Materials	Fumiyasu Oba
A	DSG10	How to cope with the heterogeneity of data sets in inorganic materials science?	Yuzuru Tanaka
B	DSG11	Exploratory Visual Analytics Platform with Multiple Coordinated Views for Materials Informatics	Jun Fujima
A	DSG12	Correlation between local structures and positron annihilation parameters for vacancy clusters in nitride semiconductor alloys	S. Ishibashi, A. Uedono, H. Kino, T. Miyake, and K. Terakura
B	DSG13	Construction of neural network potential to analyze ion migration and phonon behaviors	Satoshi Watanabe
A	DSG14	Sparse modeling of EXAFS	Y. IGARASHI, K. IWAMITSU, T. OKAJIMA, I. AKAI and M. OKADA

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Time	No.	Title	Author
B	DSG15	A Framework for Generating Descriptors to Represent Crystalline Materials	Van-Doan Nguyen, Tien-Lam Pham, and Hieu-Chi Dam
A	DSG16	Critical role of the descriptors in IMFP found by machine learning approach	Xun Liu, Zhufeng Hou, Bo Da, Hideki Yoshikawa, Shigeo Tanuma and Zejun Ding
B	DSG17	Electron spectroscopy study on carbon materials of HOPG, Diamond, Carbon Glassy and Fiber	Lu Dabao, Da Bo, Hideki Yoshikawa, Shigeo Tanuma, Goto Keisuke and Zejun Ding
Re-entrusted institute / 再委託先			
A	REI01	Transfer learning: a key driver to accelerated materials discovery with machine learning	Hironao Yamada, Chang Liu, Stephen Wu, Ryo Yoshida
Topological Analysis Group / トポロジカル解析グループ			
A	TAG01	Overview of Topological Analysis Team	Kazuto Akagi
B	TAG02	Feature extraction from observed microscopic images	Kazuto Akagi
A	TAG03	Origin of the mixed alkali effect in the silicate glass	Yohei Onodera, Yasuyuki Takimoto, Hiroyuki Hijiya, Taketoshi Taniguchi, Shingo Urata, Seiji Inaba, Sanae Fujita and Shinji Kohara
B	TAG04	Topological order in amorphous InGaZnO ₄	S. Tahara, S. Kohara, Y. Onodera, L. S. R. Kumara, A. Yang, C. Song, K. Ohara, H. Tajiri, T. Ina, Jens R. Stellhorn, S. Hosokawa, I. Obayashi, Y. Hiraoka, K. Ishikawa, H. Hiramatsu, H. Hosono, T. Kamiya, and O. Sakata
A	TAG05	Network modification in binary vanadium phosphate glass revealed by data driven structure modelling	Y. Onodera, S. Kohara, T. Aoyagi, T. Naito, M. Kodama, T. Onodera, D. Takamatsu, S. Tahara, O. Sakata, T. Miyake, K. Suzuya, K. Ohara, T. Usuki, Y. Hayashi, H. Takizawa
B	TAG06	Topological analysis of magnetic domain structures based on persistent homology	Masato Kotsugi
A	TAG07	Topological analysis of grain boundary structure	F. Ogushi, K. Inoue, Y. Hiraoka and K. Akagi
B	TAG08	Synergic collaboration of quantum beam measurements, modelling, and mathematics to unravel liquid matter: towards a collaboration with microgravity in space	A. Masuno, S. Kohara, Y. Onodera, I. Obayashi, S. Tahara, Y. Hiraoka, T. Ishikawa, C. Koyama
Materials Exploration Group / マテリアルズ探索グループ			
A	MEG01	Research Activity in Materials Exploration Group	Tamio Oguchi and Koji Nakamura
B	MEG02	Database of Gibbs energy, derived quantities, and phase diagrams for data science	Taichi ABE
A	MEG03	Exploration for paraelectric materials with high dielectric constant in collaboration with company	Hiroki Moriwake, Hiroyuki Hayashi, Ayako Taguchi, Isao Tanaka

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B	MEG04	First-Principles Calculations of Solid Solution States in Mixed-Anion Compounds	Kazuki Shitara, Ayako Taguchi, Akihide Kuwabara
A	MEG05	Analysis of atomic-layer alignment dependence of magnetic properties of thin films	K. Nakamura
B	MEG06	Development of Crystal Structure Prediction Tool	Tomoki Yamashita, Shinichi Kanehira, Nobuya Sato, Hiori Kino, Koji Tsuda, Takashi Miyake, and Tamio Oguchi
A	MEG07	Development of linearly independent descriptor generation method for empirical law discovery	Hitoshi Fujii, Tetsuya Fukushima, and Tamio Oguchi
B	MEG08	Electric field effects in magnetic metal ultrathin films	Y. Suzuki, J. Cho, S. Miwa, K. Yakushiji, H. Kubota, A. Fukushima, S. Yuasa, and C.-Y. You
A	MEG09	A new understanding of complex carbides formation in creep resistant chromium steels	R. Sahara, M. Souissi, T. Matsunaga, M. H. F. Sluiter, M. Tabuchi and M J. Mills
Materials Descriptor Platform Group / 物質・材料記述基盤グループ			
B	MDPG01	Activity Summary of the Materials Descriptor Platform group	Liu, C., Koyama, Y., and Yoshida, R.
A	MDPG02	XenonPy: Python Library for Materials Informatics	C. Liu, R. Yoshida, Y. Koyama
Data Platform Group / データプラットフォームグループ			
A	DPFG01	Data Platform Group	Yibin XU, Junko HOSOYA, Isao KUWAJIMA, Yuta SAKAIRI, Hiroyuki YAMASATO, and Toshinori IZUMI
B	DPFG02	Fee-based Inorganic Materials Database "AtomWork-adv"	Yibin XU, Junko HOSOYA, Isao KUWAJIMA, Yuta SAKAIRI
A	DPFG03	Specific Heat Prediction on Web	Yibin XU, Yuta SAKAIRI, Toshinori IZUMI, Testuya BABA and Erina FUJITA
B	DPFG04	Linking Materials Information: Substance Dictionary & Material Record Format	Yibin XU and Yuta SAKAIRI
A	DPFG05	The Recent Progress of CompES-X Database and its Application	Zhufeng HOU, Yibin XU, Junko HOSOYA, Ryo MATSUMOTO, Kiyoyuki TERAURA, and Yoshihiko TAKANO
Cooperation Organization / 連携協定			

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B	CO01	Hyogo-Prefectural Initiatives to Address Industrial Utilization of Synchrotron Radiation and Materials Informatics	Scientific Advancement Division, Hyogo Prefectural Government, Synchrotron Radiation Nanotechnology Center, University of Hyogo, Center for Materials Research by Information Integration, Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science
A	CO02	The application study of machine learning to XANES data analysis: A case of Nickel metal hydride rechargeable batteries	Shuuichi Doi, Lei Li, Soichi Nose, Naoki Fukuyama, Tamio Oguchi
B	CO03	MI2 approach to modelling Aluminum corrosion using synchrotron measurement	Takahiro Ozawa, Shintaro Yamamoto, Yuya Takara, Motoki Sudou, Masashi Yoshimura, soichi Nose, Tomoki Yamamoto, Yuta Kajio, Kazushi Yokoyama, Hitoshi Fujii, amio Oguchi, Naoki Fukuyama
Consortium WWG / コンソーシアム			
B	CWWG01	Practice of machine learning	Workflow WG members Norio Tomotsu