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Group A 2月19日（水）12：30－13：30 中会議室 1 ～ 4

Group B 2月20日（木）12：30－13：30 中会議室 1 ～ 4

Group	No.	Title	Author
Battery Materials Group／蓄電池材料グループ			
A	BMG01	Activity report of Battery Materials Group, FY2019	M. Nakayama, Y. Tateyama, K. Sodeyama
B	BMG02	Machine-learning Algorithms for Efficient Exploration of Interface Structures	Masayuki Karasuyama, Tomohiro Yonezu, Tomoyuki Tamura, and Ichiro Takeuchi
A	BMG03	Liquid electrolyte informatics for secondary batteries	Keitaro Sodeyama
B	BMG04	High-throughput construction of force-fields for solid state electrolyte materials	Ryo KOBAYASHI, Y. Miyaji, K. Nakano, M. Nakayama
A	BMG05	Search for oxide-based solid electrolytes	Kazunori Takada
B	BMG06	Li+ Transport Mechanism at the Heterogeneous Cathode/Solid Electrolyte Interface in an All-Solid-State Battery via the First- Principles Structure Prediction Scheme	GAO BO, Randy Jalem, Yanming Ma, Yoshitaka Tateyama
A	BMG07	Investigating the effects of local chemistry on diffusion in Spinels; simulating cooperative diffusion in MgAl2O4	Robyn E. Ward, Masanobu Nakayama
B	BMG08	Machine learning prediction of coordination energies for alkali group elements in battery electrolyte solvents	Atsushi Ishikawa, Keitaro Sodeyama, Yasuhiko Igarashi, Tomofumi Nakayama, Yoshitaka Tateyama and Masato Okada
A	BMG09	Active-learning-based efficient prediction of ab initio atomic energy	Tomoyuki Tamura, Masayuki Karasuyama
B	BMG10	Bayesian Optimization Technology for Efficient Battery Material Discovery	Ichiro Takeuchi, Kosei Sato, Kenta Kanamori, Yu Inatsu, Kazuaki Toyoura, Masanobu Nakayama
Magnet Materials Group／磁石材料グループ			
A	MMG01	Magnet Materials Group	Takashi Miyake and Hiori Kino
B	MMG02	Automation of the first-principles calculation to search functional materials in high entropy alloys	Hiori Kino
A	MMG03	Structuring knowledge — Case study for magnetic materials	Riichiro Mizoguchi and Hiori Kino
B	MMG04	Estimation of materials parameters based on the information from microstructure	Toshiyuki Koyama、Shun Suzuki、Daiki Kato、Yuhki Tsukada
Thermal Management Materials Group／伝熱制御材料グループ			
A	TMMG01	Progresses in thermal management materials accelerated by MI	Yibn XU
B	TMMG02	Corelation between Thermoelectric Properties of Si-Au Thin Films and Process Parameters	Yoshikazu Shinohara
A	TMMG03	Ultra-narrowband wavelength-selective thermal emitter with multilayered metamaterials designed by Bayesian optimization	Atsushi Sakurai, Kyohei Yada, Tetsushi Simomura, Shenghong Ju, Makoto Kashiwagi, Hideyuki Okada, Tadaaki Nagao, Koji Tsuda, Junichiro Shiomi
B	TMMG04	Designing Thermal Function Materials via Materials Informatics	Yuxuan Liao, Shenghong Ju, Atsushi Sakurai, Ryo Yoshida, Koji Tsuda, and Junichiro Shiomi

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Group	No.	Title	Author
A	TMMG05	High-Throughput Screening of Novel Functional Thin Films by Combinatorial Sputter Coating System (COSCOS).	Masahiro Goto, Sasaki Michiko, Yibn XU
B	TMMG06	Combinatorial Gradient Material Screening	Sasaki Michiko, Yibn XU, Masahiro Goto
A	TMMG07	Machine Learning Assisted Synthesis of Fe-Al-Si Thermoelectric Material (FAST)	Yoshiki Takagiwa, Zhufeng Hou, Yoshikazu Shinohara, Yibin Xu, Koji Tsuda
B	TMMG08	Thermal Management and Development of Composite Thin Films by Material Informatics	Yen-Ju Wu, Yibin Xu, Michiko Sasaki, Masahiro Goto
A	TMMG09	The summary of the our themes in the past five years 1. New absolute measurement method for thermal conductivity 2. New production method of nanodots	Yoichi Okamoto,
B	TMMG10	Development of thermophysical property database for materials informatics	Tetsuya Baba,
A	TMMG11	Data driven approach to materials design for high thermal conductivity materials	Kenta Hongo,
B	TMMG12	Preparation of Processable High Thermal Conductive Polyimide films	Yuka Tamao, Masa-aki Kakimoto, Stephen Wu, Ryo Yoshida, Yibin Xu and Junko Morikawa
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	Phase diagram construction by machine learning	Ryo Tamura, Kei Terayama and Koji Tsuda
B	DSG03	Structure determination of catalytic nanomaterials based on genetic algorithm	Toshiaki Taniike
A	DSG04	Development and Application of Computational Methods for Data-Driven Exploration of Electronic Materials	Fumiyasu Oba, Akira Takahashi, Yu Kumagai
B	DSG05	Construction of neural network potential to examine complicated systems and phenomena	Satoshi Watanabe
A	DSG06	Media Platform for Materials Informatics	Jun Fujima
B	DSG07	Development of unexplored materials by combining DFT calculation, machine learning and experiment	Isao Ohkubo, Zhufeng Hou, Koji Tsuda
A	DSG08	Correlation analysis of local quantities in disordered alloys	Shoji Ishibashi
B	DSG09	Objective and Rapid Crystal Structure Analysis by Integration of Measurement Informatics and Database	Masashi Ishii, Testuya Ozawa
A	DSG10	Symmetry-based segmentation of heterogeneous data sets of inorganic crystal materials into homogeneous ones for better regression	Yuzuru Tanaka, Jun Fujima, Keisuke Takahashi
B	DSG11	Data science application for exploration of 2D magnets, analysis on XAS, and identification of OCM reaction	Itsuki Miyazato, Keisuke Takahashi
A	DSG12	Development of a linear-scaling DFT code and machine-learning forces	Tsuyoshi Miyazaki, Ryo Tamura
B	DSG13	Sparse modeling for a data-driven approach in material sciences	Yasuhiko Igarashi,
A	DSG14	Sparse phase retrieval algorithm for coherent x-ray diffraction imaging	Yuichi Yamasaki, Y. Yokoyama, T. Arima, and M. Okada

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Group	No.	Title	Author
B	DSG15	Monte Carlo tree search for materials design	Dieb Sae, Tsuda Koji
A	DSG16	Ontology and Materials Informatics: Scientists' Cognitive Representation and Standardization of Materials Data and Knowledge	Lauren Nicole Takahashi,
B	DSG17	Materials and Catalyst Informatics: Searching for Novel Materials and Catalysts	Keisuke Takahashi
A	DSG18	Data-driven spectral analysis method in electron-beam based techniques	Da Bo, J.W. Liu, H. Yoshikawa, and S. Tanuma
B	DSG19	Automated generation of reconstructed nonpolar stoichiometric slab models	Yoyo Hinuma, Takashi Kamachi, and Nobutsugu Hamamoto
A	DSG20	Development of explainable material informatics core technologies	Dam Hieu-Chi, Hiori Kino, Takashi Miyake, and Kiyoyuki Terakura
B	DSG21	MateriApps - A Portal to Materials Science Simulation	Synge Todo
	Topological Analysis Group／トポロジカル解析グループ		
A	TAG01	Overview of Topological Analysis Team	Kazuto Akagi, Shinji Kohara, Yasuaki Hiraoka
B	TAG02	Topological data analysis of magnetic domain structure	Masato Kotsugi, Yohei Onodera, Shinji Kohara, Shuta Tahara, Motoki, Shiga, Akihiko Hirata, Ippei Obayashi, Yasuaki Hiraoka, Osami Sakata
A	TAG03	Understanding diffraction patterns of glassy, liquid and amorphous materials via persistent homology analyses	Atsunobu Masuno
A	TAG04	Very sharp diffraction peak in liquid Er2O3 with crystal-like homology	Shuta Tahara, Yohei Onodera, Shinji Kohara, Atsunobu Masuno, Ippei Obayashi, Yasuaki Hiraoka, Osami Sakata
A	TAG05	Origin of mixed alkali effect in silicate glass	Yohei Onodera, Ippei Obayashi, Yasuaki Hiraoka, Shinji Kohara
A	TAG06	Ring persistency in permanently densified silica glass	Shinji Kohara, Motoki, Shiga, Yohei Onodera, Akihiko Hirata, Ippei Obayashi, Yasuaki Hiraoka
B	TAG07	Topological data analysis of Grain Boundary structures	Fumiko Ogushi, Kazutoshi Inoue, Yasuaki Hiraoka, and Kazuto Akagi
	Materials Exploration Group／マテリアルズ探索グループ		
B	MEG01	Research Activity in Materials Exploration Group	Tamio Oguchi and Koji Nakamura
A	MEG02	Development of Crystal Structure Prediction Method	Tomoki Yamashita, Shinichi Kanehira, Nobuya Sato, Hiori Kino, Koji Tsuda, Takashi Miyake, Tamio Oguchi
B	MEG03	Data analysis and prediction of structural and magnetic properties in metal multilayer films	Kohji Nakamura
A	MEG04	First-principles calculations on the thermodynamic stability of High Entropy Alloy	Masanori Enoki, Hiroshi Ohtani
B	MEG05	Machine learning potential and structure optimization	Atsuto Seko
A	MEG06	Accurately predicting grain boundary thermal conductivities in MgO from local atomic structures	Susumu Fujii, Tatsuya Yokoi, Craig A. J. Fisher, Hiroki

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Group	No.	Title	Author
B	MEG07	Recommender system of processing conditions for inorganic compounds based on a parallel	Hiroyuki Hayashi, Atsuto Seko, Isao Tanaka
A	MEG08	Experimental search for perpendicular magnetic anisotropy heterostructures	Seiji Mitani
B	MEG09	MLCC material exploration with private company	HIROKI MORIWAKE, Hiroki MORIWAKE, Hiroyuki HAYASHI, Isao TANAKA
A	MEG10	CALPHAD thermodynamics prepared for open science	TAICHI ABE
B	MEG11	Solid States in Mixed Anion Compounds: A First-Principles Study	SHITARA Kazuki
A	MEG12	Voltage control of magnetism	Yoshishige Suzuki
	Materials Descriptor Platform Group／物質・材料記述基盤グループ		
A	MDPG01	XenonPy: Python Platform for Materials Informatics	Liu, C., Koyama,Y., and Yoshida, R.
B	MDPG02	Machine Learning of Crystal Growth Simulation	Yukinori Koyama
A	MDPG03	SPACIER: designing molecules using iQSPR coupled with first-principles calculation	Liu Chang, Yoh, Noguchi, Wu, Stephen, Ryo, Yoshida
B	MDPG04	iQSPR in XenonPy: a Bayesian molecular design algorithm and its application to polymer design	Stephen Wu, Yoh Noguchi, Wu Stephen, Ryo Yoshida, Chang Liu, Hironao Yamada, Yoh Noguchi, Guillaume Lambard, Ryo Yoshida
	Data Platform Group／データプラットフォームグループ		
B	DPFG01	MI2I data infrastructure	Yibin XU, Junko Hosoya, Yuta Sakairi, Hiroyuki Yamasato
A	DPFG02	Report of Mi2i Data Platform	Hiroyuki Yamasato, Junko Hosoya, Isao Kuwajima, Yuta Sakairi, Yibin Xu
B	DPFG03	Inorganic Materials Database "AtomWork-Adv"	Yuta Sakairi, Yibin Xu, Junko Hosoya, Isao Kuwajima
A	DPFG04	Specific Heat Prediction On Web	Yuta Sakairi, Yibin XU, Tetsuya BABA, Erina FUJITA
B	DPFG05	Template Oriented Atomic Simulation Toolkit (TOAST): A python-based automatic framework for high-throughput electronic structure calculations	Junko Hosoya, Masao Arai, Nobutaka Nishikawa, Isao Kuwajima and Yibin Xu
	Cooperation Organization, Consoritium WWG, MaDIS／連携, コンソーシアム, MaDIS		
A	CO01	データ駆動材料開発パートナーシップ	Uchibori Chihiro
B	CO02	Intellectual property issues in Materials Informatics	TAKADA Masahide
A	CO03	MI2 approach to modeling atmospheric corrosion of steel using synchrotron measurement	小澤 敬祐, 山本 慎太郎, 漆原 良昌, 芦 聡,李 雷, 横山 和司, 高山 裕貴, 福山 直樹
B	CO04	Automatic translation of measurement data on materials data platform: M-DaC (Materials Data Conversion Tools)	Mineharu Suzuki, Hiroko Nagao, Shigeyuki Matsunami, and Hideki Yoshikawa

都合により発表はありません。

※ポスター発表は予告なく変更される場合があります。 V11