

AMDS 2024 Program

Plenary Session

2024.11.14

| Time | Speaker | Affiliation | Presentation Title |
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| Opening Ceremony (15:30-16:00) | | | |
| Plenary Session Chairs: Prof. Tongyi Zhang, Dr. Yibin Xu | | | |
| 16:00 -16:30 | Yong-hak Huh | The Korea Research Institute of Standards and Science, Korea | Issues and Strategies for Materials Data Sharing |
| 16:30-17:00 | Satoshi Minamoto | National Institute for Materials Science, Japan | Operation of Materials Data Platform in NIMS |
| 17:00-17:30 | Peng Wang | Chinese Society for Testing & Materials, China | Construction of the (CSTM) Material Data Standard System |
| 17:30-18:00 | Heiko B. Weber | University of Erlangen-Nuremberg, Germany | Experimental Research Data in Materials Science and Solid-State Physics: Challenges, Strategies and Solutions |

Symposium: Materials Data Management and Image Data

Convenors: Prof Haiqing Yin, Prof Xuejing Shen, Prof Dawei Zhang

2024.11.15

| Time | Speaker | Affiliation | Presentation Title |
|---|-----------------|---|--|
| Materials Data Management (1) Chairs: Prof. Hong Wang, Dr. Kwang-Ryeol Lee | | | |
| 8:30-9:00 | Kwang-Ryeol Lee | Korea Institute of Science and Technology, Korea | Standardization of Materials R&D Data Scheme and Vocabulary |
| 9:00-9:25 | Hong Wang | Shanghai Jiao Tong University, China | The standard system for AI ready materials data |
| 9:25-9:50 | Yi Zhang | China National Building Materials Group Co, Ltd., China | Exploration and application of digital transformation in the inorganic non-metallic materials industry |
| 9:50-10:15 | Takuya Kadohira | National Institute for Materials Science, Japan | Management of experimental data in NIMS |
| Coffee break | | | |
| Materials Data Management (2) Chairs: Prof. Lanting Zhang, Prof. Siqi Shi | | | |
| 10:35-11:00 | Siqi Shi | Shanghai University, China | Constructing high-performance Machine Learning Models depends on high-quality materials data |
| 11:00-11:25 | Isao Kuwajima | National Institute for Materials Science, Japan | Data collection and retrieval system in NIMS |

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| 11:25-11:50 | Lanting Zhang | Shanghai Jiao Tong University, China | Some key considerations on materials data ecology in the context of large models |
| 11:50:12:10 | Zhigang Yu | Shanghai University, China | An unbiased recommendation framework mining the optimal combination of data subsets and algorithms |
| Luncheon | | | |
| Materials Data Management (3) Chairs: Dr. Lingling Ren, Prof. Jie He | | | |
| 13:30-14:00 | Lingling Ren | Materials measurement laboratory, National Institute of Metrology of China | Metrology and traceability of materials big data |
| 14:00-14:25 | Cheng Xu | University of Science and Technology Beijing, China | Toward Collaborative Intelligence: Secure Big-data Sharing and Computing in Materials Genomics Engineering |
| 14:25-14:50 | Xing Wu | Shanghai University, China | A Spatial-frequency Domain-based image Noise Suppression Model and Application in Silicon Chip Defect Detection |
| 14:50-15:15 | Xingjian Huang | Huawei Technologies Co. LTD | Ecological construction practices for industrial software simulation materials data |
| 15:15-15:35 | Jie He | University of Science and Technology Beijing, China | MGED-Assistant: Smart Material Database Powered by LLM |
| Coffee break | | | |
| Materials Image Data Chairs: Dr. Jaimyun Jung, Prof. Xiaojuan Ban | | | |
| 15:55-16:25 | Jaimyun Jung | Korea Institute of Materials Science, Korea | Inverse design of 3D microstructures using latent diffusion model |
| 16:25-16:50 | Xiaojuan Ban | University of Science and Technology Beijing, China | An approach to efficiently extracting microstructures via visual large model |
| 16:50-17:15 | Sangil Hyun | Korea Institute of Ceramic Engineering and Technology, Korea | Virtual characterization models developed by multiphysics computer simulation & data-driven AI for ceramic manufacturing process |
| 17:15-17:40 | Yuxing Han | Shanghai University, China | Research on Machine Learning Methods for Mining Material Properties from Material Images |
| 17:40-18:00 | Jianfeng Jin | Northeastern University, China | A Web-based System for Automated Microstructure Recognition and Mechanical Properties Prediction of Polycrystalline Alloys |
| 18:00-18:20 | Weiho Wan | The NCS Testing Technology Co., Ltd, China | A high-throughput statistical mapping characterization method for microstructure based on multi-element coupling |

Symposium: Data Driven Materials Design

Convenors: Prof Haiqing Yin, Prof Woo Jin CHOI, Prof Wei Ren
2024.11.15

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|---|---------|-------------|--------------------|
| Materials Calculation and Data Chairs: Prof. Lei Shen, Prof. Yong Du | | | |

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| 8:30-9:00 | Seungwu Han | Seoul National University, Korea | SevenNet: a pretrained universal machine learning force fields |
| 9:00-9:25 | Yong Du | Central South University, China | Intelligent design of Al alloy by integrating CALPHAD, machine learning and key experiments |
| 9:25-9:50 | Lei Shen | National University of Singapore, Singapore | High-throughput calculations of 2D heterostructures |
| 9:50-10:15 | In Kim | Korea Institute of Ceramic Engineering and Technology, Korea | Advancing the Development of Polymer Composites through Artificial Intelligence |
| Coffee break | | | |
| Data-driven Materials Design (1) Chairs: Dr. Yibin Xu, Dr. Jungho Shin | | | |
| 10:35-11:00 | Yibin Xu | National Institute for Materials Science, Japan | Data-driven Exploration for Li Ionic Conductor |
| 11:00-11:25 | Jungho Shin | Korea Research Institute of Chemical Technology, Korea | Web-based Interface for Search and Analysis of Materials Data: ChemDX and MatDX |
| 11:25-11:50 | Zhe Liu | Northwestern Polytechnical University, China | Design and Screening of Functional Organic Molecules for Perovskite Solar Cells via Machine Learning |
| 11:50-12:10 | Heechae Choi | Xi'an Jiaotong-Liverpool University, China | TBD |
| Luncheon | | | |
| Data-driven Materials Design (2) Chairs: Dr. Ho Won Lee, Dr. Guojun Wang, Prof. Deng Pan | | | |
| 13:30-14:00 | Ho Won Lee | Korea Institute of Materials Science, Korea | Overcoming Small Dataset Challenges in Semantic Segmentation of Metallographic Microscopy Images |
| 14:00-14:25 | Guojun Wang | Chinalco Materials Application Research Institute Co., Ltd, China | Design and development of high performance aluminum alloy based on integrated computing and machine learning |
| 14:25-14:50 | Xiaodong Xiang | Southern University of Science and Technology | New AI Algorithm for Materials Science |
| 14:50-15:15 | Deng Pan | Shanghai University, China | KAN Made Learning Physics Laws Simple |
| 15:15-15:35 | Song Sun | Anhui University, China | Material Genome Engineering in Catalysis |
| Coffee break | | | |
| Data-driven Materials Design (3) Chairs: Dr. Sehyeok Oh, Prof. Yi Liu | | | |
| 15:55-16:25 | Sehyeok Oh | Korea Institute of Materials Science, Korea | Innovative Applications of AI to Mechanical /Materials Processing |
| 16:25-16:50 | Yi Liu | Shanghai University | "What you need is pre-attention": Small-data machine learning with center-environment features |
| 16:50-17:15 | Hoheok Kim | Korea Institute of Materials Science, Korea | Deep learning application for modeling the heat treatment condition-microstructure-property relationship |

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| 17:15-17:40 | Haiqing Yin | University of Science and Technology Beijing, China | Screening strategy for refractory high-entropy alloys |
| 17:40-18:00 | Yuan Tian | Shanghai University, China | Noise-aware active learning to develop high-temperature shape memory alloys with large latent heat |
| 18:00-18:20 | Haiyou Huang | University of Science and Technology Beijing, China | Finding New High-Temperature Superconductors Based on Crystal Graph Neural Networks |

FMGE-AMDS Joint Symposium: Materials Big Data and AI for Science

Convenors: Prof Yanjing Su, Prof. Dezhen Xue, Prof Yi Wang

2024.11.15

| Time | Speaker | Affiliation | Presentation Title |
|--|---------------|---|--|
| AI Algorithm for Materials(1) Chairs: Prof. Xiang Chen, Prof. Xiaoyu Chong | | | |
| 8:30-8:55 | Turab Lookman | AiMaterials Research, LLC | How can theory guide data science? |
| 8:55-9:20 | Alex Ganose | Imperial College London, UK | Computational Materials Discovery in the Age of Automation |
| 9:20-9:45 | Xiang Chen | Tsinghua University, China | Artificial Intelligence Design of Lithium Battery Electrolytes |
| 9:45-10:10 | Jiayu Peng | University at Buffalo, USA | Bridging physics-informed and data-driven materials designs to catalyze deep decarbonization |
| Coffee break | | | |
| AI Algorithm for Materials(2) Chairs: Prof. Huadong Fu, Prof. Yi Wang | | | |
| 10:25 -10:55 | Hongming Weng | Institute of Physics, Chinese Academy of Sciences, China | Data Resource Construction for Condensed matter quantum material science and AI empowerment |
| 10:50-11:15 | Yue Li | The Max Planck Institute for Sustainable Materials, Germany | Artificial intelligence-enhanced atom probe microscopy: Local chemical ordering analysis |
| 11:15-11:40 | Shanshan Wang | National University of Defense Technology, China | Machine learning empowered material atomic structural understanding |
| 11:40-12:05 | Jie Xiong | Shanghai University, China | Domain Knowledge Embedded Materials Data Mining |
| Luncheon | | | |
| Large Language Models for Materials Chairs: Prof. Dezhen Xue, Prof. Yicong Ye | | | |
| 13:30-13:55 | Tongqi Wen | The University of Hong Kong, China | Small and Large Atomic/Language Models for Materials Science |
| 13:55-14:20 | Yicong Ye | National University of Defense Technology, China | MatPilot, an AI Materials Scientist Empowered by Large Language Models: Intelligent R&D Practice for Functional Ceramics |
| 14:20-14:45 | Xue Jiang | University of Science and Technology Beijing, China | Steel design based on a large language model |

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| 14:45-15:10 | Zhaoyan Sun | Changchun Institute of Applied Chemistry, China | Genetic Engineering of Polymer Materials: Small Data, Model Interpretability, and Large Language Models |
| 15:10-15:35 | Yue Liu | Shanghai University, China | Empowering Material Knowledge Extraction with Large Language Models |
| 15:30-15:50 | Jue Wang | Chengdu Caizhi Technology Co., Ltd, China | Enhancing Materials Research through LLM: Building a Comprehensive Platform and Facilitating Knowledge-Led Innovation |
| Coffee break | | | |
| Materials Design and Optimization Chairs: Prof. Yuan Wu, Prof. Chenchong Wang | | | |
| 16:05-16:30 | Yuan Wu | University of Science and Technology Beijing, China | Multi-objective co-design strategy of low modulus and high yield strength for high entropy alloys |
| 16:30-16:55 | Xiaoyu Chong | Kunming University of Science and Technology, China | The Design and Application of Noble Metal-Based Superalloys Driven by the Synergy of Physical Models and Machine Learning |
| 16:55-17:20 | Lixian Lian | Sichuan University, China | Multi-objective intelligent optimization design and development of new superalloys |
| 17:20-17:45 | Ziyuan Rao | Shanghai Jiao Tong University, China | Alloy Design Based on Artificial Intelligence and Machine Learning |
| 17:45-18:10 | Ruihao Yuan | Northwestern Polytechnical University, China | Deep learning strengthening mechanism for high fidelity inverse design of microstructure |

**The 3rd Workshop towards Materials Data Standards on
Challenges and opportunities of large language model on materials science
2024.11.16**

Chairs: Prof. Hong Wang, Prof. Haiqing Yin

| Time | Speaker | Affiliation | Presentation Title |
|--|-------------------------------|--|--|
| 8:30-8:55 | Ryo Maezono | Japan Advanced Institute of Science and Technology, JAIST, Japan | AI-recognition of XRD pattern using auto-encoder |
| 8:55-9:20 | Lei Zhang | Nanjing University of Information Science and Technology, China | Data-driven language models for materials science |
| 9:20-9:45 | Byungju Lee | Korea Institute of Science and Technology, Korea | Accelerating materials language processing with large language models |
| 9:45-10:10 | Yuzhi Zhang | DP Technology Co., Ltd, China | New-generation materials design platform empowered by AI foundation models |
| Coffee break | | | |
| 10:30-12:10 | Round Table Discussion | | |
| Prof. Ryo Maezono, Prof. Lei Zhang, Dr. Byungju Lee, Dr. Yuzhi Zhang Prof. Shuichi Iwata (The University of Tokyo) Dr. Yibin Xu (National Institute for Materials Science, Japan) Dr. Satoshi Minamoto (National Institute for Materials Science, Japan) Dr. Yong-hak Huh (Korea Research Institute of Standards and Science) Dr. Kwang-Ryeol Lee (Korea Institute of Science and Technology) Prof. Hong Wang (Shanghai Jiaotong University) Dr. Peng Wang (Chinese Society for Testing & Materials, China) | | | |

