Materials Data Standards Serial Workshops

The 1st Workshop on Materials Data Standards System



As the digitalization has created new opportunities and challenges around the world, material data become crucial for material innovation and intelligent manufacturing. The Materials Data Standards serial workshops, organized by the Beijing Advanced Innovation Center for Materials Genome Engineering, aim to promote the exchange of opinions on materials data and materials data standards from the multi-stakeholders and to enable people around the world to explore the most recent progress on materials data standards, serving as an important international benchmark for research, quality, safety, and trust on materials data.

The 1st Workshop on Materials Data Standards System will be held on Aug 30th, online. Four speakers from US, Japan, Korea and China will give excellent presentations followed by a online round-table discussion with eight experts.

Time: August 30, 8:30-12:00am （Beijing, GMT+8）
August 30, 9:30am-1:00pm （Tokyo & Seoul, GMT+9）
August 29, 8:30-12:00pm （New York, GMT-4）

Venue: Zoom: Meeting ID: 898 6951 4541, Passcode: 628564
https://us06web.zoom.us/j/89869514541?pwd=QU5qcXpFWnNXMldpRWJQUDR5RjhQQT09

KouShare: https://www.koushare.com/lives/room/519421

北京科技大学 University of Science and Technology Beijing

北京材料基因工程高精尖创新中心 BEIJING ADVANCED INNOVATION CENTER FOR MATERIALS GENOME ENGINEERING

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Program

TIME	SUBJECT	CONTRIBUTOR
8:30-8:40	Opening remarks	Prof. Dawei Zhang
8:40-9:20	Knowledge Graphs Supporting Accelerated Materials Innovation	Prof. Surya R. Kalidindi
9:20-10:00	A Literature Database for Battery Materials with Integrated Substance and Material Data	Dr. Yibin Xu
10:00-10:40	Establishment of Materials Research Data Standard and a Platform for the Data Usage	Dr. Yong-Hak Huh
10:40-11:20	The standard system for the AI-ready material data	Prof. Hong Wang
11:20-11:50	Round-Table discussion Prof. Surya R. Kalidindi Dr. Yibin Xu Dr. Yong-Hak Huh Prof. Hong Wang Prof. Shuichi Iwata（University of Science and Technology Beijing / The University of Tokyo / MPDS / EEI） Prof. Lei Zhang （University of Science and Technology Beijing） Dr. Lingtian Tang （China Iron & Steels Research Institute Group） Dr. Peng Wang（Chinese Society for Testing & Materials, Zhonguancun）	
11:50-12:00	Closing remarks	Prof. Shuichi Iwata

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Prof. Surya R. Kalidindi Georgia Institute of Technology, USA



Title: **Knowledge Graphs Supporting Accelerated Materials Innovation**

In order to maximize the use of the materials data being generated by various researchers and organizations, it is necessary to store the data such that it is findable, accessible, interoperable, and reusable (FAIR). Although current materials data repositories and databases partly address the FAIR principles, they do not adequately capture the critical metadata that represents the contextual information (e.g., relationship between materials data and terms typically used by materials scientists such as process, structure, and property). The collection and organization of this metadata along with the original data would allow advanced queries that implicitly improve FAIR characteristics. This paper introduces a new materials graph and develops the associated materials graph ontology needed to address this grand challenge. Specifically, this talk discusses the critical elements needed for the conceptual description of a broad variety of materials data, the findability and usability of the different graph-connected material concepts and data, and formalizes a novel materials data ingest framework that can potentially drive autonomous materials innovation in the future.

Dr. Yibin Xu National Institute for Material Science, Japan



Title: **A Literature Database for Battery Materials with Integrated Substance and Material Data**

The purpose of data-driven materials research is to improve material property and performance by designing and optimizing material chemical composition, structure and process conditions. For this purpose, interlinked data of material composition, structure and property for comprehensive material systems from element, compound to substance and material, are needed. Material identification is considered the key issue of data integration. To solve this problem, standardization of material descriptors at different levels are required. In this talk, our current work on construction of a materials database for battery will be introduced. In this work we try to link experimental data of complex material systems such as process condition and property to substance data such as crystal structure and electronic structure. Examples of data-driven studies on ionic conductivity of crystal and grain boundary with integrated materials and substances data will be introduced.

Dr. Yong-Hak Huh
Korea Research Institute of Standards and Science, Korea



Title: **Establishment of Materials Research Data Standard and a Platform for the Data Usage**

Materials research data standard, including data schema and vocabularies, must be essential for sharing and linking the data between the systematically networked data infrastructures. So, a lot of global effort have been put into standardizing the data. Recently, in Korea, standard vocabularies and schema for the data have been defined, and the platform for the collection and service of the data is being established. A schema concept called 'materials system' was proposed to systematically organize the data on materials of diverse structures. The materials system is made up of two hierarchies, including Materials and System. The Material hierarchy consists of structure (chemical information) , process and properties data, while the System hierarchy contains configuration, process and performance data. Furthermore, standard data vocabularies and their formats have been defined, which were done through a Materials Data Standardization Process. Elements of the data consist of a value, uncertainty and measurement (condition). Based on the standard materials research data vocabularies and schema, the data platform, which is called K-MDS, is being developed for the data exploration, data analysis and visualization, and data sharing.

Prof. Hong Wang
Shanghai Jiaotong University, China



Title: **The Standard System for the AI-ready Material Data**

The core of material genome engineering lies in the data-driven mode featuring "data + artificial intelligence (AI)". Material data is characterized by large quantity, multi-sources and heterogeneous in forms. Data standard provides an key assurance for the construction of AI-ready data (set). The recently proposed China Standards of Testing and Materials (CSTM) "General Rules for Materials Genome Engineering Data" is a first attempt to standardize the content of data in principle. The data is divided into three classes of sample information, source data , and processed data. The information is assigned a unique and permanent resource identification code. Listing the sample information as a class of data is a unique choice, the greatest advantage of which is to make the samples themselves conforming to FAIR principles, so that samples can be found, shared, and reused. The General Rule of Materials Genome Data provides high level principles for the content of materials data. For full regulation of materials data, a standard system consisting of a large set of standards needs to be designed from top down, to cover all aspects in data generation, collection, storing, sharing, exchanging, and application, etc. To establishing the whole system of standards involves great complexity, wide range of expertise, as well as tremendous workload, which can only be accomplished with the participation of the whole materials community.