



NSF FAIROS Materials Research Data Alliance Working Groups to hold Town Hall Meeting at 2024 MRS Spring Meeting & Exhibit

<https://www.marda-alliance.org>

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Two Working Groups of the Materials Research Data Alliance (MaRDA) will hold a Town Hall Meeting at the 2024 MRS Spring Meeting & Exhibit in Seattle, Wash., on Monday, April 22, 4–6 p.m. (PST), Summit-Seattle Convention Center, Level 3, Room 326 to which all attendees are invited. The Working Groups will review their draft recommendations and gather feedback from the materials community.

As part of the US National Science Foundation's (NSF) Findable, Accessible, Interoperable, Reusable, Open Science Research Coordination Networks (FAIROS RCN) program, Northwestern University and Duke University hosted a Virtual Meeting in December 2022 to initiate a community discussion on FAIR data in two areas: materials microscopy and laboratory information management systems (LIMS). The meeting began with invited presentations by recognized experts in these two areas with considerable impact in the domain. The first presentation by Mitra L. Taheri (Johns Hopkins University) on FAIR Data and Microscopy detailed how the widespread use of microscopy and the breadth of its applications create challenges to forming a consensus on critical metadata, while also providing fertile ground to facilitate data sharing across multiple organizations with varying capabilities. The second presentation by June W. Lau (National Institute of Standards and Technology) emphasized Laboratory Information Management Systems (LIMS) as an essential infrastructure

to aggregate, organize, and exchange microscopy data in a FAIR way, as well as to support data analysis, including artificial intelligence and machine learning, and reuse. After the workshop, participants were invited to join two MaRDA Working Groups that would be established in 2023, and conduct their work within an 18-month period.

By March 2023, two new MaRDA Working Groups (Microscopy Metadata and FAIR LIMS Data) were formed to develop draft recommendations for consideration by the materials community. These groups have brought together materials scientists and researchers from across academia, industry, and government with a broad range of focus areas and a goal to generate outputs that are useful to the entire materials research community, rather than limited to specific domains. The LIMS Working Group is led by Co-chairs Eric A. Stach (University of Pennsylvania) and Joshua A. Taillon (National Institute of Standards and Technology) and has 10 additional members. The Microscopy Metadata Working Group is led by Co-chairs Edward S. Barnard (Lawrence Berkeley National Laboratory), Maria K.Y. Chan (Argonne National Laboratory), and Mitra L. Taheri (Johns Hopkins University) and has 10 additional members. Representatives of MaRDA Council, Laura M. Bartolo (Northwestern University), L. Cate Brinson (Duke University), Peter W. Voorhees (Northwestern University), and June W. Lau (National Institute of Standards and

Technology) serve as Ex-officio members of both Working Groups. The two MaRDA Working Groups are distinct in focus yet are working in concert to produce complementary recommendations to maximize their joint benefits for the materials community.

Two joint in-person 1.5-day meetings for the working groups were hosted by Northwestern University in May and October 2023 with multiple virtual meetings held by each working group during the intervening months. Details on MaRDA Working Groups are available at <https://www.marda-alliance.org/working-groups/> and preliminary draft reports and requests for feedback have been scheduled for release in March 2024. The following are summaries on the efforts of the two MaRDA Working Groups, which will be presented in greater detail at a Town Hall Meeting scheduled for the 2024 MRS Spring Meeting & Exhibit in Seattle, Wash., on Monday, April 22, 4–6 p.m. (PST), Summit-Seattle Convention Center, Level 3, Room 326 with requests for feedback from Meeting attendees.

The **Microscopy Metadata Working Group** has focused on common metadata requirements for electron microscopy experiments in materials science. As a foundational step toward recommended minimal, common, lightweight metadata for materials electron microscopy, the working group has conducted a review of existing recognized electron microscopy metadata practices

in cognate disciplines, for example, life sciences, materials science, and chemistry. The working group will review key features of selected domain metadata practices with regard to sample information, microscope configuration, user, time, and persistent identifiers. Additionally, it will compare existing metadata standards and provide references to help researchers find the example metadata that could be used or modified in materials microscopy. The group has also established a demonstration project on several common samples, examined by multiple methods and instruments, to share microscopy data and metadata and to reproduce results across microscopy facilities. The results of this study will be made available to the materials community and could be updated by future working groups as additional resources become available. While starting with electron microscopy, the findings will serve as an extensible model that may eventually broaden into the full array of imaging and spectroscopy methods.

The **FAIR LIMS Data Working Group** focuses on LIMS as essential components of modern materials research laboratory operations, providing the digital infrastructure to support essential services such as research data management, sample tracking, and result reporting. Implementing LIMS in existing research workflows requires considerable planning, preparation, and an understanding of the available technological solutions, the laboratory's needs, and the organization's overarching goals. The draft recommendations of the FAIR LIMS Data Working Group will address three primary areas: (1) comparison of *costs versus benefits* involved with implementing LIMS; (2) evaluation of *desired capabilities* for successful LIMS implementation; and (3) structure and content of a

metadata schema to be used to catalog information within a LIMS for materials research. The recommendations will additionally include a set of checklists to assist with planning the implementation of a LIMS, including: (a) *Organization's Prerequisites*: what an organization should have in place before installing a LIMS; (b) *LIMS Capabilities*: what functionality should a LIMS include to operate efficiently and to support FAIR Data Principles; and (c) *Research Data Management Activities*: what data management activities should be considered when research projects use a LIMS.

A **Town Hall Meeting** will be held at the 2024 MRS Spring Meeting & Exhibit on **Monday, April 22, 2024, 4–6 p.m. (PST), Summit-Seattle Convention Center, Level 3, Room 326** where the Working Groups will review their draft recommendations and gather feedback from the materials community. All attendees of the 2024 MRS Spring Meeting & Exhibit are invited and encouraged to participate. This session will provide an important two-hour venue for in-person, in-depth discussions about building recommended materials community-driven best practices on microscopy and LIMS. After the 2024 MRS Spring Meeting & Exhibit, the Working Groups will reconvene to review and incorporate participants' responses in order to develop updated community-based and community-driven recommendations related to Microscopy Metadata and LIMS. Final recommendations of both Working Groups will be released and widely disseminated through numerous communication channels by the end of the Working Groups' time period, in September 2024.

Acknowledgments

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Network (MaRCN), as part of NSF's Findable, Accessible, Interoperable, Reusable, Open Science Research Coordination Networks (FAIROS RCN) program, works to advance and coordinate findable, accessible, interoperable, reusable (FAIR) data. To support open-science materials research nationally and internationally, MaRCN aims to bridge the fundamental gap between materials data and data-intensive methods including artificial intelligence and machine learning. The MaRCN project involves six institutions: Johns Hopkins University (lead institution); University at Buffalo, The State University of New York; Duke University; Northwestern University; Purdue University; and The University of Chicago.

Endnotes

1. MaRDA LIMS Working Group Members: John Allison (University of Michigan), Carelyn Campbell (National Institute of Standards and Technology), Jennifer Carter (Case Western Reserve University), Kamal Choudhary (National Institute of Standards and Technology), Cory Czarnik (Gatan), Dieter Isheim (Northwestern University), Derk Joester (Northwestern University), Roberto dos Reis (Northwestern University), Richard Sheridan (Duke University), Douglas Stauffer (Bruker Corporation).
2. MaRDA Microscopy Metadata Working Group Members: Eva Campo (Campostella Research and Consulting, LLC), Fernando Castro (Gatan), Miaofang Chi (Oak Ridge National Laboratory), John Damiano (Protochips Inc.), Anthony DiGiovanni (US Army Research Laboratory), Tom Isabell (JEOL USA, Inc.), Robert Klie (University of Illinois at Chicago), Ying Jia (Northwestern University), Prashant Singh (Ames National Laboratory), Maureen E. Williams (National Institute of Standards and Technology). □

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