Facilitating the Development of Modular Data Models in Materials Science

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ABSTRACT

The Materials Data Curation System [1,2] has the potential to accelerate interoperable data exchange within materials science and engineering. This platform is designed to enable the typical PI to easily disseminate diverse datasets with sufficient domain-specific metadata through various access methods. In order to use the Materials Data Curation System, the user must compose a "Template", which is a comprehensive description of the structure of metadata, data, and files under consideration, within their unique project. Although the Materials Data Curation System Composer allows the user to create a Template from scratch, this approach results in redundant efforts and limited interoperability. An alternative approach would be to develop and disseminate broadly applicable data models, which could be assembled, at the user's discretion, into Templates. This approach both decreases the burden on the user and increases the interoperability and discoverability, while still providing flexibility for users to define a unique Template. The focus of this project is to coordinate effort and convene experts to address relevant challenges. We are currently focused on three areas:

- Development of foundational data models for concepts used throughout the field
- Development of modular data models for specific modeling, synthesis and measurement techniques
- Facilitating integration of the Materials Data Curation System within new and established research projects

This effort should reduce the barrier of adoption among new users and significantly expand the breadth of materials data currently discoverable and accessible.

REFERENCES

- [1] https://mgi.nist.gov/materials-data-curation-system
- [2] https://github.com/usnistgov/MDCS