Working toward Interoperability: Nanomine to Metamine and Ontologies

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Data-driven methods can help accelerate materials design given the vast array of past research data. Data resources that hold these research data in a findable, accessible, integratable, and reusable (FAIR) way are essential to the success. NanoMine is an ontology-based, open-source data resource that follows the FAIR principles for the polymer nanocomposite community. During the development of NanoMine, a standalone API service entitled ChemProps was developed to solve the database indexing issue caused by the lack of uniformity in polymer names, which integrates seamlessly into NanoMine platform and enables more interoperability across many polymer data sites.

Beyond being a contribution only to the polymer nanocomposite community with the NanoMine Knowledge Graph, NanoMine has the vision to create the Materials Knowledge Graph as a stable, user-friendly data and knowledge framework for materials through the development of an extensible semantic infrastructure with customized and customizable user templates and semi-automatic curation tools for data entry and associated data validation protocols, along with ontology-enabled design tools and custom user dashboards.

The first sibling of the NanoMine Knowledge Graph under the Materials Knowledge Graph framework is the MetaMine Knowledge Graph, which extends from the NanoMine schema and ontology, which by itself is also an extension of the work done in modeling entirely different domains, including epidemiology and bioinformatics. By building off an existing science ontology (Semantic-science Integrated Ontology, or SIO), the extension into a related metamaterials domain is smooth, since most of the modeling was done and only a few tasks including how to describe metamaterials geometries, and how to represent modulus tensors are left to be considered.