NanoMine: A Knowledge Graph for Nanocomposite Materials Science

Jamie P. McCusker[1(✉)], Neha Keshan[1], Sabbir Rashid[1], Michael Deagen[3], Cate Brinson[2], and Deborah L. McGuinness[1]

[1] Department of Computer Science, Rensselaer Polytechnic Institute, Troy, NY, USA
{mccusj2,keshan,rashis}@rpi.edu, dlm@cs.rpi.edu

[2] Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, USA
cate.brinson@duke.edu

[3] College of Engineering and Mathematical Sciences, University of Vermont, Burlington, VT, USA
Michael.Deagen@uvm.edu

Abstract. Knowledge graphs can be used to help scientists integrate and explore their data in novel ways. NanoMine, built with the Whyis knowledge graph framework, integrates diverse data from over 1,700 polymer nanocomposite experiments. Polymer nanocomposites (polymer materials with nanometer-scale particles embedded in them) exhibit complex changes in their properties depending upon their composition or processing methods. Building an overall theory of how nanoparticles interact with the polymer they are embedded in therefore typically has to rely on an integrated view across hundreds of datasets. Because the NanoMine knowledge graph is able to integrate across many experiments, materials scientists can explore custom visualizations and, with minimal semantic training, produce custom visualizations of their own. NanoMine provides access to experimental results and their provenance in a linked data format that conforms to well-used semantic web ontologies and vocabularies (PROV-O, Schema.org, and the Semanticscience Integrated Ontology). We curated data described by an XML schema into an extensible knowledge graph format that enables users to more easily browse, filter, and visualize nanocomposite materials data. We evaluated NanoMine on the ability for material scientists to produce visualizations that help them explore and understand nanomaterials and assess the diversity of the integrated data. Additionally, NanoMine has been used by the materials science community to produce an integrated view of a journal special issue focusing on data sharing, demonstrating the advantages of sharing data in an interoperable manner.

Keywords: Knowledge graph · Semantic science · Knowledge representation

Supported by the National Science Foundation.

J. Z. Pan et al. (Eds.): ISWC 2020, LNCS 12507, pp. 144–159, 2020.
https://doi.org/10.1007/978-3-030-62466-8_10

1 Introduction

Polymer nanocomposites are materials made with particles that have at least one dimension that is less than 100 nm [15] that have been embedded in a polymer base, or matrix. Polymer nanocomposites exhibit complex, nonlinear responses to changes in material composition and processing methods. Additionally, these materials are used in many different applications, which means that a wide array of properties have been investigated, including mechanical, thermal, electrical, and others. This complexity makes it difficult to predict the properties of polymer nanocomposites from the performance of their consituents. The diversity of materials used, the ways in which they can be prepared, and the different kinds of properties that could be measured resulted in a complex XML-based data standard that was difficult to understand and query. The NanoMine project attempts to support researchers in their quest to explore new options for nanomaterials by providing an integrated resource where they can explore existing data about nanomaterials and their interrelationships. The biggest challenge facing NanoMine was how to create an extensible data standard that meets the needs of the present and future, while avoiding over-complexity of that standard so that the data can be queried and explored without expanding the software as new data types are added.

The foundation of materials science is the analysis of the processing, structure, and properties (PSP) interrelationships of materials. Materials scientists follow this paradigm to invent new kinds of materials that have a desired performance in real world applications.

Processing describes the sequence of steps needed to create and prepare a material. These might include mixing, melting, cooling, heating, or other methods, and each step can have many parameters.

Structure describes the composition of a material in terms of its parts, and how those constituent parts are arranged within the material. In the case of polymer nanocomposites, this usually consists of a polymer *matrix*, or base material, that has nanoparticles of different types added to it. These nanoparticles are collectively referred to as *filler*.

Properties are measured values describing how the material responds to mechanical, electrical, thermal, or other observable events. A property can indicate how strong a material is, how well it insulates or conducts electricity, how it stores or transmits heat, etc.

Originally, the NanoMine resource was conceived as a repository of XML files that describe polymer nanocomposite experiments. However, the representation needed to adequately describe experiments was complex and difficult to navigate [18]. Finding a specific piece of data required detailed knowledge of the schema, and typically included a sometimes cumbersome process of navigating built-in hierarchies of properties and different representations of measurements. We needed a way to simplify access and querying of data by providing a consistent representation for material processing methods, material composition or structure, and material properties. As a result, we built the following semantically-enabled resources for polymer nanocomposite materials science:

NanoMine Knowledge Graph: The NanoMine knowledge graph provides access to experimental data, including full PSP data, citation information, and provenance.

NanoMine Ontology: The NanoMine Ontology extends the Semanticscience Integrated Ontology (SIO) [3] and provides classes for 141 material properties, 25 processing methods, and 171 material types, compatible with and extending the NanoMine XML Schema.

NanoMine Whyis Instance: A website to search and visualize curated experiments through faceted search, full text search, a SPARQL endpoint, and user-contributed visualizations.

2 Availability

The NanoMine knowledge graph is published at http://nanomine.org, using the Whyis knowledge graph framework. The NanoMine ontology is published as part of the knowledge graph and is available at http://nanomine.org/ns. All entities in the graph are published as 5 star linked data aligned with SIO, Dublin Core Terms, and the W3C Provenance ontology, PROV-O. A read-only SPARQL API is available at https://materialsmine.org/wi/sparql, providing access to all material data and its provenance, as well as how it was transformed into RDF.

This knowledge graph is currently used by the polymer nanocomposite research community to explore their data, and will be featured in a special data issue of ACS Macro Letters [1].

Table 1. Namespace prefixes used in this paper.

Prefix	URI
nanomine	http://nanomine.org/ns/
sio	http://semanticscience.org/resource/
prov	http://www.w3.org/ns/prov#
np	http://www.nanopub.org/nschema#
setl	http://purl.org/twc/vocab/setl/
bibo	http://purl.org/ontology/bibo/

3 Modeling Materials Science

The NanoMine XML schema describes the parts of PSP for nanomaterials that materials scientists considered essential for understanding those nanomaterials [18]. As we have stated, the resulting XML files were complex and difficult to query. The NanoMine knowledge graph is designed to enable consistent representation across data types for properties, material composition, and material processing that are appropriate for nanocomposite materials research, while providing simple methods for querying and visualizing the data. To support this, we re-use representations for entities, processes, and attributes from the Semanticscience Integrated Ontology (SIO) [3]. SIO has been used in many domains, including epidemiology [10], computational biology [9,13], and sea ice data [2]. SIO provides a representation for the most commonly needed relationships and top-level classes for integrated science applications. This reuse supports interoperability with other tools and applications that also use SIO. The basic SIO classes and relationships are outlined in Fig. 1, adapted from figures in [3]. We build on these fundamental properties and classes to create the models needed for the NanoMine ontology and knowledge graph. The namespace prefixes used in this paper are listed in Table 1.

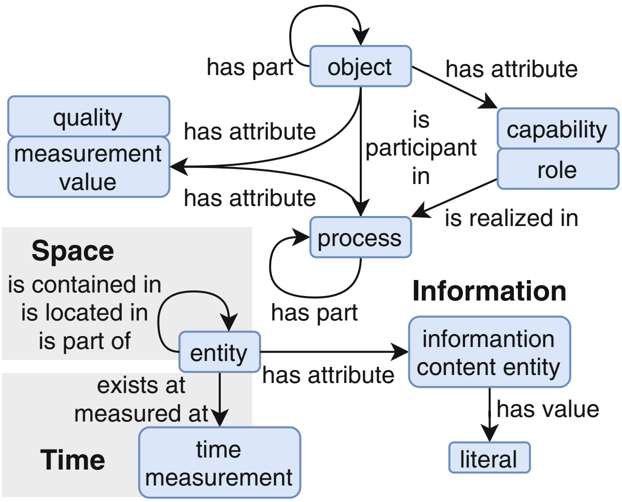

Fig. 1. The basic relationships of SIO include properties for representing attributes, values, parts, and temporal measurements. All classes and properties are part of SIO. Structures in "Space", "Time", and "Information" are the parts of SIO used to model those particular aspects of knowledge. Adapted from [3].

3.1 Properties

The physical properties of materials are at the heart of materials science. Numerous means of measuring and expressing physical properties exist. The NanoMine project represents the common electrical, mechanical, thermal, crystalline, volumetric, and rheological (flow) properties of nanomaterials as instances, following the modeling approach of SIO. Each property is represented as a single value,

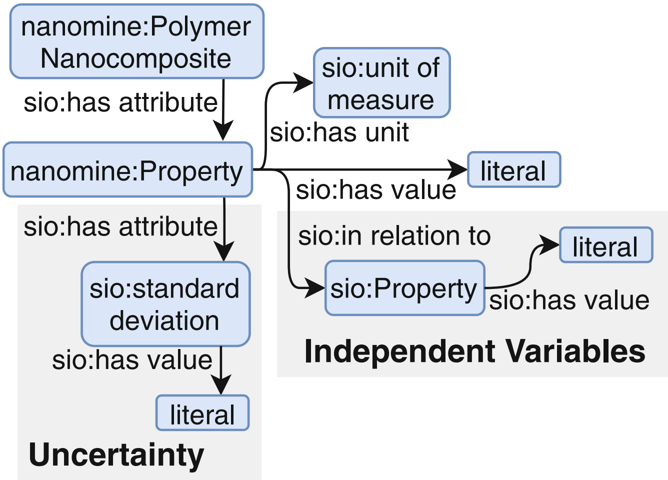

Fig. 2. Modeling properties of polymer nanocomposites. A property is a subclass of *sio:quantity*. Properties with uncertainty ranges have their own attribute of a standard deviation. A property curve has its independent variable linked to the property by *sio:'in relation to'*. Note that SIO uses lowercase labels, while the NanoMine Ontology uses capitalized labels. This distinction is preserved in our figures and visualizations.

a value with an uncertainty range, or a dependent variable that exists in relation to one or more independent variables. The model needed to represent these kinds of properties is shown in Fig. 2.

3.2 Material Composition

Polymer nanocomposites consist of a matrix, or base material, made of polymers like epoxy or latex, that is combined with different kinds of particles, such as graphite or silica. These particles are called fillers, and sometimes multiple filler types are added to the matrix. Fillers can be given surface treatments of different types, which can also change how they interact with the matrix. All of these components have their own properties, like density, volume or mass fraction, and dimensionality to individual particles. Some of these constituent properties are complex, and have a mean and standard deviation (like particle dimension), so we use the same property templates available for the aggregate, nanocomposite representation, as shown in Fig. 2. We represent polymer nanocomposities in terms of their constituents - fillers, matrices, and surface treatments, while linking them to the main nanocomposite using *sio:'has component part'* and *sio:'is surrounded by'*, as shown in Fig. 3. The actual consituent materials are given types, like "silica" or "graphene," based on the kind of material it is. That certain materials are fillers versus matrices is represented using subclasses of *sio:role*.

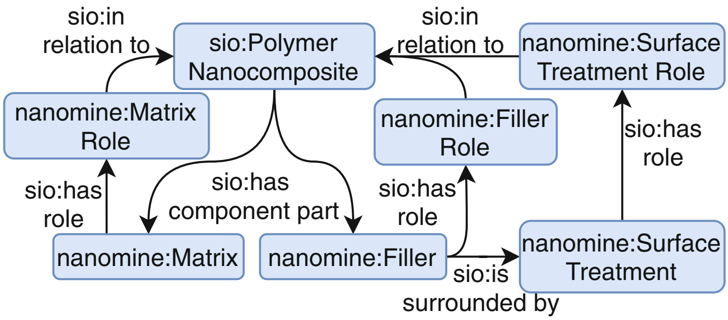

Fig. 3. Modeling composition of polymer nanocomposites. Constituent materials are given a type corresponding to the physical material type (silica, graphene, BPA, etc.), while the roles of filler or matrix is represented as *sio:role* instances.

3.3 Material Processing

The processing methods associated with a polymer nanocomposite are as important to its properties as the materials used to create it. Depending on how the material was prepared, its properties can be wildly different. Analogous to baking a cake, where a precise sequence of recipe steps leads to a tasty result, preparation of polymer nanocomposites requires a sequence of processing steps under controlled conditions in order to achieve the desired material properties. Similarly for polymer nanocomposites, changes in conditions can result in different interactions between the filler and matrix.

The ontology supports the encoding of processing methods using subclasses of *sio:procedure* to represent different kinds of mixing, heating, cooling, curing, molding, drying, and extrusion. Some of these processes, like extrusion, require complex parameters and descriptions of equipment. These are expressed as objects that are used in a process in addition to the process input, and attributes on the process and equipment. This takes advantage of process modeling in both SIO (from a science modeling perspective) and PROV-O (from a provenance perspective) [7]. Figure 4 illustrates this modeling approach for processing polymer nanocomposites.

In the curated XML files, processing steps are able to be expressed as a plain list, but experimental methods often have multiple flows and partial ordering. The use of the SIO hasInput/hasOutput properties allows us to expand the expression of processing workflows beyond the current representations.

3.4 Provenance

Provenance is crucial to an effective openly available knowledge graph with community contributions. The Whyis knowledge graph does not allow additions of knowledge without that addition being wrapped in at least minimal provenance, such as who contributed the knowledge and at what time. In NanoMine, all samples are curated from specific journal articles and unpublished data. Therefore,

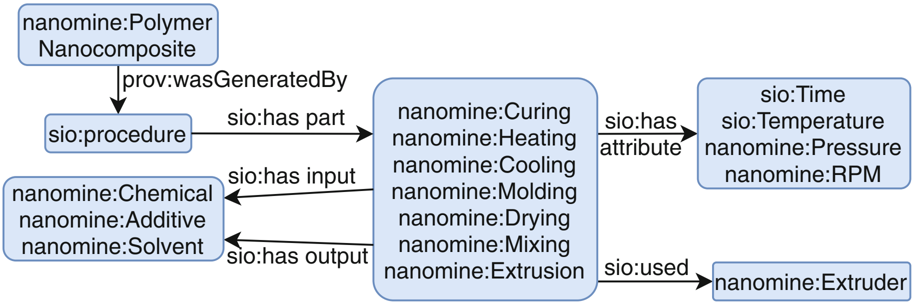

Fig. 4. Modeling processing of polymer nanocomposites. Each sample is marked as being generated by a top level procedure that is composed of numerous steps. Each step has inputs and outputs, and the use of one step's output as another step's input provides partial ordering to the overall workflow.

it is important to track where the sample information comes from. We rely on nanopublications [5] to provide structure for that provenance. This allows us to link a provenance named graph to the general assertion named graph. Provenance includes the processing (how the sample was created) and characterization (how the measurements were made) methods, as well as DOI-compatible metadata for the papers that the samples are curated from. Further details on the representation are shown in Fig. 5.

4 Curating the NanoMine Knowledge Graph

NanoMine has a data curation pipeline (Fig. 6) that takes data from papers and datasets and converts it into a knowledge graph through a collaboration of materials scientists, software engineers, and knowledge graph engineers. Our pipeline is optimized to support contributions by many different collaborators with differing levels of technical skill. Curators on the project generally use a web tool to manually extract information from published papers, and use the WebPlotDigitizer[1] to extract data from figures. Curators and collaborators can fill in an Excel file template, modeled after the XML schema, with these data. The Excel files are uploaded to NanoMine[2] and converted into XML. Once curation is complete, the system uploads the XML files to the NanoMine Whyis instance. This instance is configured to recognize NanoMine XML files and run a Semantic ETL script using SETLr [8] to convert the XML files into the RDF representation described in Sect. 3. The output of this script is added to the knowledge graph. Additionally, we created the NanoMine Ontology using the approach developed for the CHEAR Ontology [10], where we extend SIO, add concepts on-demand, and use a spreadsheet and SETLr to compile the ontology into OWL. Most of the concepts in the NanoMine Ontology were contributed

[1] https://automeris.io/WebPlotDigitizer/.
[2] https://materialsmine.org/nm#/XMLCONV.

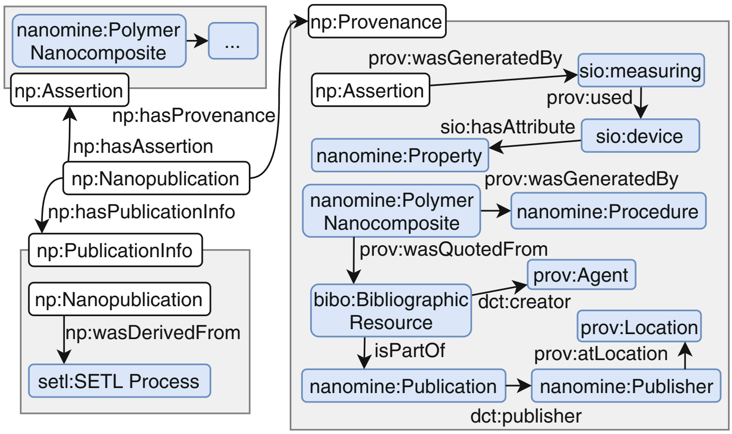

Fig. 5. Modeling the provenance of polymer nanocomposites. Named graphs are indicated as grey boxes. The provenance graph contains information about the methods used to produce the characteristics in the provenance, the processing graph from Fig. 4, and bibliographic information. The Publication Info graph contains statements about how the nanopublication itself was created, usually as a result of a Semantic ETL (SETL) process.

and defined by domain experts, and then integrated into SIO by our ontology experts.

We determined that a knowledge graph was needed instead of an XML file repository because it was difficult to search and visualize the data without custom software. The same properties were stored in many different ways, depending on if they had dependent variables or not, and whether or not there were uncertainty values. It was also difficult to tell if the XML files were curated in a consistent way - as it turns out many chemical names and units of meaures were entered in different ways. Converting the data to a knowledge graph also provides us with an opportunity to enhance the data progressively. For instance, we will be able to search for samples that can be used in different kinds of simulations and computational analyses to produce computed properties. Additionally, we will be providing conversions to preferred units of measure from the ones that were reported in the original papers.

5 Resource Evaluation

We evaluate the ontology by the ability to search, explore, and visualize polymer nanocomposites and their properties from many different experiments. Additionally, we evaluate the knowledge graph itself through the ability for materials scientists to explore nanomaterials using a faceted browser, and the ability of semantics-trained materials scientists to create custom visualizations to share with others.

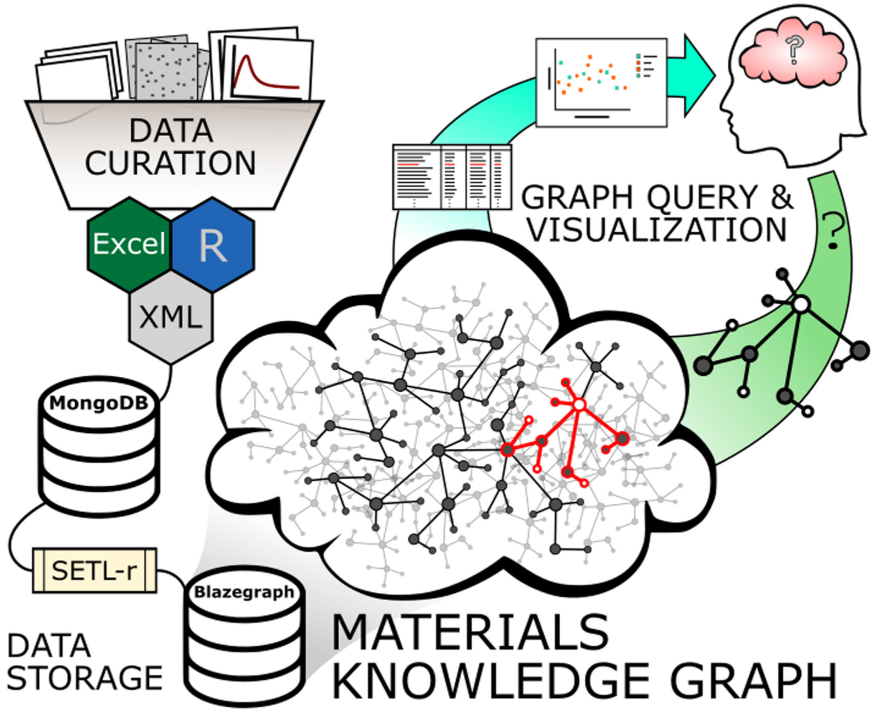

Fig. 6. Overview of the NanoMine curation process. Data is curated from papers by the NanoMine team and other materials science contributors into XML files and Excel spreadsheets (sometimes using R for to improve data quality) and stored in a MongoDB database. The files are copied over to Whyis to be converted into nanopublications that express sample properties. This knowledge graph is then used to visualize properties on demand by users, and further properties are inferred from additional data, including images of the materials.

5.1 Ontology Evaluation

We were able to formally map the NanoMine schema into the NanoMine Ontology using the approaches expressed above. The NanoMine Ontology is fully integrated into SIO and PROV-O. All classes are subsumed by classes in SIO or PROV-O, and no additional properties were needed beyond the ones in those ontologies. This makes it easier for tools that understand SIO or PROV-O to be re-used on NanoMine data, and for NanoMine-specific tools to be used with other scientific or provenance-related data. The NanoMine Ontology is in $ALEOF$, and contains 318 classes and no new Object or Datatype Properties. It is also self-consistent (including the imported ontologies of SIO and PROV-O) as confirmed by both Hermit and Pellet.

The modeling used with the ontology has supported a number of key data exploration features that previously would have been difficult or impossible. For instance, it is now possible to provide summary statistics across groupings of properties, as well as individual property types, as shown in Fig. 8. These views are important for curation quality control, as we can assess if there are any unexpected property names being used in the XML files. We are also able to analyze the use of different materials as fillers and matrices, as shown in Fig. 9. It is important to note that, while the XML Schema and its translation into RDF has evolved over the course of several years, the underlying representation in RDF has not had to change to support those improvements, suggesting that the representation may be durable against future changes. The use of the PROV-O-based partial ordering representation expands on the kinds of experimental procedures we can represent from simple lists of steps to complex workflows. Use of this representation also allows for quick analysis of what kinds of processing steps co-occur, as shown in Fig. 7. Table 2 provides a summary of the total subclasses and instances of the major classes in the knowledge graph.

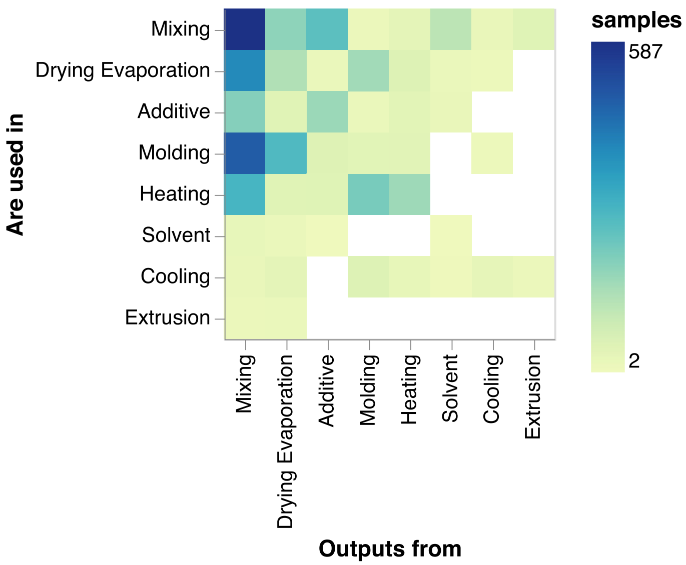

Fig. 7. A co-occurrence matrix of processing steps. Outputs of processing steps from the X axis are fed as inputs into processing steps on the Y axis. This lets users see how common certain methods are and what they tend to be used with, available at http://nanomine.org/viz/b2b74728f1751f2a.

5.2 Visualizing the Knowledge Graph

We provide two primary means of visualizing the knowledge graph - a faceted browser and a custom visualizer. Our general purpose faceted browser for browsing and visualizing samples in the graph allows users to find, select, and visualize

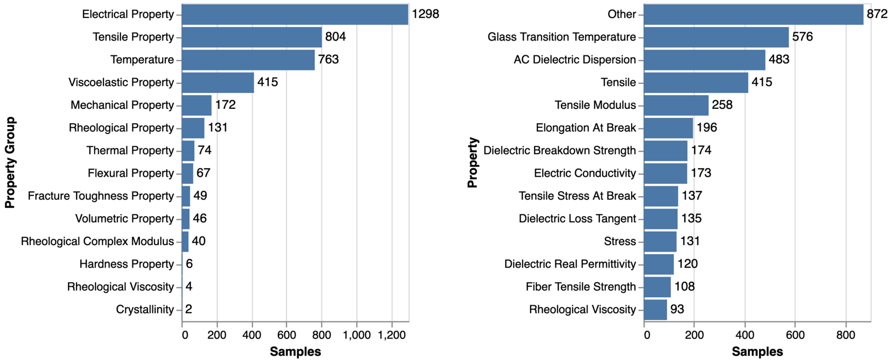

Fig. 8. Material property types by frequency, both by immediate superclass (left) and overall, available at http://nanomine.org/viz/77a5fa51556d064b.

Table 2. Summary of instances and subclasses of the major classes in the NanoMine Ontology. Note that units of measure in SIO are instances, not classes, and that the kinds of polymer nanocomposites are determined by their composition, so there are no current subclasses used for the overall nanomaterial (Polymer Nanocomposite).

Class	Subtypes	Instances
Polymer Nanocomposite	–	1,725
Property	97	733,155
Matrix	62	1,787
Filler	35	1,560
Surface Treatment	88	478
procedure	8	7,471
unit of measure	–	81
Bibliographic Resource	4	183

data about polymer nanocomposites. In Fig. 10, we can see a user plotting properties against each other to determine the effects of certain values on their performance. This browser is a general purpose tool available to any developers of Whyis knowledge graphs. It is heavily customized from the SPARQL Faceter [6], and can autogenerate facet configurations by introspecting the knowledge graph.

Advanced users can also create custom visualizations using the Vega and Vega-Lite tools [14]. In Fig. 12, a materials scientist with training in SPARQL has created a linked visualization using the Vega-Lite framework. In Whyis, the user can publish and share this visualization for others to see their analysis. Figure 11 shows the chart from Fig. 7 being edited. Other plots have been produced using this approach, and are available in the NanoMine visualization gallery.[3]

[3] Available from the main NanoMine page at http://nanomine.org.

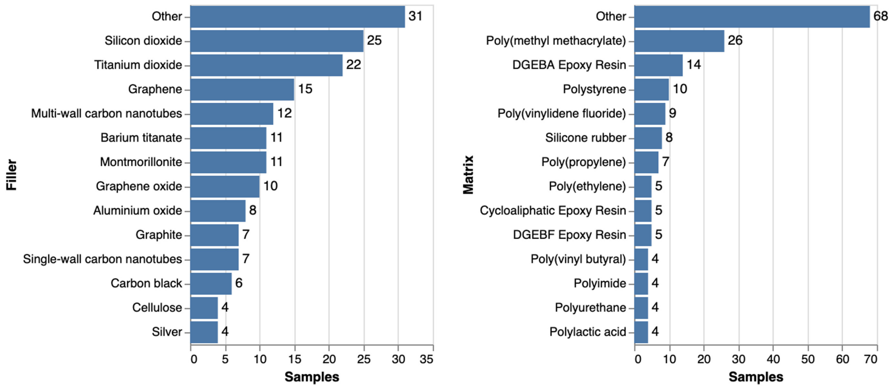

Fig. 9. Particle filler and polymer matrix types in the NanoMine knowledge graph, available at http://nanomine.org/viz/e037b3b61ab26244.

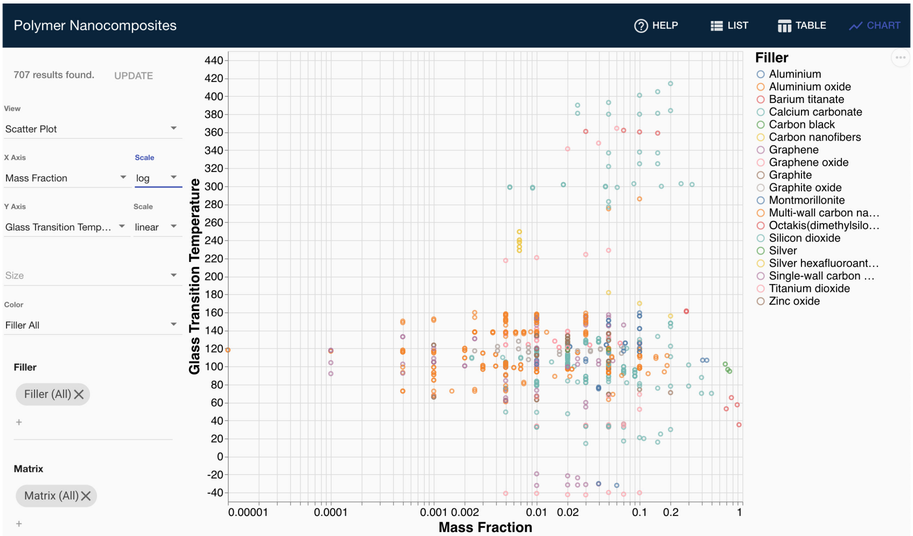

Fig. 10. Users can search for nanomaterial samples of interest and visualize their properties using simple controls. Here, a common view of the data, comparing the mass fraction (amount of nanoparticles by mass) of more than 700 samples to its glass transition temperature (the temperature below which a material becomes glassy and brittle). Users can select from any properties, constituent properties, material types, processing methods, and publication data to filter and visualize.

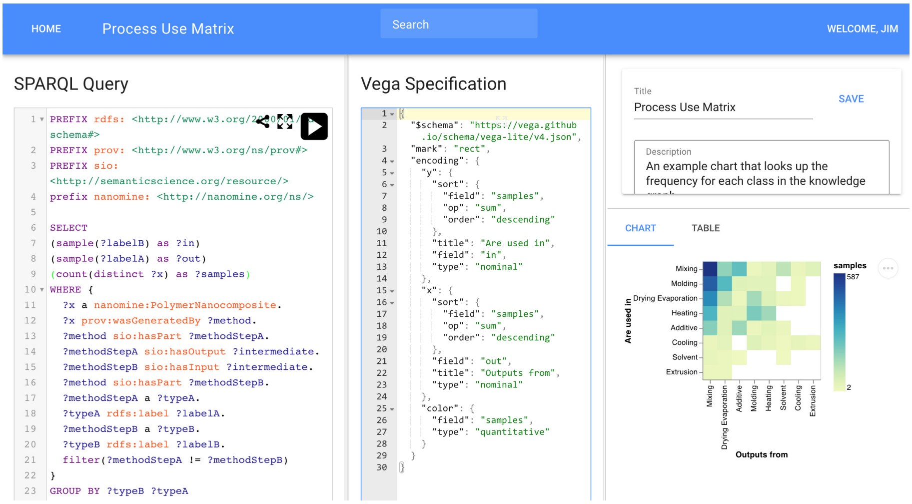

Fig. 11. Editing the Fig. 7 visualization in Whyis. Users can iterate over the SPARQL query and Vega specification to produce their preferred plot.

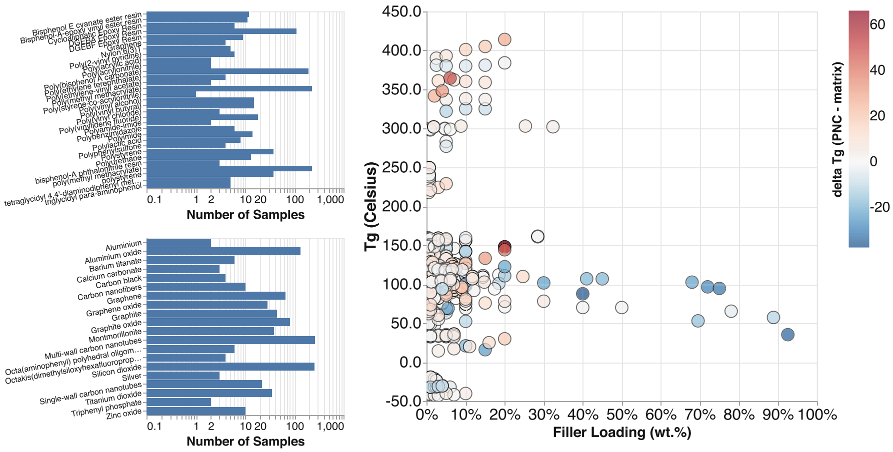

Fig. 12. A user-created custom visualization, created by a materials scientist. In this linked plot example, the heat map dynamically updates as the user selects matrix and filler materials from the bar charts below. Collaborators can use the resulting plot to identify overall trends in how the glass transition temperature, Tg, may change as filler particles are added to the matrix material. Available at http://nanomine.org/viz/10720c80b5b41ab8.

6 Related Work

There are several polymer data resources, but none focus on polymer nanocomposites, nor have publicly accessible APIs. These include the CRC POLYMER-

SnetBASE by the Taylor and Francis Group [4], the Polymer Property Predictor and Database (PPPDB) by the University of Chicago,[4] and the PolyInfo database from NIMS of Japan [12]. All of these data resources distribute curated polymer data from publications and polymer handbooks, with detailed annotations of chemical properties and characteristics. However, there are limitations for those data resources; for PolyInfo and PPPDB, the lack of application program interface (API) access prevents the application of a user-defined search and exploration of data, the CRC POLYMERSnetBASE requires paid access, and PPPDB covers only a few properties (notably the chi parameter and glass transition temperature) and is focused on polymer blends. In all those data resources, very few records are related to composites or nanocomposites, and those data resources rarely contain the complete information needed to describe the nanocomposite processing parameters, microstructure, and properties. Other materials science knowledge graphs include the Metallic Materials Knowledge Graph (MMKG) [17], which subsets DBpedia from seed entities. It does not attempt to manage the properties of those materials, only aggregate terms of interest. Another materials science knowledge graph is propnet [11], which constructs a graph of related materials based on their properties, but does not create a graph that contains representations of those properties, nor does it seem to handle complex composite materials. The Bosch Materials Science Knowledge Base is an internal project to produce a knowledge base of materials produced by the manufacturing company [16], but is not publicly available. Generally, these knowledge graphs provide conceptual models of material types, but do not manage or visualize experimental data from actual or simulated materials.

7 Future Work

There are a number of image analysis tools that the NanoMine team has developed for computing additional properties of nanomaterials. We plan to integrate these as autonomous agents that can perform these analyses automatically when a sample is added with the appropriate image type. Because Whyis allows deep metadata about any kind of file, including the context of how the file was produced, it is simple to identify the relevant image files for analysis. We also plan to introduce quality metrics for sample data that can determine if curation errors have been introduced. This can come from providing additional metadata about specific property types, and then checking for consistency with that metadata. We are also working to provide more consistent naming and identification of the chemicals used in creating the nanomaterials. Many chemicals have multiple names, and no current chemical databases have compete coverage of the materials used. We plan to improve the user experience of the Whyis interface through a usability study. Finally, we are continually seeking to curate more materials into the resource, and are currently working on expanding it to support similar capabilities for metamaterials. This new resource, which will encompass NanoMine, will be called MaterialsMine.

[4] https://pppdb.uchicago.edu.

8 Conclusion

We introduced the NanoMine *ontology, knowledge graph, and Whyis instance* as complementary semantically-enabled resources that help materials scientists explore the known effects of polymer nanocomposite design on their many properties. This resource is published as Linked Data and through a SPARQL endpoint, using the Whyis knowledge graph framework. Scientists can filter and visualize polymer nanocomposite samples to find relationships between aspects of those samples to gain further insights into nanocomposite design. Additionally, materials scientists, with some semantic training, can create and have created advanced visualizations using the Vega and Vega-Lite libraries. The use of nanopublications in the knowledge graph allows for the management of the knowledge graph as curation improves. The resources are in use today by a number of material science groups and the resources provide a semantic foundation for a consolidated data resource of data related to a special issue of a material science journal. While we have focused here on nanomaterials, we believe this model can be used by a wide range of efforts that need to model and explore content that rely on the process-structure-property linkages, which is most of material science. We plan to continue to evolve and improve the NanoMine knowledge graph and ontology as our team and collaborators identify and curate more polymer nanocomposite experiments into the graph, and to expand the framework of NanoMine to provide similar support for metamaterials research.

References

1. Brinson, L.C., et al.: Polymer nanocomposite data: curation, frameworks, access, and potential for discovery and design. ACS Macro Lett. **9**, 1086–1094 (2020)
2. Duerr, R.E., et al.: Formalizing the semantics of sea ice. Earth Sci. Inf. **8**(1), 51–62 (2014). https://doi.org/10.1007/s12145-014-0177-z
3. Dumontier, M., et al.: The semantic science integrated ontology (SIO) for biomedical research and knowledge discovery. J. Biomed. Semant. **5**(1), 14 (2014)
4. Ellis, B., Smith, R.: Polymers: A Property Database. CRC Press (2008)
5. Groth, P., Gibson, A., Velterop, J.: The anatomy of a nanopublication. Inf. Serv. Use **30**(1–2), 51–56 (2010)
6. Koho, M., Heino, E., Hyvönen, E., et al.: SPARQL faceter-client-side faceted search based on SPARQL. In: LIME/SemDev@ ESWC (2016)
7. Lebo, T., Sahoo, S., McGuinness, D.: PROV-O: The PROV Ontology (2013). http://www.w3.org/TR/prov-o/
8. McCusker, J.P., Chastain, K., Rashid, S., Norris, S., McGuinness, D.L.: SETLr: the semantic extract, transform, and load-r. PeerJ Preprints 6, e26476v1 (2018)
9. McCusker, J.P., Dumontier, M., Yan, R., He, S., Dordick, J.S., McGuinness, D.L.: Finding melanoma drugs through a probabilistic knowledge graph. PeerJ Comput. Sci. **3**, e106 (2017)
10. McCusker, J.P., et al.: Broad, interdisciplinary science in tela: an exposure and child health ontology. In: Proceedings of the 2017 ACM on Web Science Conference, pp. 349–357 (2017)
11. Mrdjenovich, D., et al.: Propnet: a knowledge graph for materials science. Matter **2**(2), 464–480 (2020). https://doi.org/10.1016/j.matt.2019.11.013

12. Otsuka, S., Kuwajima, I., Hosoya, J., Xu, Y., Yamazaki, M.: Polyinfo: polymer database for polymeric materials design. In: 2011 International Conference on Emerging Intelligent Data and Web Technologies, pp. 22–29. IEEE (2011)
13. Piñero, J., et al.: Disgenet: a comprehensive platform integrating information on human disease-associated genes and variants. Nucleic Acids Res. gkw943 (2016)
14. Satyanarayan, A., Moritz, D., Wongsuphasawat, K., Heer, J.: Vega-lite: a grammar of interactive graphics. IEEE Trans. Vis. Comput. Graph. **23**(1), 341–350 (2016)
15. Schadler, L., Brinson, L.C., Sawyer, W.: Polymer nanocomposites: a small part of the story. JOM **59**(3), 53–60 (2007)
16. Strötgen, J., et al.: Towards the bosch materials science knowledge base. In: ISWC Satellites (2019)
17. Zhang, X., Liu, X., Li, X., Pan, D.: MMKG: an approach to generate metallic materials knowledge graph based on DBpedia and Wikipedia. Comput. Phys. Commun. **211**, 98–112 (2017). https://doi.org/10.1016/j.cpc.2016.07.005. High Performance Computing for Advanced Modeling and Simulation of Materials
18. Zhao, H., et al.: Nanomine schema: an extensible data representation for polymer nanocomposites. APL Mater. **6**(11), 111108 (2018)