



Award #: OAC-1835677

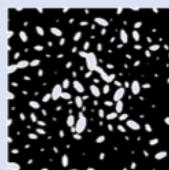
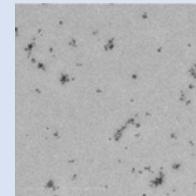
## CSSI Element: Nanocomposites to Metamaterials A Knowledge Graph Framework

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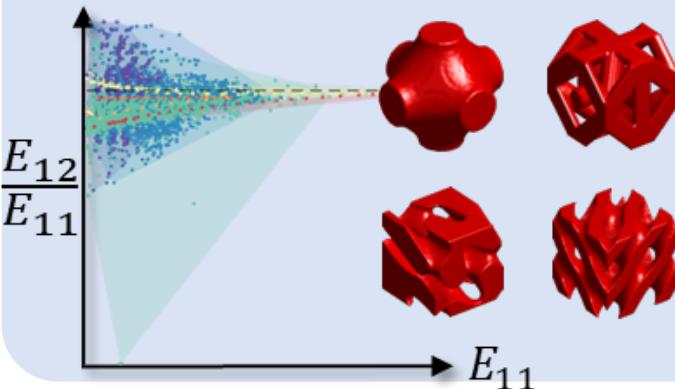
Institutions: <sup>1</sup>Duke University, <sup>2</sup>Northwestern,  
<sup>3</sup>Rensselaer Polytech. Inst., <sup>4</sup>Caltech, <sup>5</sup>Univ. Vermont

### Polymer Nanocomposites

< 1% nanoparticle  
→ dramatic changes in physical properties



### Structural Metamaterials



Geometric structure patterns → “impossible” properties, eg band gaps

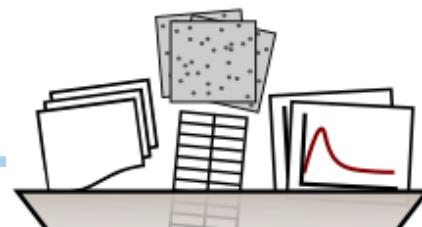
NSF CSSI PI Meeting, Seattle, WA, Feb. 13-14, 2020

# MaterialsMine

An open data resource for materials scientists

### DATA CURATION

Materials structure, processing, and property data extracted from literature, individual experiments



Organized data + Metadata

Excel template  
Flattened  
Configurable

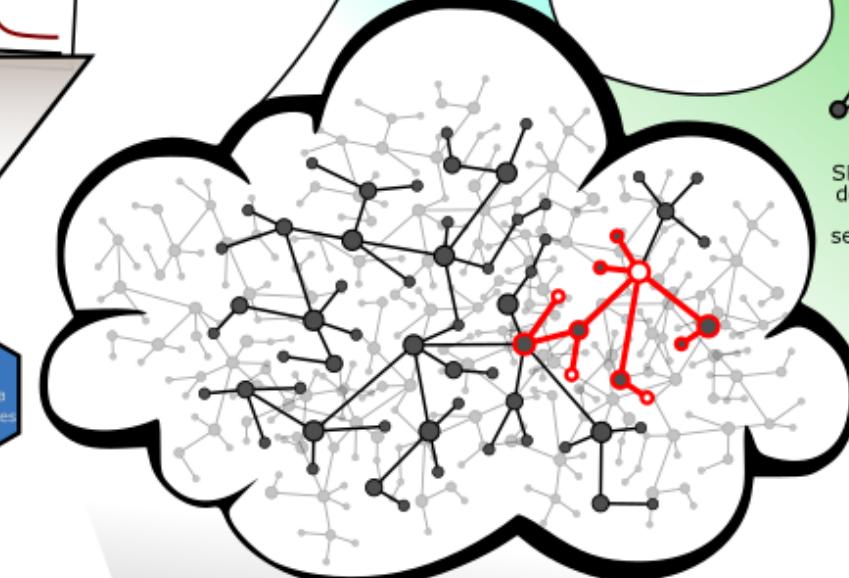
R tools  
Wrangle data  
Output datafiles  
Tidy data

XML schema  
Unified data structure  
Auto-generated metadata (DOI, ChemProps)

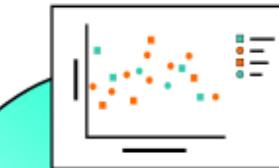
MongoDB  
XML documents & supplementary datafiles

Conversion of XML data to RDF

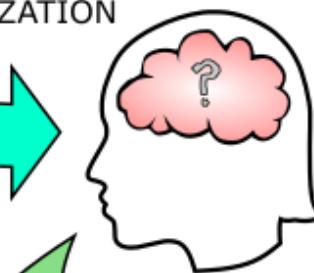
Bindings to SPARQL query returned in tabular format



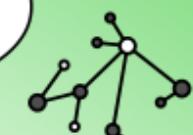
### SEARCH & VISUALIZATION



Search results presented to user as customizable visual plots



Faceted browser lets user select parameters of interest



SPARQL query defines graph pattern to search against Knowledge Graph

Metadata descriptors  
Volume fraction  
Radius  
Shape  
Particle size  
Particle spacing  
Interfacial area

Correlation function

Microstructure Characterization & Reconstruction  
3-D reconstruction

### DATA STORAGE

Blazegraph  
RDF triple store

### MODULAR ANALYSIS & SIMULATION TOOLS