Making materials science resources discoverable and accessible with the NIST Materials Resource Registry

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TMS Annual Meeting
March 15, 2018
Phoenix, AZ

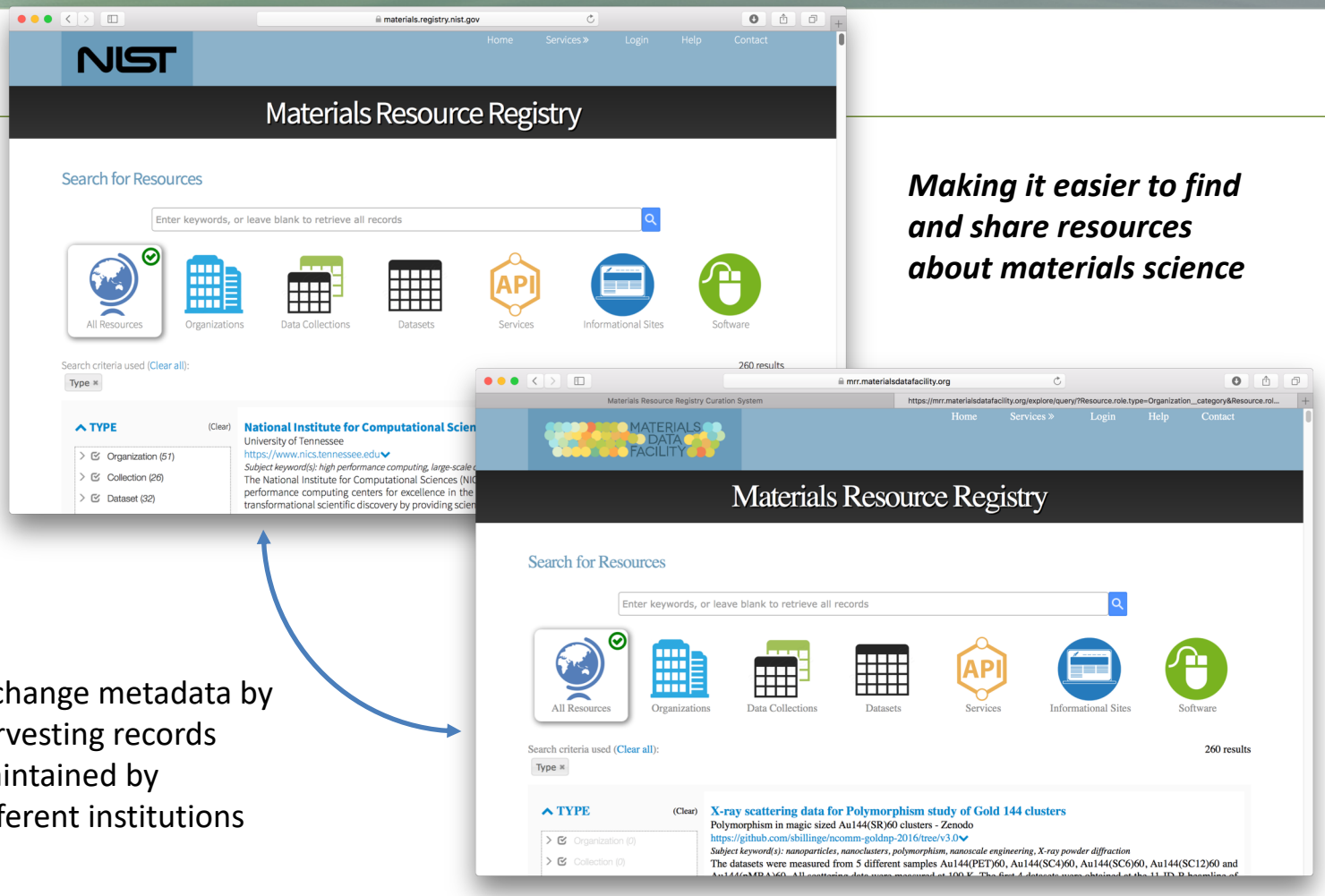
Goals for Materials Resource Registry

Materials data is proliferating, and finding/using it can be time-consuming

Help users find data-related resources to improve design, research and collaboration by:

- Defining and building consensus around minimum required metadata for materials science data discovery
- Deploying metadata schema using a pilot registry infrastructure developed by NIST
- Validating with materials science data collections at organizations participating in the Working Group

- Support development of an ecosystem around making data and metadata available and machine-actionable
  - From multiple sources (MDF, Materials Commons, nanoHub, researcher repositories, etc.)
  - Where each institution can control how they distribute the data



Making it easier to find and share resources about materials science

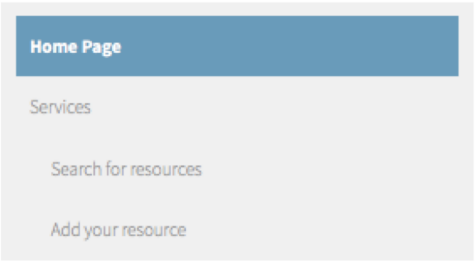
Exchange metadata by harvesting records maintained by different institutions

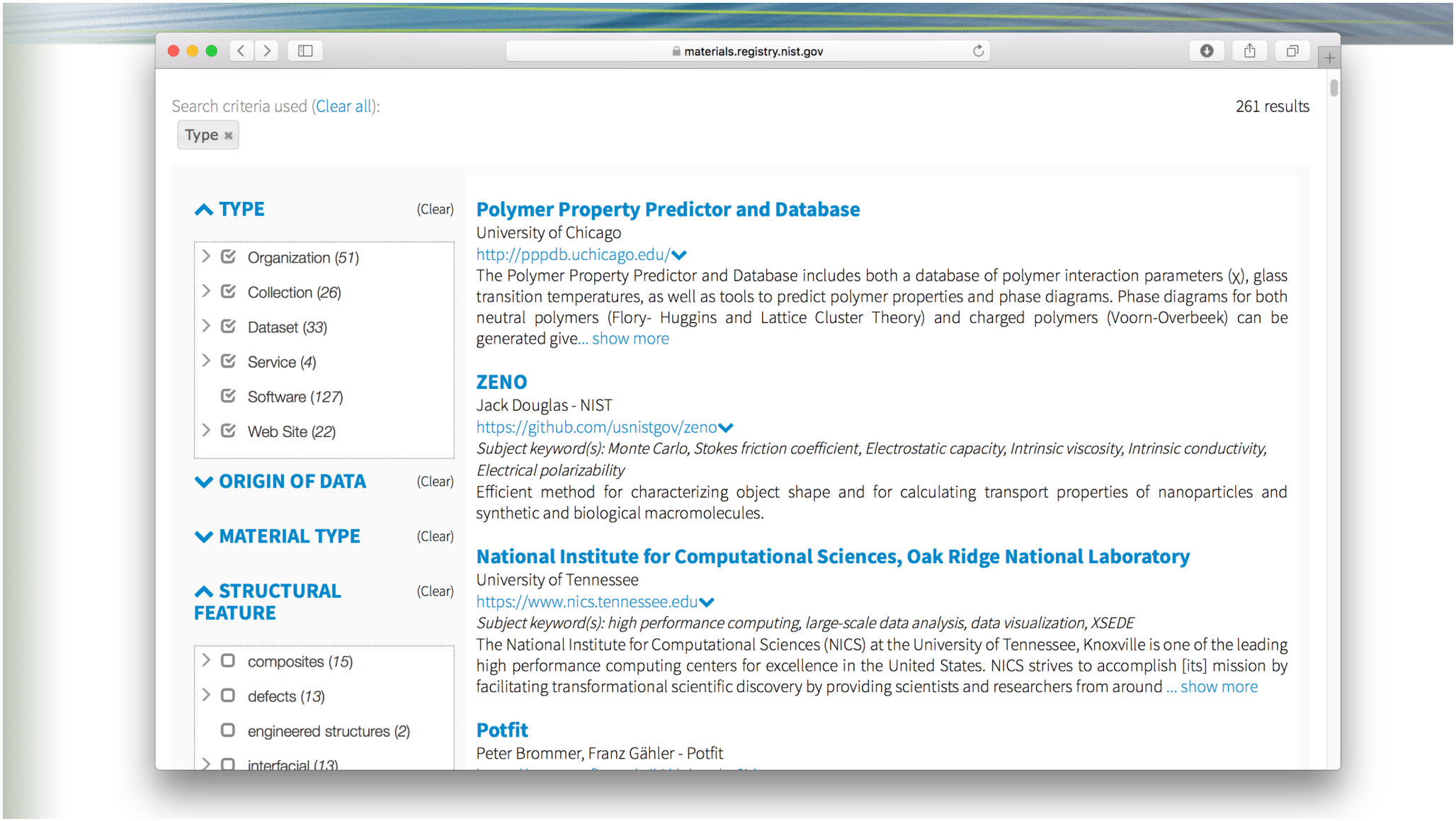
Materials Resource Registry Application

Find Materials Data

This system allows for the registration of materials resources, bridging the gap between existing resources and the end users. The Materials Resource Registry functions as a centrally located service, making the registered information available for research to the materials community.

This is being developed at the National Institute of Standards and Technology and is made available to




materials.registry.nist.gov
Search criteria used (Clear all):
Type ×
261 results
TYPE (Clear)
Organization (51)
Collection (26)
Dataset (33)
Service (4)
Software (127)
Web Site (22)
ORIGIN OF DATA (Clear)
MATERIAL TYPE (Clear)
STRUCTURAL FEATURE (Clear)
composites (15)
defects (13)
engineered structures (2)
interfacial (13)
Polymer Property Predictor and Database
University of Chicago
http://pppdb.uchicago.edu/
The Polymer Property Predictor and Database includes both a database of polymer interaction parameters (χ), glass transition temperatures, as well as tools to predict polymer properties and phase diagrams. Phase diagrams for both neutral polymers (Flory- Huggins and Lattice Cluster Theory) and charged polymers (Voorn-Overbeek) can be generated give... show more
ZENO
Jack Douglas - NIST
https://github.com/usnistgov/zeno
Subject keyword(s): Monte Carlo, Stokes friction coefficient, Electrostatic capacity, Intrinsic viscosity, Intrinsic conductivity, Electrical polarizability
Efficient method for characterizing object shape and for calculating transport properties of nanoparticles and synthetic and biological macromolecules.
National Institute for Computational Sciences, Oak Ridge National Laboratory
University of Tennessee
https://www.nics.tennessee.edu
Subject keyword(s): high performance computing, large-scale data analysis, data visualization, XSEDE
The National Institute for Computational Sciences (NICS) at the University of Tennessee, Knoxville is one of the leading high performance computing centers for excellence in the United States. NICS strives to accomplish [its] mission by facilitating transformational scientific discovery by providing scientists and researchers from around ... show more
Potfit
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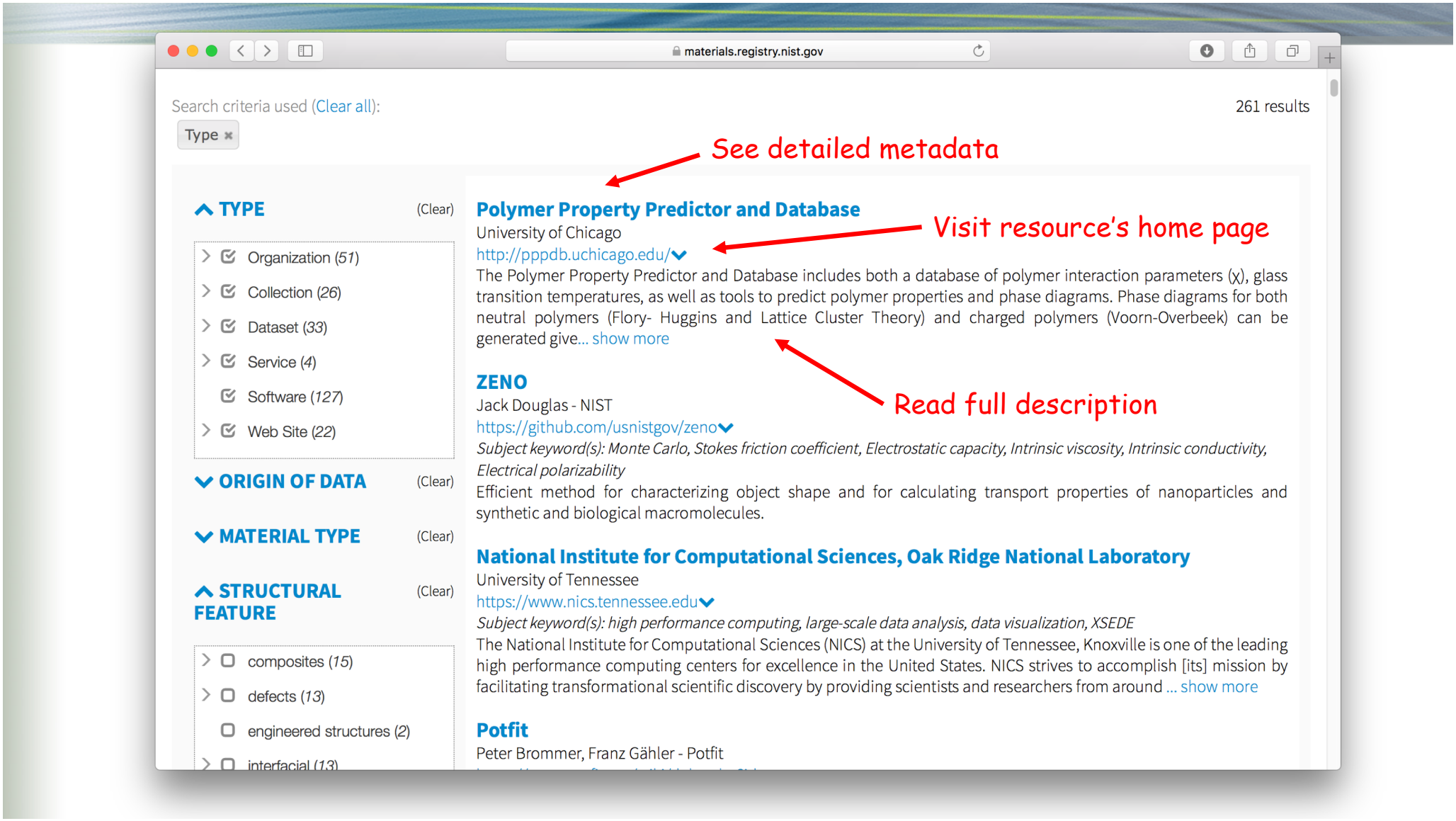
materials.registry.nist.gov
Search criteria used (Clear all):
Type ×
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See detailed metadata
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Collection (26)
Dataset (33)
Service (4)
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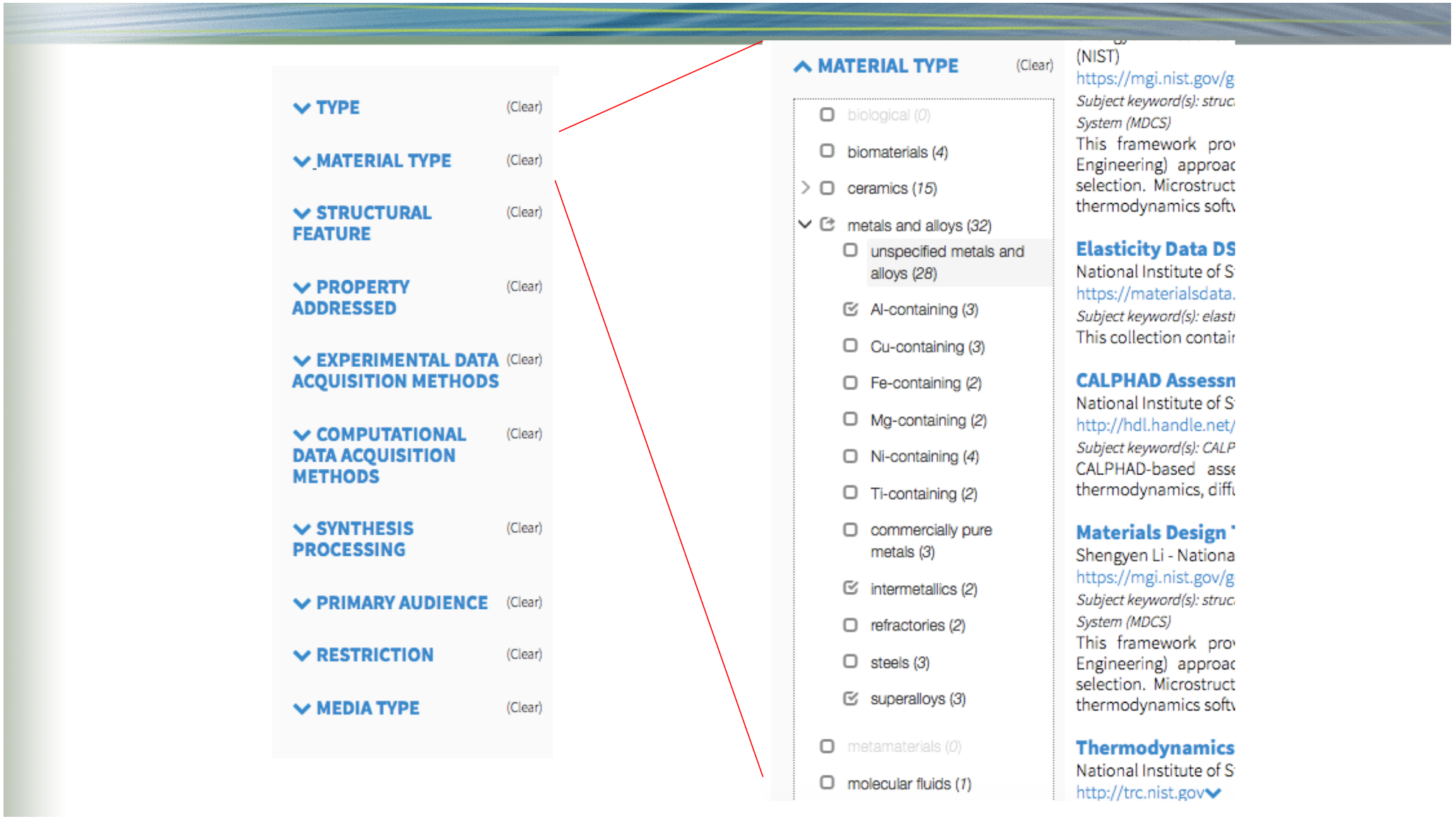
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STRUCTURAL FEATURE (Clear)
PROPERTY ADDRESSED (Clear)
EXPERIMENTAL DATA ACQUISITION METHODS (Clear)
COMPUTATIONAL DATA ACQUISITION METHODS (Clear)
SYNTHESIS PROCESSING (Clear)
PRIMARY AUDIENCE (Clear)
RESTRICTION (Clear)
MEDIA TYPE (Clear)
MATERIAL TYPE (Clear)
biological (0)
biomaterials (4)
ceramics (15)
metals and alloys (32)
unspecified metals and alloys (28)
Al-containing (3)
Cu-containing (3)
Fe-containing (2)
Mg-containing (2)
Ni-containing (4)
Ti-containing (2)
commercially pure metals (3)
intermetallics (2)
refractories (2)
steels (3)
superalloys (3)
metamaterials (0)
molecular fluids (1)
(NIST)
https://mgi.nist.gov/g
Subject keyword(s): struc
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Elasticity Data DS
National Institute of S
https://materialsdata.
Subject keyword(s): elast
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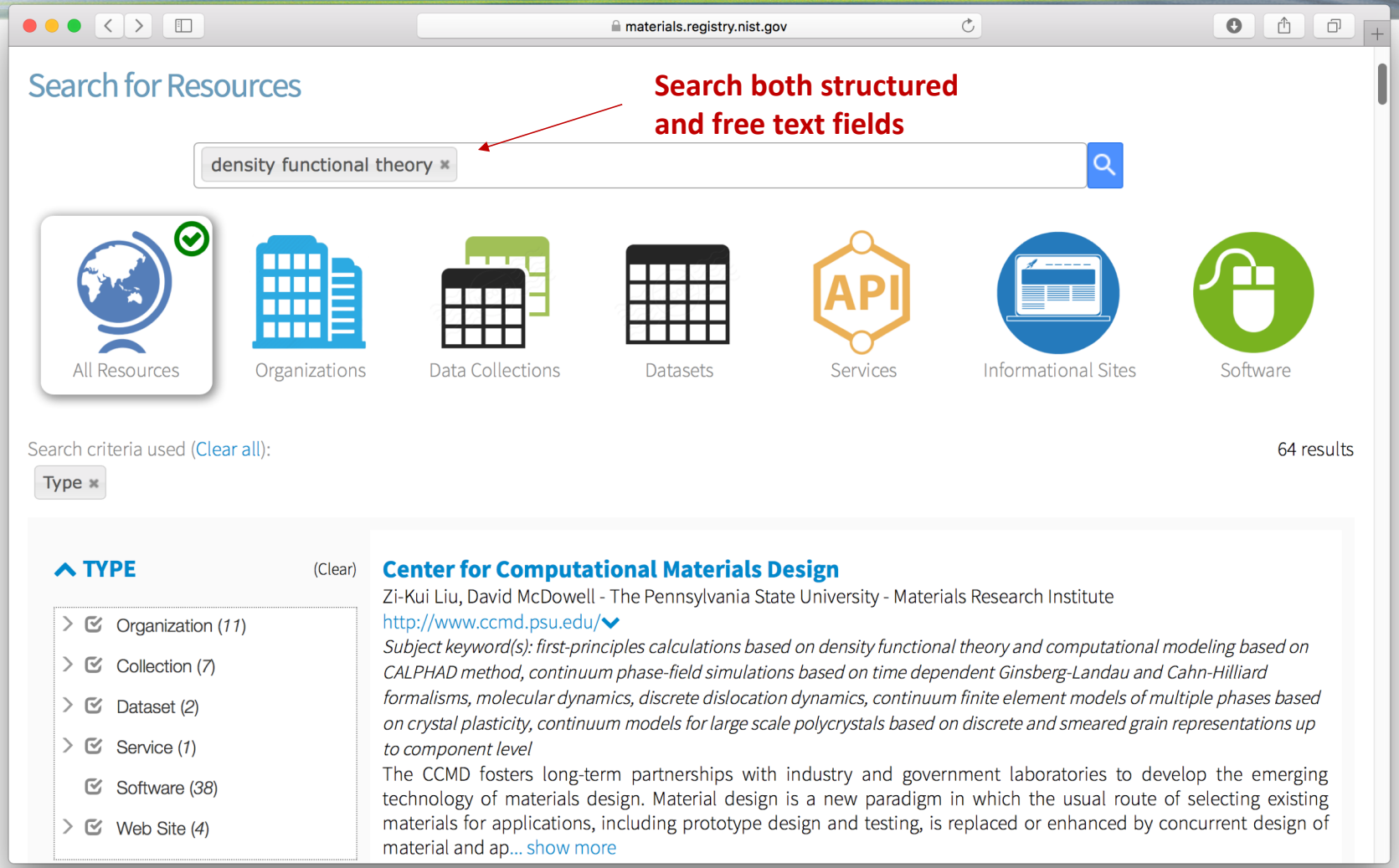

materials.registry.nist.gov
Search for Resources
Search both structured and free text fields
density functional theory
All Resources
Organizations
Data Collections
Datasets
API
Services
Informational Sites
Software
Search criteria used (Clear all):
Type
64 results
TYPE
(Clear)
Organization (11)
Collection (7)
Dataset (2)
Service (1)
Software (38)
Web Site (4)
Center for Computational Materials Design
Zi-Kui Liu, David McDowell - The Pennsylvania State University - Materials Research Institute
http://www.ccmd.psu.edu/
Subject keyword(s): first-principles calculations based on density functional theory and computational modeling based on CALPHAD method, continuum phase-field simulations based on time dependent Ginsberg-Landau and Cahn-Hilliard formalisms, molecular dynamics, discrete dislocation dynamics, continuum finite element models of multiple phases based on crystal plasticity, continuum models for large scale polycrystals based on discrete and smeared grain representations up to component level
The CCMD fosters long-term partnerships with industry and government laboratories to develop the emerging technology of materials design. Material design is a new paradigm in which the usual route of selecting existing materials for applications, including prototype design and testing, is replaced or enhanced by concurrent design of material and ap... show more

Materials Resource Registry

Select a Resource type to add


Organization


Data Collection


Dataset

Service


Informational


Software

Organization - a group of people that come together to contribute to or participate in a federated data operation. Organizations can be hierarchical: an organization can contain or sponsor other organizations. Organizations can also aggregate or participate with other organizations in broader collaborations.

Data Collection - An aggregation of one or more datasets, possibly spanning many research projects or teams.

- Repository - A data collection service that specializes in hosting data from many different research teams and projects.
- Project Archive - A large collection of data resulting from a project that produces and publishes data over an extended period of time and made accessible through a common portal or interface.
- Database - A collection of data that is not formally file-based but stored in a database system. Here, a database is not assumed to be relational and can be quite complex in structure.

Dataset - a set of data (can be one or more separate files or other digital objects) that is unified by a common set of research goals and/or results. This is intended to be a single publishable unit of scientific output that might be described in a single journal article.

Service - A set of stand-alone services not associated with a particular collection of data but which can either operate on data or produce data. Such a resource

Running instances

Two instances running to date, collectively containing 360+ records, searchable from either interface:

- NIST Materials Resource Registry
  - https://materials.registry.nist.gov
  - NIST records plus a number of records related to the U.S. Materials Genome Initiative (MGI)
- Center for Hierarchical Materials Design (CHiMaD) Materials Resource Registry
  - https://mrr.materialsdatafacility.org
  - Records associated with CHiMaD efforts, including Midwest Data Spoke
- Records represent many institutions and types of resources

Working with several other institutions to exchange records from existing infrastructures

Do I have to give you my data? No.

Metadata – Key to Federating

Federate registries by exchanging resource description records

A common description schema makes this possible

This project has adopted an XML-based approach

- OAI-PMH for searching and exchanging records
  - Supports distributed search and future releases will have increased support for access control
- XML Schema for defining record format/syntax

Building extensible metadata

- Defining concepts, vocabularies in format-free way
- Encode into XML using techniques that allow for future extension and evolution

Developed high-level MSE vocabulary to support searching across systems; working through Research Data Alliance with other international efforts

Concept Categories

- Data origin
- Material types
- Structural features
- Properties addressed
- Characterization methods *(covering experimental methods/techniques)*
- Computational methods
- Synthesis and processing

Properties addressed

Tier 1

chemical
colligative
corrosion
crystallographic
durability
electrical
kinetic
magnetic
mechanical
optical
rheological
structural
thermodynamic
toxicity
transport

Tier 2

chemical:
composition
functional ligands
impurity concentration
molecular weights

corrosion:
crevice
erosion-corrosion
galvanic
high temperature
intergranular
pitting
selective leaching
stress corrosion
uniform

crystallographic:
crystalline lattice
orientation maps
space groups
textures

durability:
aging
coefficient of friction
thermal shock resistance
water absorption
wear resistance

kinetic:
grain growth
phase evolution
phase transitions and ordering

electrical:
band structure
conductivity
current and energy density
dielectric constant and spectra
dielectric dispersion
electrostrictive
piezoelectric
power conversion efficiency
pyroelectric
resistivity
spin polarization
superconductivity
thermoelectric

Supporting software descriptions

Resulting from merging in another NIST registry effort: MGI Code Catalog

- A registry of materials science and engineering related software
- Funded under the US Materials Genome Initiative
- Needed to merge metadata schemas used

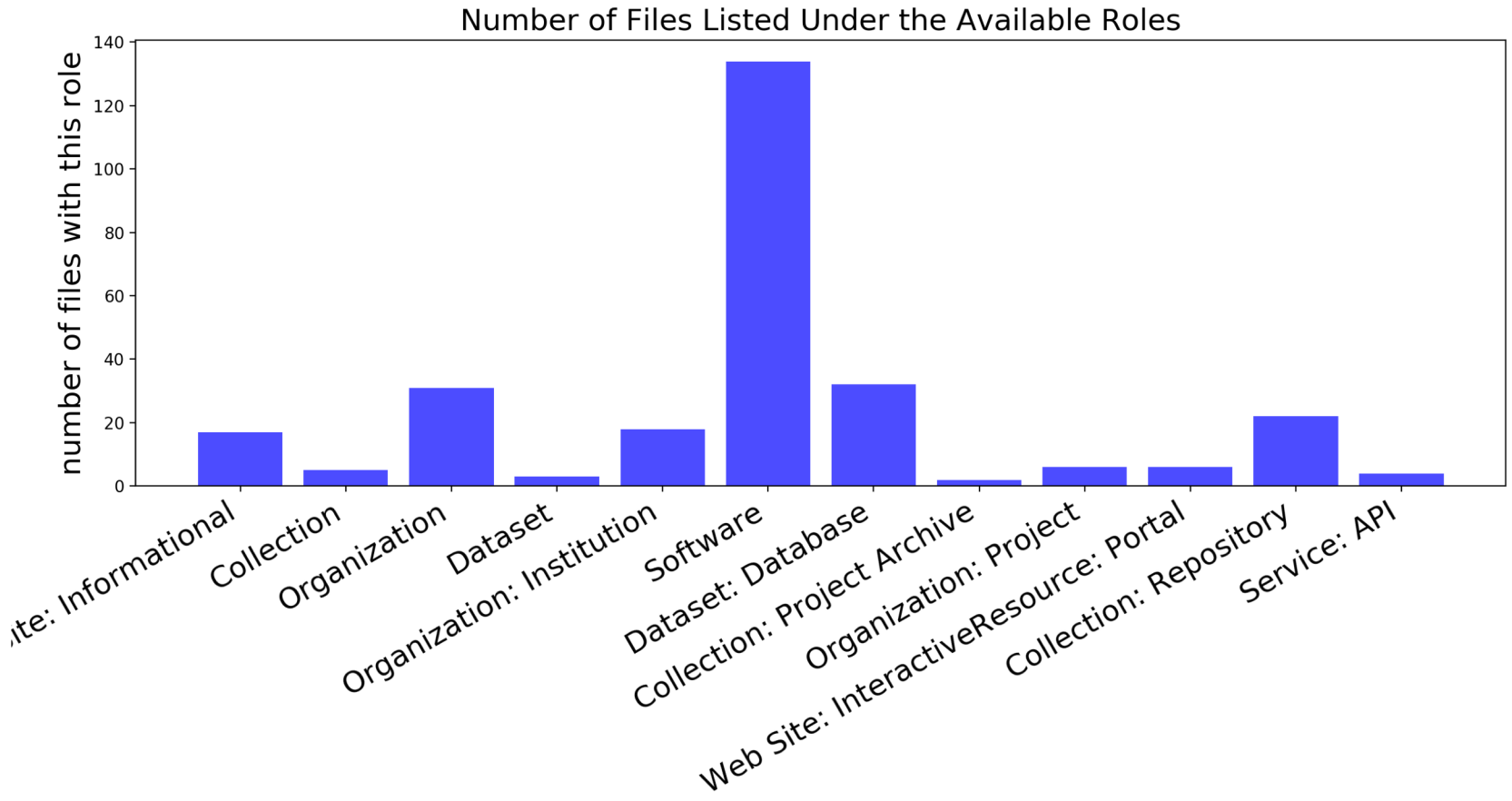
Some metadata additions are generic (not specific to materials)

- e.g. code language, supported OS, license, etc.

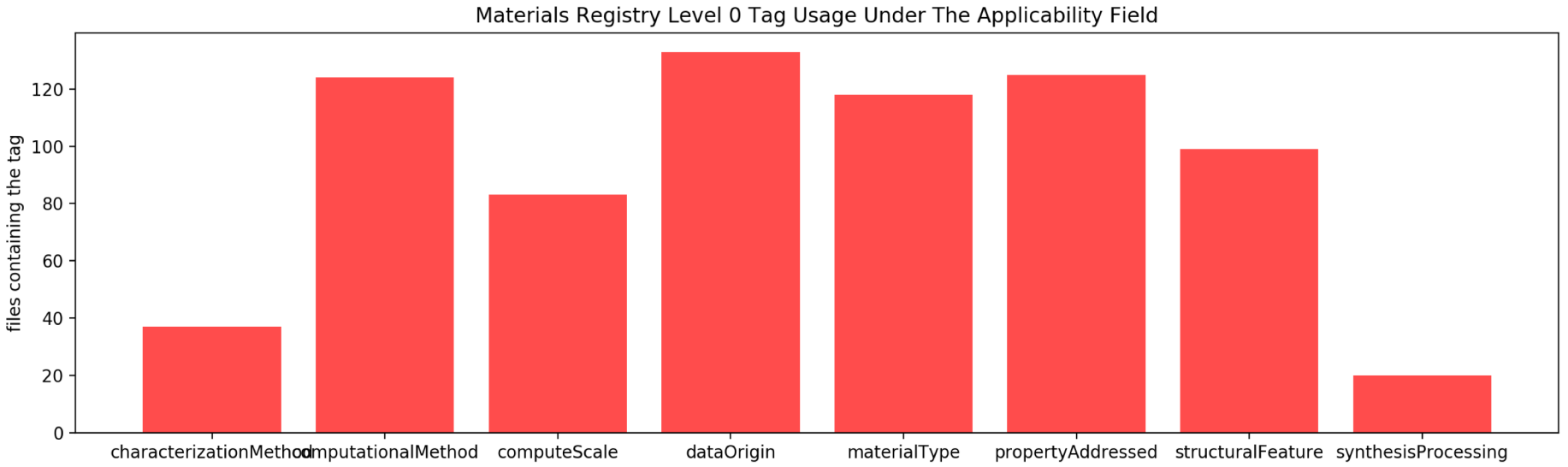
Compute scale – physical scale a computation models/simulates

electronic scale, nanoscale (atomic), microscale, mesoscale, structural scale, multiscale

Types of resources (NIST instance)



Categories represented in the NIST instance (Number of records)



Summary

Basic functionality in place for registering resources, harvesting between instances, and searching

The newest version of the schema, supporting software, and vocabulary are available

Currently populating the MRR with records and continuing to test the components and system

Examining ways to populate records more easily and consistently

Working with other institutions to link into their existing infrastructures

https://materials.registry.nist.gov

Interested in running an instance or advertising your resource?

- We can help.