Materials Resource Registries Working Group Breakout session

21 September 2017

Moderators: Jim Warren, Laura Bartolo, Chandler Becker, Ray Plante

Agenda

1) Problem description and results (20 minutes)

2) Discussion re resources, contributions, identification of partners, and future plans (40 minutes)

3) Discussion to identify action items (20 minutes)

4) Summary of results and actions identified (10 minutes)

Problem Description

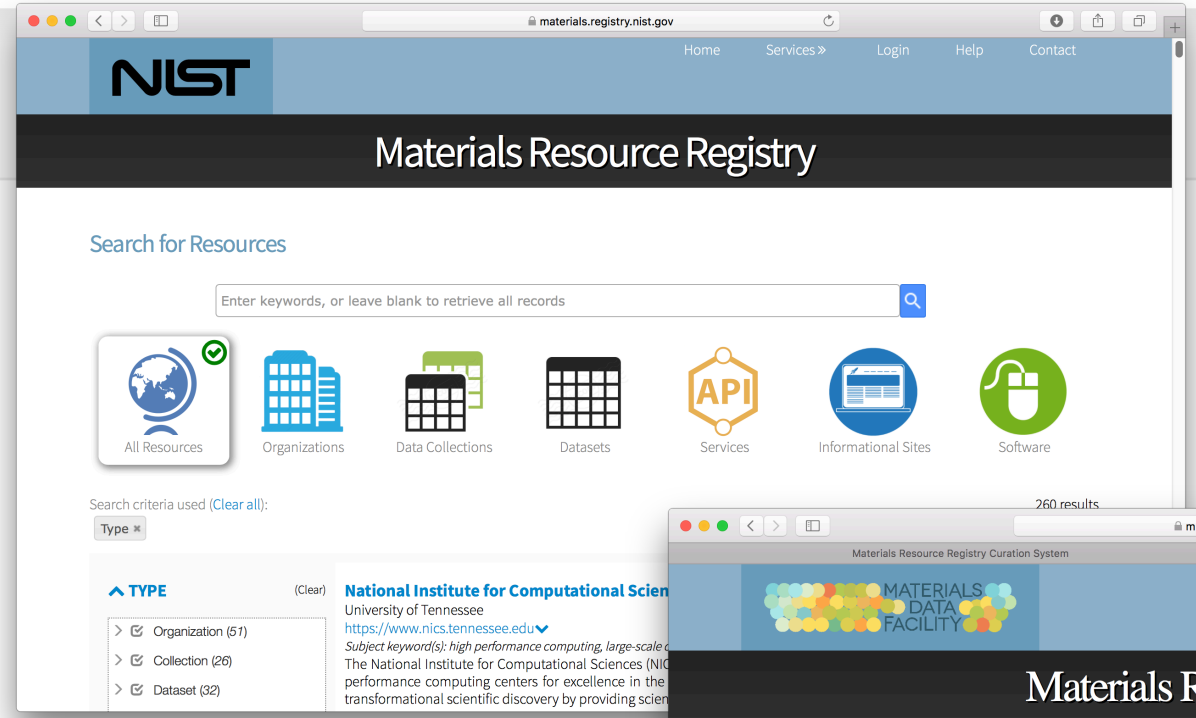
- Materials science is very broad and interdisciplinary
  - Primarily comes from: metallurgy, ceramics, polymer science
  - Plus: physics, chemistry, chemical engineering, geology, electronics, optics, biology
- Engineers need to answer questions like:
  - "What structural properties and processing methods are required to develop new lightweight materials that significantly improve fuel efficiency yet meet safety standards satisfied by traditional materials in use today?"
- Materials data is proliferating, but it is difficult and time-consuming to find and use

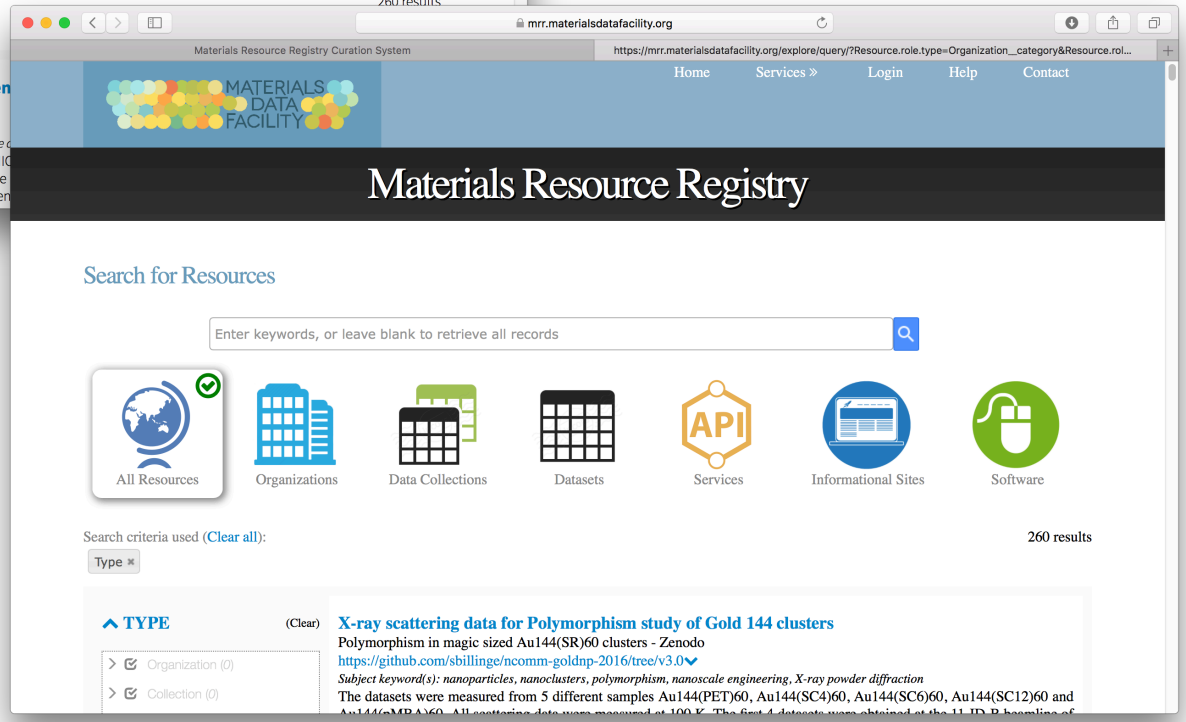
Goals for MRR

- 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

Goals for this meeting

- Solicit resource contributions
- Review software development, enhancements, and timetable.
- Identify registry partners for an International Resource Registry Federation.
- Identify contributors to Best Practices & Final Report documents





Making it easier to find and share resources about materials science

Exchange metadata by harvesting records maintained by different institutions

Metadata – Key to Federating

- Federate registries by exchanging resource description records
- A common description schema makes this possible
- This working group has adopted an XML-based approach
  - OAI-PMH for exchanging records
  - 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

Materials Science Metadata

- Showed prototype schema at RDA6 [Fall 2015] through registry application
  - Used to filter records based on materials science concepts
  - Illustrate use for MS metadata
- Subsequent development as Materials Science vocabulary
  - Development boosted by VO-CAMP workshop (Dec. 2016)
  - Approach: Concept categories + two-tier level of terms

    Ex: **Material Types:** ceramics: oxides
  - Balance the need for specificity against not overwhelming users with options
  - Note: we are trying to describe high-level resources

    e.g. Repositories, databases, web sites; not individual datasets or measurements
- WG Workshop: 23 Feb 2017
  - Vocabulary presented and updated
- Vocabulary presented at RDA9 in April 2017 and feedback requested
- Further changes incorporated in response to feedback through Summer ‘17

MRR status

- First version of the schema, supporting software, and vocabulary are being released
- Basic functionality in place for registering resources, harvesting between instances, and searching
- Initial deployments at two institutions
  - National Institute of Standards and Technology (NIST)
  - Center for Hierarchical Materials Design (CHiMaD headquartered at Northwestern Univ. and U Chicago)
- Currently populating the MRR with records and continuing to test the components and system

Timeline

- Month 1 (Jul ’16)
  - recruit domain specialists to participate in WG
- Month 2 (Aug/Sep ’16)
  - initiate discussions about conducting a survey of existing materials science data providers
  - develop 20 typical data discovery queries to inform metadata discussions
- Month 3 (Sep/Oct ’16)
  - hold meeting to draft 1st version of metadata extensions to Dublin Core
- Months 4-8 (Oct ’16 - Feb ’17)
  - disseminate draft to the materials science community, both within and external to RDA, and solicit feedback
- Month 8 (Feb ’17)
  - hold teleconference to refine metadata extensions and establish implementation pilot program
- Months 9-12 (Mar – Jun ’17)
  - Evaluate & give feedback on MatSci Vocabulary BY 01 May 2017
  - Implement pilot federated registry and recruit testers/evaluators
  - Write best practices guidelines document
- Months 13-15 (Jul – Sep ’17)
  - Adoption & Recommendations BY 01 SEPTEMBER 2017
  - Document metadata development process: what worked well, what didn’t expand content of pilot registry
- Months 16-18 (Oct – Dec ’17)
  - Prepare final document for delivery to RDA

Concept Categories

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

Data Origin

Tier 1

experiments
informatics and data science
simulations
theory

Material Types

Tier 1

biological
biomaterial
ceramics
metals and alloys
metamaterials
molecular fluids
organic compounds
organometallics
polymers
semiconductors

Tier 2

ceramics:
carbides
cements
nitrides
oxides
perovskites
silicates

metals and alloys:
Al-containing
commercially pure metals
Cu-containing
Fe-containing
intermetallics
Mg-containing
Ni-containing
rare earths
refractories
steels
superalloys
Ti-containing

polymers:
copolymers
elastomers
homopolymers
liquid crystals
polymer blends
rubbers
thermoplastics
thermosets

semiconductors:
II-VI
III-V
extrinsic
intrinsic
n-type
p-type

Material types

organic compounds:

alcohols
aldehydes
alkanes
alkenes
alkynes
amines
carboxylic acids
cyclic compounds
cycloalkanes
esters
ketones
nitriles

Contributions in red primarily from CHiMaD Polymer Data Core group

Structural features

Tier 1

composites
defects
engineered structures
interfacial
microstructures
molecular structures
morphologies
phases

Tier 2

composites:
biological or green
fiber-reinforced
metal-matrix
nanocomposites
particle-reinforced
polymer-matrix
structural

defects:
cracks
crazing
debonding
disclinations
dislocations
inclusions
interstitials
point defects
pores
vacancies
voids

interfacial:
grain boundaries
interfacial surface area
interfacial tension or energy
interfacial thickness
magnetic domain walls
ordering boundaries
phase boundaries
stacking faults
surfaces
twin boundaries

microstructures:
BCC spheres
cellular
clustering
compound
crystallinity
defect structures
dendritic
dispersion
eutectic
grains
gyroid
HEX cylinders
lamellae
nanocrystalline
particle distribution
particle shape
polycrystalline
~~polydispersity~~
porosity
precipitates
quasicrystalline
single crystal
twinned

Structural features

Tier 1

composites
defects
engineered structures
interfacial
microstructures
molecular structures
morphologies
phases

Tier 2

molecular structure:
alternating copolymer
block copolymer
bottlebrush
dendrimer
end-group composition
functionalization
gradient copolymer
long-chain branching
molecular weight
polydispersity
random copolymer
short-chain branching
surfactants
tacticity

morphologies:
aligned
amorphous
anisotropic
clusters
complex fluids
glass
isotropic
layered
nanoparticles or nanotubes
one-dimensional
open-framework
particles or colloids
percolated
porous
quantum dots or wires
random
semicrystalline
thin film
two-dimensional
wires
woven

phases:
crystalline
disordered
gas
liquid
melt
metastable
nonequilibrium
ordered

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

Properties addressed

Tier 1

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

Tier 2

magnetic:
coercivity
Curie temperature
magnetization
permeability
saturation magnetization
susceptibility

mechanical:
acoustic emission
bulk modulus
compression response
creep
deformation mechanisms
ductility
elasticity
fatigue
flexural response
fracture behavior
fracture toughness
hardness
impact response
phonon modes
plasticity
Poisson's ratio
shear response
strength
stress-strain behavior
tensile response
tensile strength
visoelasticity
yield strength

optical:
index of refraction
luminescence
photoconductivity

rheological:
complex modulus
monomer friction coefficient
viscoelasticity
viscosity

Properties addressed

Tier 1

chemical
colligative
corrosion
crystallographic
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optical
rheological
structural
thermodynamic
toxicity
transport

Tier 2

thermodynamic:
calorimetry profile
critical temperatures
crystallization temperature
degradation temperature
density
glass transition temperature
grain boundary energies
heat capacity
heat of fusion
heat of solidification
interfacial energies
liquid crystal phase transition temperature
melting temperature
molar volume
phase diagram
phase stability
specific heat
superconductivity
surface energies
thermal conductivity
thermal decomposition temp.
thermal expansion

transport:
diffusivity
grain boundary diffusivity
interdiffusion
intrinsic diffusivity
mobilities
surface diffusivity
tracer diffusivity

Characterization methods

Tier 1

charge distribution
chromatography
dilatometry
electrochemical
mechanical
microscopy
optical
osmometry
profilometry
scattering and diffraction
spectrometry
spectroscopy
thermochemical
tomography
ultrasonic
viscometry

Tier 2

charge distribution:
pulsed electroacoustic method

chromatography:
critical and supercritical chromatography
gas-phase chromatography
ion chromatography
liquid-phase chromatography

electrochemical:
amperometry
potentiometry
voltammetry

mechanical:
compression tests
creep tests
dynamic mechanical analysis
fatigue testing
hardness testing
in-situ testing
nanoindentation
shear or torsion tests
tension tests
wear tests

Characterization methods

Tier 1

charge distribution
chromatography
dilatometry
electrochemical
mechanical
microscopy
optical
osmometry
profilometry
scattering and diffraction
spectrometry
spectroscopy
thermochemical
tomography
ultrasonic
viscometry

Tier 2

microscopy:
analytical electron microscopy
atomic force microscopy
confocal microscopy
electron probe microanalysis
environmental scanning electron microscopy
field emission electron probe
optical microscopy
photoluminescence microscopy
scanning Auger electron microscopy
scanning electron microscopy
scanning Kelvin probe
scanning probe microscopy
scanning tunneling microscopy
transmission electron microscopy
x-ray optical interferometry

optical:
differential refractive index
dynamic light scattering
ellipsometry
fractography
light scattering
quasi-elastic light scattering

osmometry:
freezing point depression
membrane osmometry
vapor pressure depression osmometry

Characterization methods

Tier 1

charge distribution
chromatography
dilatometry
electrochemical
mechanical
microscopy
optical
osmometry
profilometry
scattering and diffraction
spectrometry
spectroscopy
thermochemical
tomography
ultrasonic
viscometry

Tier 2

scattering and diffraction:
electron backscatter diffraction
neutron [elastic] scattering
neutron [inelastic] scattering
small angle x-ray scattering and USAXS
small-angle neutron
synchrotron
x-ray diffraction
x-ray reflectivity
x-ray topography
XRD grazing incidence

spectrometry:
alpha spectrometry
energy dispersive x-ray spectrometry
gamma spectrometry
ion mobility spectrometry
IR/FTIR spectrometry
mass spectrometry
secondary ion mass spectrometry
x-ray fluorescence spectrometry

Characterization methods

Tier 1

charge distribution
chromatography
dilatometry
electrochemical
mechanical
microscopy
optical
osmometry
profilometry
scattering and diffraction
spectrometry
spectroscopy
thermochemical
tomography
ultrasonic
viscometry

Tier 2

spectroscopy:
dielectric and impedance spectroscopy
dynamic mechanical analysis
electron energy-loss spectroscopy
EXAFS
Fourier-transform infrared spectroscopy
neutron spin echo spectroscopy
NEXAFS
nuclear magnetic resonance
Raman spectroscopy
x-ray absorption spectroscopy
x-ray emission spectroscopy
x-ray photoelectron spectroscopy
XPS variable kinetic

thermochemical:
calorimetry
differential scanning calorimetry
differential thermal analysis
microcalorimetry
thermogravimetry

tomography:
atom probe tomography
x-ray tomography

Computational methods

Tier 1

boundary tracking or level set
CALPHAD
cellular automata
cluster expansion
crystal plasticity
density functional theory or electronic structure
discrete element method
dislocation dynamics
dissipative particle dynamics
finite element analysis
machine learning
micromagnetics simulations
molecular dynamics
Monte Carlo methods
multiscale simulations
phase-field calculations
reverse Monte Carlo
self-consistent field theory
simulated experiment
statistical mechanics

Synthesis and processing

Tier 1

annealing and homogenization
casting
deposition and coating
forming
fractionation
mechanical and surface
powder processing
quenching
reactive
self-assembly
solidification

Tier 2

annealing and homogenization:
aging
dry blending
homogenization
mechanical mixing
melt mixing
normalizing
recrystallization
stress relieving
tempering
twin screw extrusion
ultrasonication

casting:
centrifugal casting
continuous casting
die casting
investment casting
sand casting
slip casting
vacuum arc melting

deposition and coating:
atomic layer deposition
carbon evaporation coating
chemical vapor deposition
electrodeposition
electron beam deposition
evaporation
gold-sputter coating
ink-jet deposition
ion beam deposition
Langmuir-Blodgett film deposition
physical vapor deposition
plasma spraying
pulsed laser deposition
splatter
spin coating
solvent casting
sputter coating

Synthesis and processing

Tier 1

annealing and homogenization
casting
deposition and coating
forming
fractionation
mechanical and surface
powder processing
quenching
reactive
self-assembly
solidification

Tier 2

forming:
cold rolling
compression molding
drawing
extrusion
forging
hot pressing
hot rolling
injection molding
milling
rotational molding
vacuum molding
~~molding~~

mechanical and surface:
doctor blade or blade coating
focused ion beam
joining
lithography
polishing
sectioning
thermal plasma processing

powder processing:
atomization
ball milling
centrifugal disintegration
hot pressing
sintering
sponge iron process

quenching:
air cooled / quench
brine quench
furnace cooled
gas cooled
ice quench
liquid nitrogen quench
oil quench
water quench

Synthesis and processing

Tier 1

annealing and homogenization
casting
deposition and coating
forming
fractionation
mechanical and surface
powder processing
quenching
reactive
self-assembly
solidification

Tier 2

reactive:
addition polymerization
condensation polymerization
curing
dissolving / etching
drying
in-situ polymerization
post-polymerization modification
reductive roasting
solution processing
~~solvent casting~~

self-assembly:
micelle formation
monolayer formation
self-assembly-assisted grafting

solidification:
crystallization
directional solidification
precipitation
rapid solidification
seeded solidification
single crystal solidification
zone refining

Supporting software descriptions

- Resulting from merging in another registry effort: NIST 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

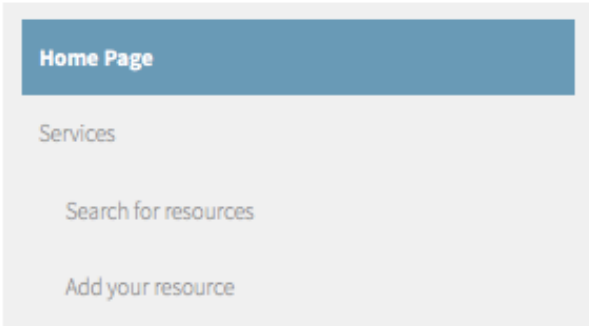
Materials Resource Registry Application



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



Running instances

- Two instances running to date, collectively containing 260+ records:
  - 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
  - Records represent many institutions and types of resources

- Interested in running an instance? Talk with Ray and Chandler. We can help get things installed and configured.

Discussion about efforts and plan

- Identification of resources
- New instances
- Reports
- Other possible search demonstrations
  - Leveraging repository-level search services

Discussion re action items

- Deployment of new instances
- Reports
- Software release (NIST)

Summary

- First version of the schema, supporting software, and vocabulary are being released
- Basic functionality in place for registering resources, harvesting between instances, and searching
- Initial deployments at two institutions
  - National Institute of Standards and Technology (NIST)
  - Center for Hierarchical Materials Design (CHiMaD headquartered at Northwestern Univ. and U Chicago)
- Currently populating the MRR with records and continuing to test the components and system

- Want to be more involved?

Screenshots

Search criteria used (Clear all):

Type ×

73 results

TYPE (Clear)

- Organization (21)
- Collection (25)
- Dataset (12)
- Service (0)
- Software (2)
- Web Site (14)

MATERIAL TYPE (Clear)

STRUCTURAL FEATURE (Clear)

- composites (6)
- defects (2)
  - unspecified defects (0)
  - cracks (0)
  - dislocations (2)
  - inclusions (0)
  - interstitials (0)

Materials Design Toolkit

Shengyen LiNational Institute of Standards and Technology (NIST) - National Institute of Standards and Technology (NIST)

https://mgi.nist.gov/generic-materials-design-toolkit

Subject keyword(s): structural materials, superalloys, Co alloys, Ni-based superalloys, two-phase microstructures, Materials Data Curation System (MDCS)

This framework provides an environment for materials design. The ICME (Integrated Computational Materials Engineering) approach is implemented for processing-structure-property correlation with a optimizer for material selection. Microstructure evolution can be simulated using the CALPHAD approach and phase based models using thermodynamics softwar... show more

Exascale Co-design Center for Materials in Extreme Environments

Tim Germann, Jim Belak, David Richards, Allen McPherson

http://www.exmatex.org/

The objective of the Exascale Co-design Center for Materials in Extreme Environments (ExMatEx) is to establish the interrelationship among algorithms, system software, and hardware required to develop a multiphysics exascale simulation framework for modeling materials subjected to extreme mechanical and radiation environments. Such a simulation cap... show more

Bilbao Crystallographic Server

Walter de Gruyter

http://cryst.ehu.es/

Subject keyword(s): Crystallography

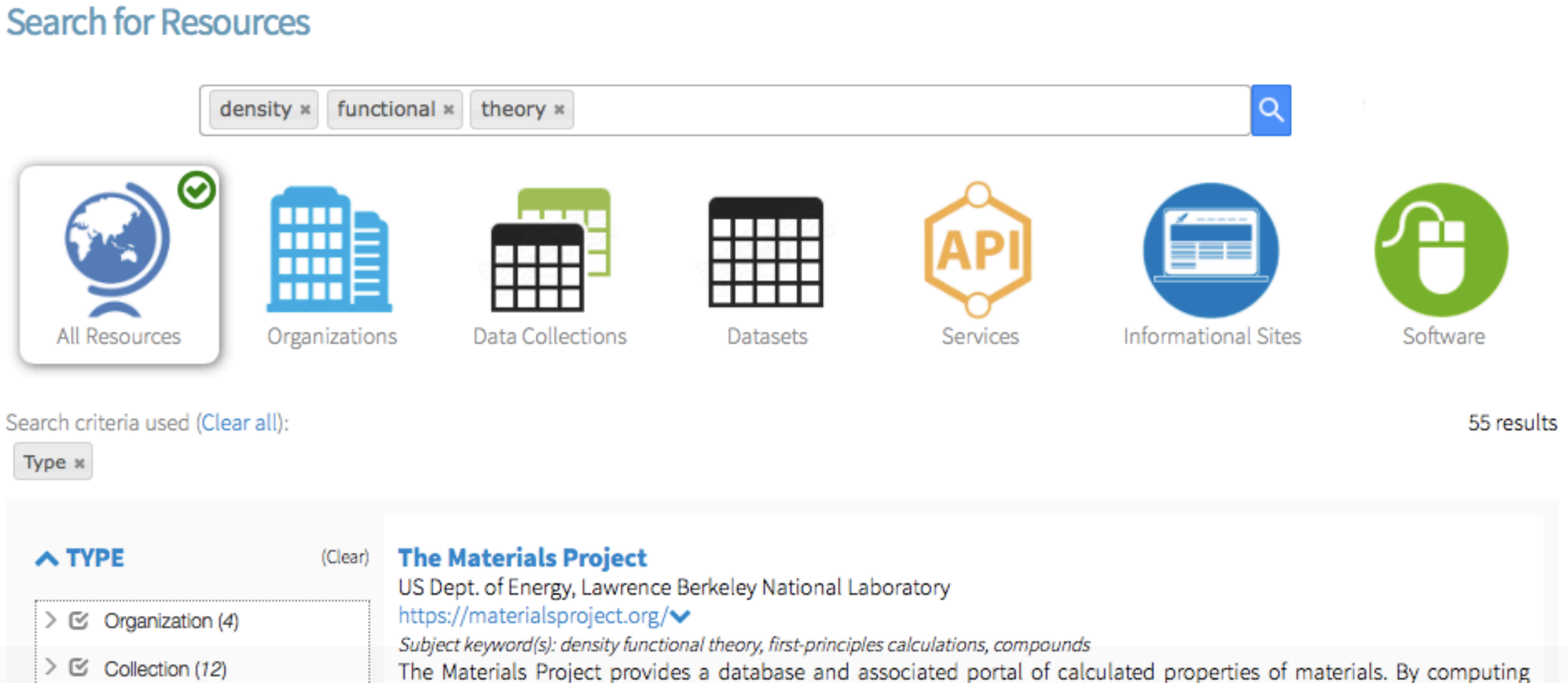
Initiated in 1997, at the Materials Laboratory of the University of the Basque Country, Spain, the Bilbao Crystallographic Server has since been offering its crystallographic and solid state programs and utilities, free of charge. The programs hosted on the server are on a wide variety of topics, and are grouped units called "shells".

DOE Data Explorer

Department of Energy

http://www.osti.gov/dataexplorer/

Subject keyword(s): DOE sponsored public data collections


Search for Resources
density
functional
theory
All Resources
Organizations
Data Collections
Datasets
API
Services
Informational Sites
Software
Search criteria used (Clear all):
55 results
Type
TYPE
(Clear)
Organization (4)
Collection (12)
The Materials Project
US Dept. of Energy, Lawrence Berkeley National Laboratory
https://materialsproject.org/
Subject keyword(s): density functional theory, first-principles calculations, compounds
The Materials Project provides a database and associated portal of calculated properties of materials. By computing

Search criteria used (Clear all):

Type ×

73 results

See detailed metadata

TYPE (Clear)

- Organization (21)
- Collection (25)
- Dataset (12)
- Service (0)
- Software (2)
- Web Site (14)

MATERIAL TYPE (Clear)

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Visit resource's home page

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Read full description

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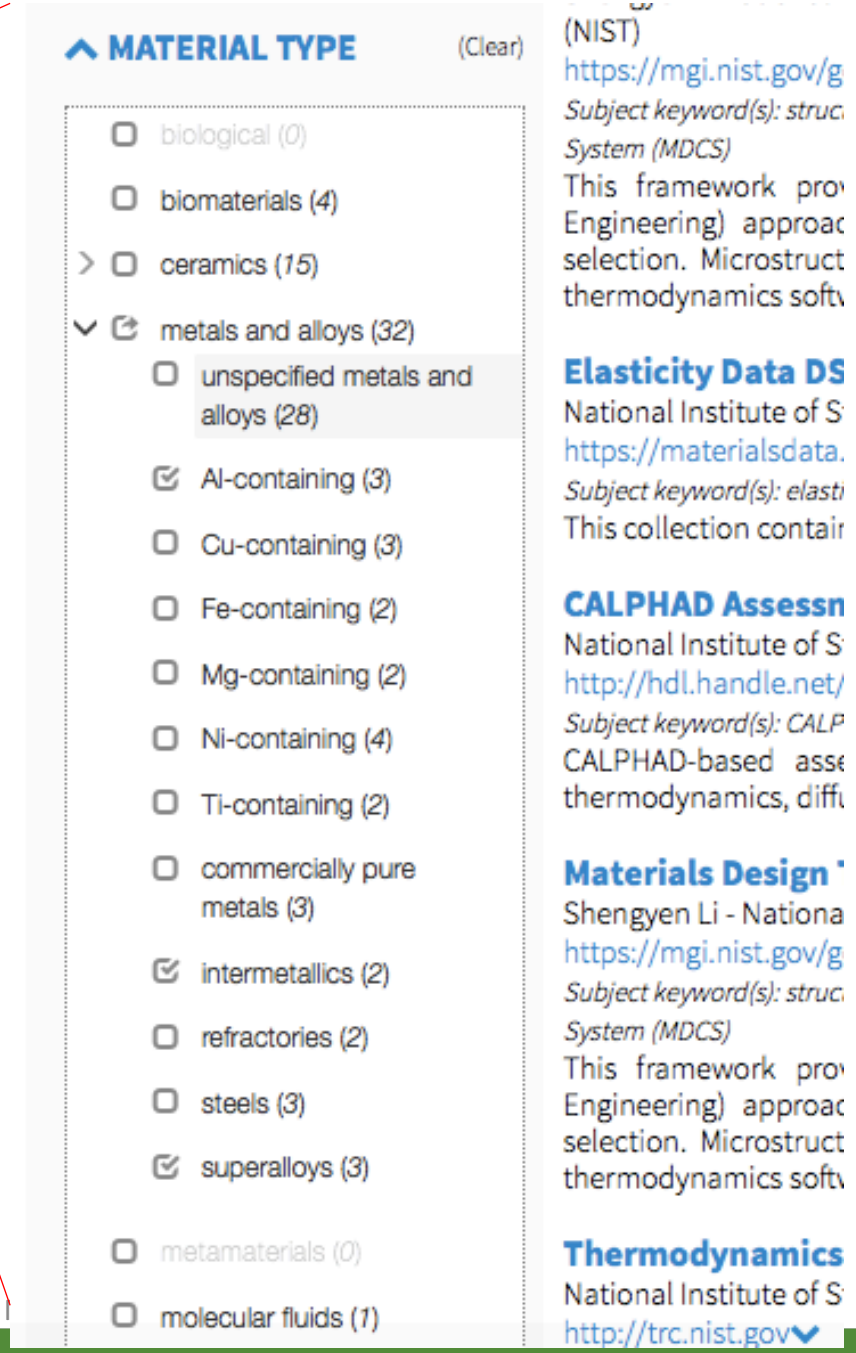
DOE Data Explorer

Department of Energy

http://www.osti.gov/dataexplorer/

Subject keyword(s): DOE sponsored public data collections


TYPE (Clear)
MATERIAL TYPE (Clear)
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
System (MDCS)
This framework pro
Engineering) approac
selection. Microstruct
thermodynamics soft
Elasticity Data DS
National Institute of S
https://materialsdata.
Subject keyword(s): elast
This collection contai
CALPHAD Assessn
National Institute of S
http://hdl.handle.net/
Subject keyword(s): CALP
CALPHAD-based asse
thermodynamics, diff
Materials Design
Shengyen Li - Nationa
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National Institute of S
http://trc.nist.gov

Materials Resource Registry

Select a Resource type to add


Organization


Data Collection


Dataset



Service


Informational


Software

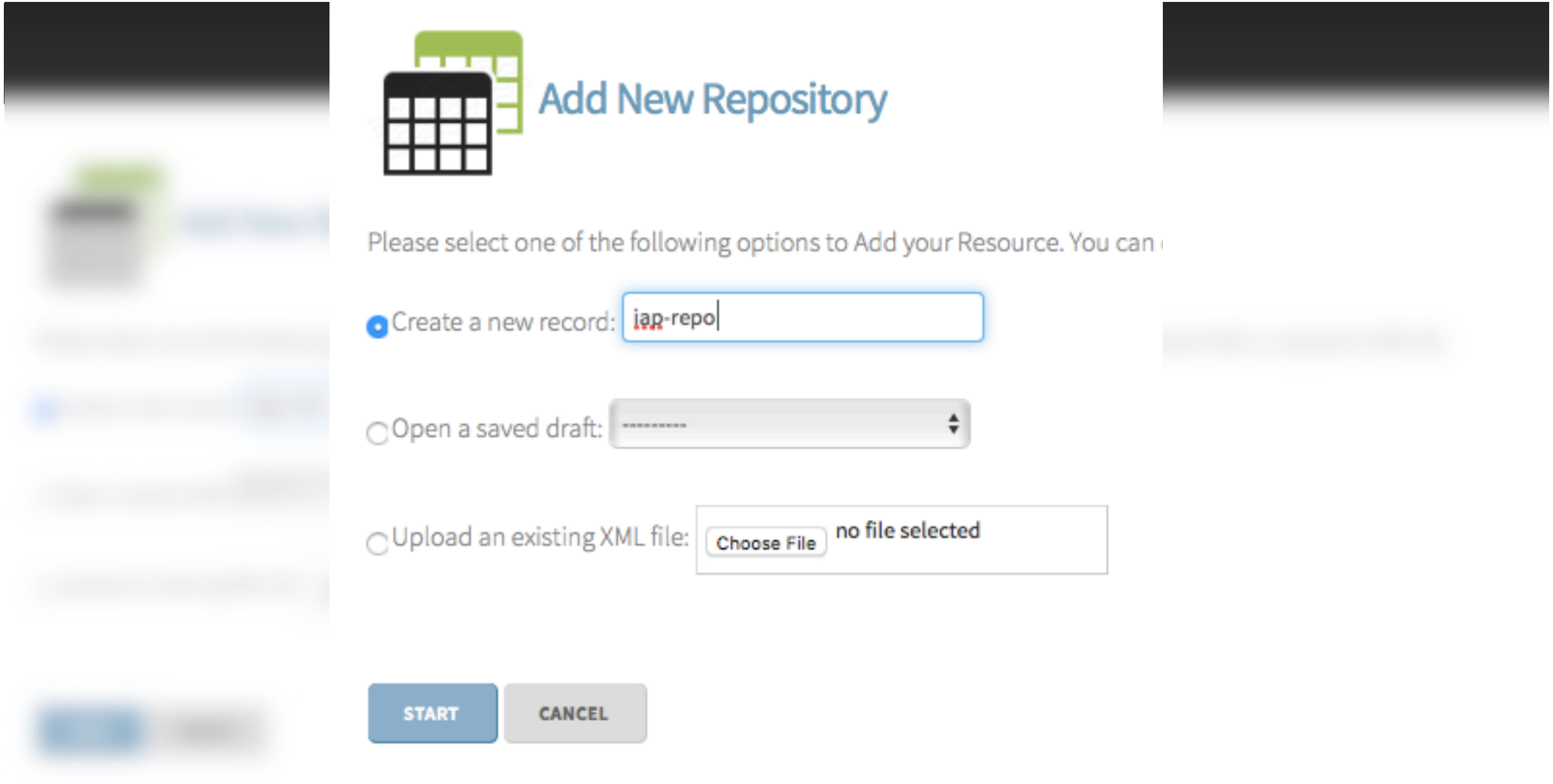
Organization - a group of people that come together to contribute to or participate in a federated data operation. Organizations can be hierarchical: an organization can contain or sponsor other organizations. Organizations can also aggregate or participate with other organizations in broader collaborations.

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

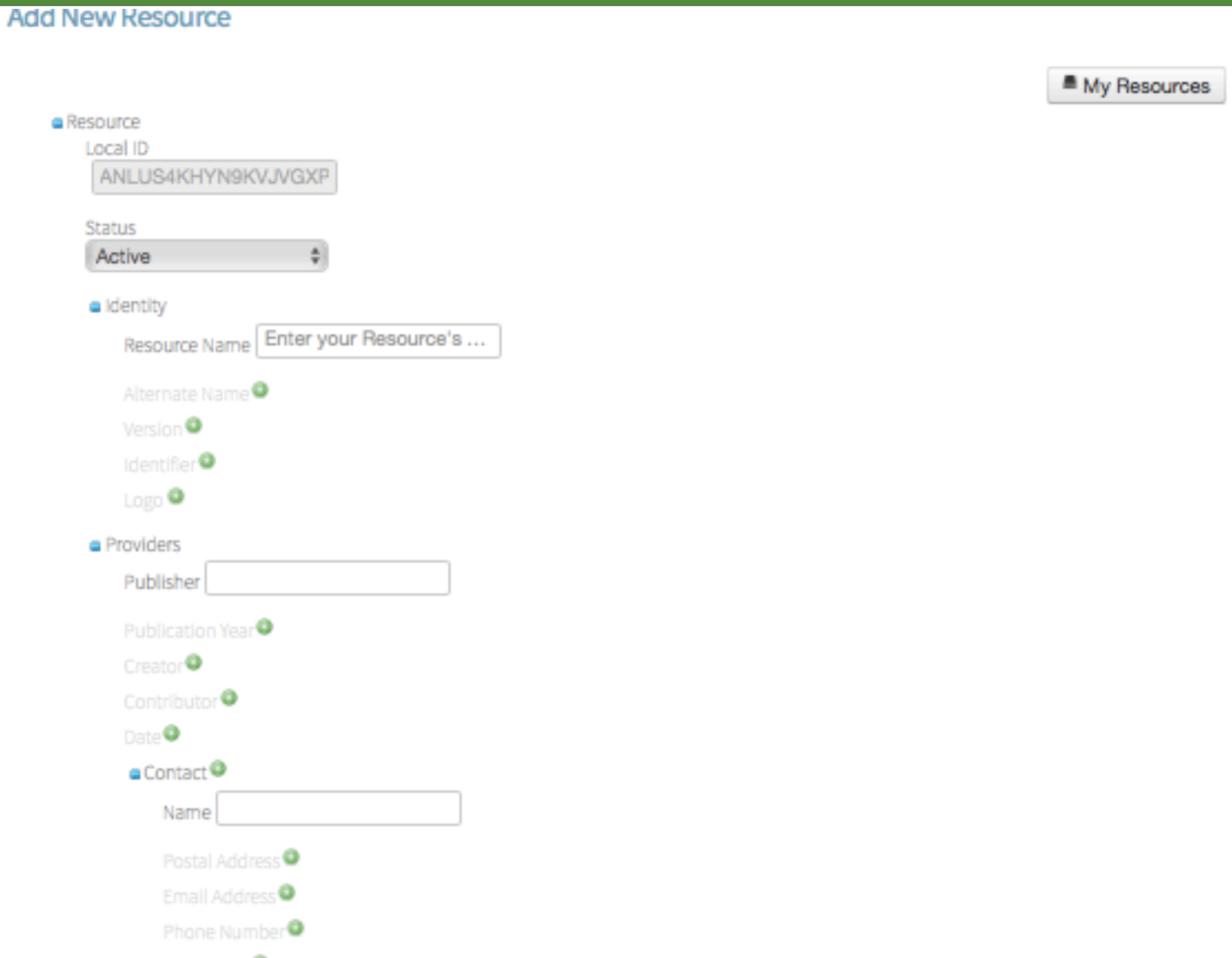
- Repository - A data collection service that specializes in hosting data from many different research teams and projects.
- Project Archive - A large collection of data resulting from a project that produces and publishes data over an extended period of time and made accessible through a common portal 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.

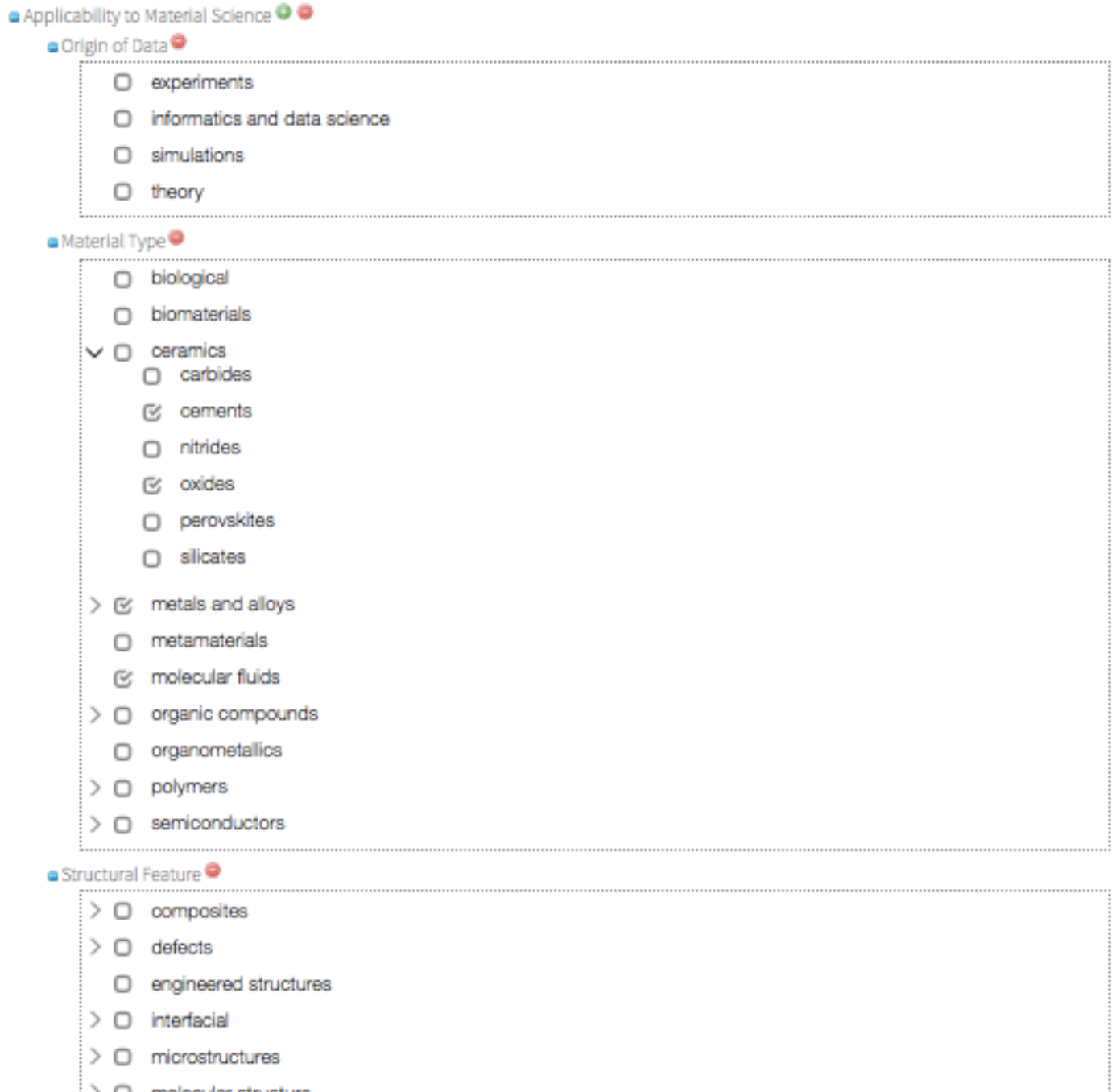
Dataset - a set of data (can be one or more separate files or other digital objects) that is unified by a common set of research goals and/or results. This is intended to be a single publishable unit of scientific output that might be described in a single journal article.

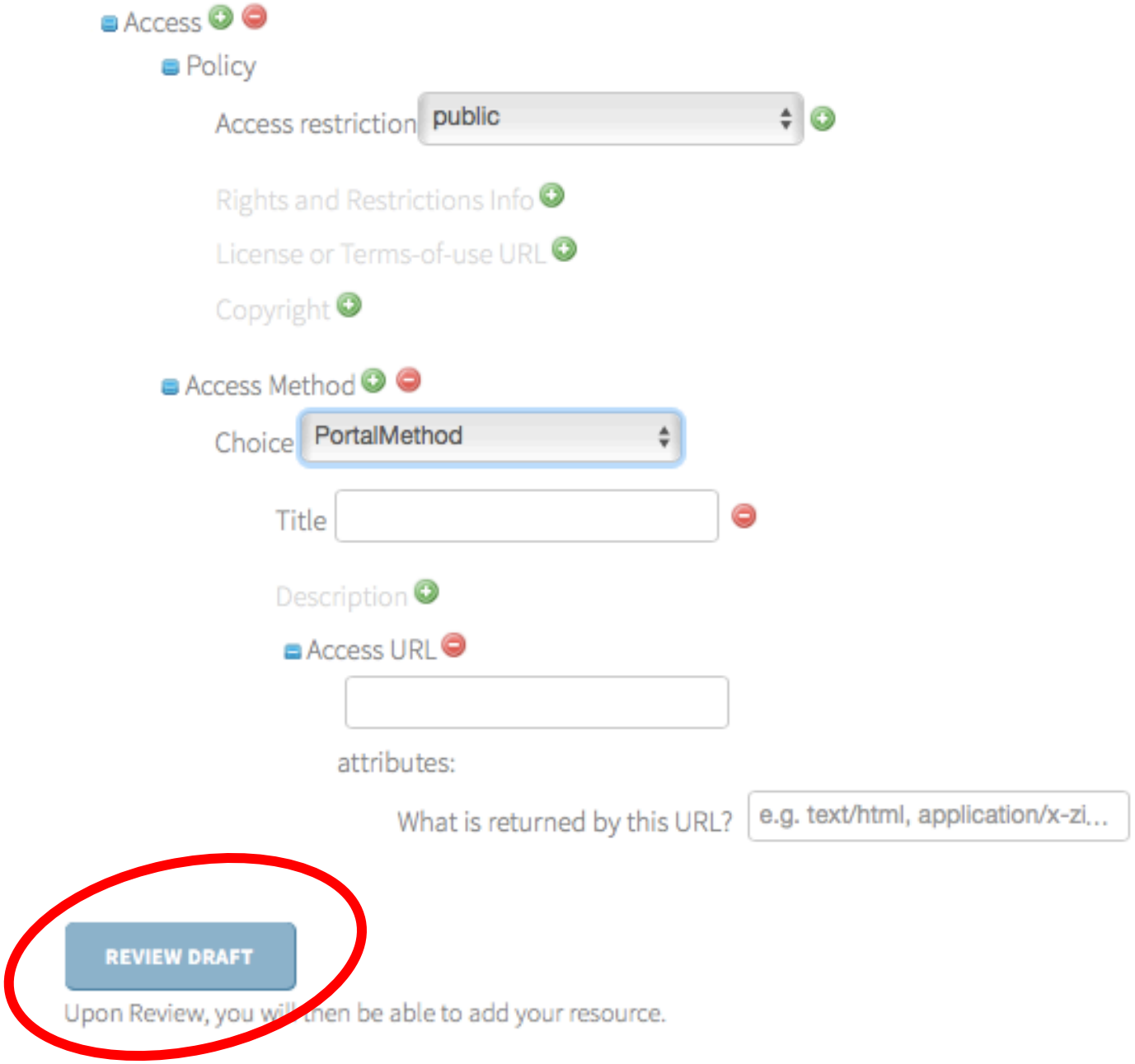
Service - A set of stand-alone services not associated with a particular collection of data but which can either operate on data or produce data. Such a resource


Add New Repository
Please select one of the following options to Add your Resource. You can
Create a new record:
iap-repo
Open a saved draft:

Upload an existing XML file:
Choose File
no file selected
START
CANCEL

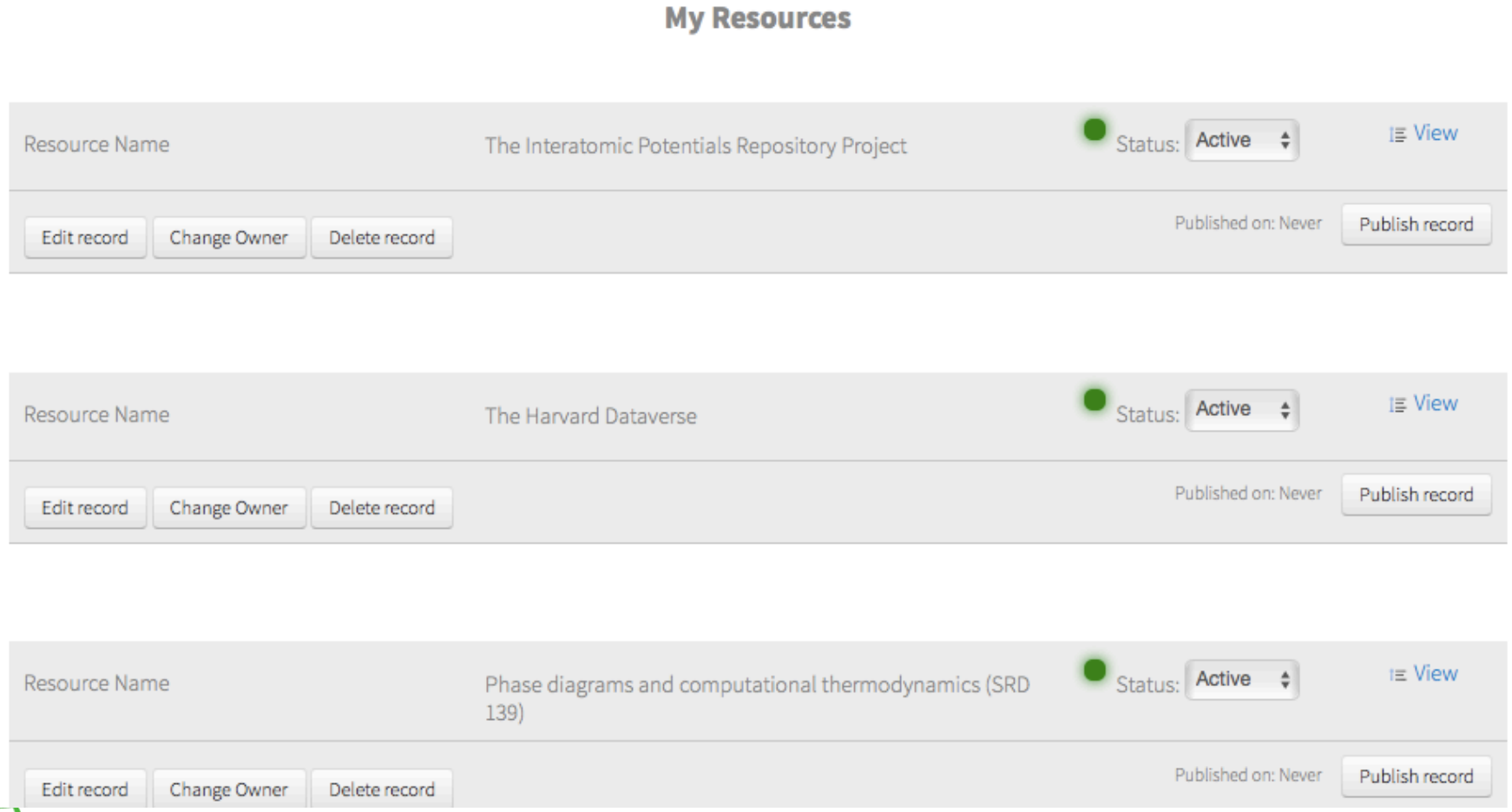

Add New Resource
My Resources
Resource
Local ID
ANLUS4KHYN9KVJVGXP
Status
Active
Identity
Resource Name
Enter your Resource's ...
Alternate Name
Version
Identifier
Logo
Providers
Publisher
Publication Year
Creator
Contributor
Date
Contact
Name
Postal Address
Email Address
Phone Number


Applicability to Material Science
Origin of Data
experiments
informatics and data science
simulations
theory
Material Type
biological
biomaterials
ceramics
carbides
cements
nitrides
oxides
perovskites
silicates
metals and alloys
metamaterials
molecular fluids
organic compounds
organometallics
polymers
semiconductors
Structural Feature
composites
defects
engineered structures
interfacial
microstructures

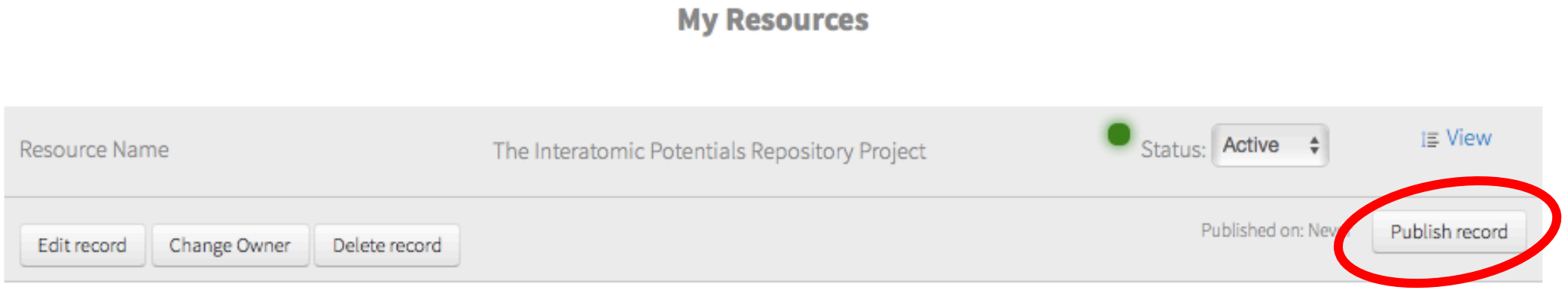

Access
Policy
Access restriction
public
Rights and Restrictions Info
License or Terms-of-use URL
Copyright
Access Method
Choice
PortalMethod
Title
Description
Access URL
attributes:
What is returned by this URL?
e.g. text/html, application/x-zi...
REVIEW DRAFT
Upon Review, you will then be able to add your resource.

Check results through the browser

- Browse your unpublished records through the Dashboard



Click “Publish”



Expected impact

- Lay the groundwork to make materials resources and data more readily discoverable, accessible, and interoperable
- Deliverables to the broader community beyond Materials Science
  - A model for a peer-to-peer federation of registries
  - Use of the OAI-PMH standard to exchange records
  - A model for interoperable metadata:
    - Includes common, non-discipline-specific metadata
    - Addition of discipline-specific metadata
  - A registry application with support for pluggable metadata
  - A vision for how a registry contributes to the search process
- Support development of an ecosystem around making data and metadata available and machine-actionable
  - E.g., data for machine learning to develop new materials