

MATERIALS RESOURCE REGISTRIES Working Group RDA Plenary 9 – Barcelona – 5 April 2017

Metadata and Software Development

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Outline

Metadata

- Intro to our approach
- Materials Science vocabulary development

Thursday's session: overview of general metadata schema

Registry Software (Demo)

- Incorporating vocabulary into the NIST Registry app
- Registering your resources

Later this session: uploading records via the REST interface



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 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
 - Latest version incorporating feedback at RDA WG site: https://www.rd-alliance.org/system/files/documents/Materials Registry vocab draft 170321.pdf

Search criteria used (Clear all): 73 results

Type ×

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>	ď	Organization (21)	
>	\subseteq	Collection (25)	
>	\subseteq	Dataset (12)	
>	\subseteq	Service (0)	
	\subseteq	Software (2)	
>	C	Web Site (14)	
~	M/	TERIAL TYPE	(Clea

▲ STRUCTURAL FEATURE

composites (6)

defects (2)

- unspecified defects (0)
- Cracks (0)
- dislocations (2)
- inclusions (0)

ar) 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 knowned/eli DOE engagered public data collections

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

organic compounds:

amines

nitriles

carboxylic acids

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

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 magnetic domain walls

ordering boundaries

phase boundaries

stacking faults

surfaces

twin boundaries

microstructures:

cellular

clustering

compound

crystallinity

defect structures

dendritic

dispersion

eutectic

particle shape polycrystalline polydispersity precipitates quasicrystalline single crystal

nanocrystalline

twinned

Structural features

Tier 2

Tier 1
composites
defects
engineered structures
interfacial
microstructures
molecular structures
morphologies
phases

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

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

toxicity

transport

Tier 2

chemical:

composition

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

wear resistance

kinetic:

grain growth

phase evolution

phase transitions and ordering

electrical:

band structure

conductivity

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

toxicity

transport

magnetic
mechanical
optical
rheological
structural
thermodynamic

Tier 2

magnetic:

coercivity
Curie temperature

magnetization

permeability

saturation magnetization

susceptibility

transport:

diffusivity

grain boundary diffusivity

interdiffusion

intrinsic diffusivity

mobilities

surface diffusivity

tracer diffusivity

optical:

index of refraction luminescence

photoconductivity

rheological:

complex modulus viscoelasticity

viscosity

strength stress-strain behavior

mechanical:

creep

ductility

elasticity

hardness

plasticity

fatigue

acoustic emission

flexural response

fracture behavior

impact response

phonon modes

Poisson's ratio

shear response

fracture toughness

compression response

deformation mechanisms

tensile response

tensile strength

visoelasticity

thermodynamic:

calorimetry profile critical temperatures

crystallization 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

surface energies

thermal conductivity

thermal decomposition

thermal expansion

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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 chromotagraphy gas-phase chromatography ion chromatography liquid-phase chromatography

electrochemical:

amperometry potentiometry voltammetry

mechanical:

compression tests
creep tests
dynamic mechanical analysis
hardness
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]

neutron [inelastic]

small angle x-ray scattering and USAXS

small-angle neutron

synchrotron

x-ray diffraction

x-ray reflectivity

x-ray topography

XRD grazing incidence

tomography:

atom probe tomography

x-ray tomography

thermochemical:

calorimetry

differential scanning calorimetry

differential thermal analysis

microcalorimetry

thermogravimetry

spectrometry:

alpha spectrometry

energy dispersive x-ray spectometry

gamma spectrometry

ion mobility spectrometry

IR/FTIR spectrometry

mass spectrometry

secondary ion mass spectrometry

x-ray flourescence spectrometry

spectroscopy:

dielectric and impedance spectroscopy

dynamic mechanical analysis

electron energy-loss spectroscopy

EXAFS

Fourier-transform infrared spectroscopy

NEXAFS

NMR

Raman

x-ray absorption spectroscopy

x-ray emission spectroscopy

x-ray photoelectron spectroscopy

XPS variable kinetic

Computational methods

Tier 1

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

See also email to WG list from Gehard Goldbeck: RoMM6: Vocabulary for Materials Modelling European Materials Modeling Council

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

homogenization

mechanical mixing

melt mixing

normalizing

recrystallization

stress relieving

tempering

ultrasonication

casting:

centrifugal casting

continuous casting

die casting

investment casting

sand casting

slip casting

vacuum arcamelting 9 -- Barcelona

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

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 drawing

extrusion

forging

hot pressing

hot rolling

milling molding powder processing:

atomization ball milling

centrifugal disintegration

hot pressing

sintering

sponge iron process

reactive:

addition polymerization

curing

dissolving / etching

drying

in-situ polymerization

post-polymerization modification

reductive roasting

solution processing

solvent casting

mechanical and surface:

doctor blade or blade coating

focused ion beam

joining

lithography

polishing

sectioning

thermal plasma processing
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quenching:

air cooled / quench

brine quench

furnace cooled

gas cooled ice quench

liquid nitrogen quench

oil quench

water quench

solidification:

crystallization

directional solidification

rapid solidification

seeded solidification

single crystal solidification

zone refining

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Other metadata updates

- Supporting descriptions of Software
 - 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

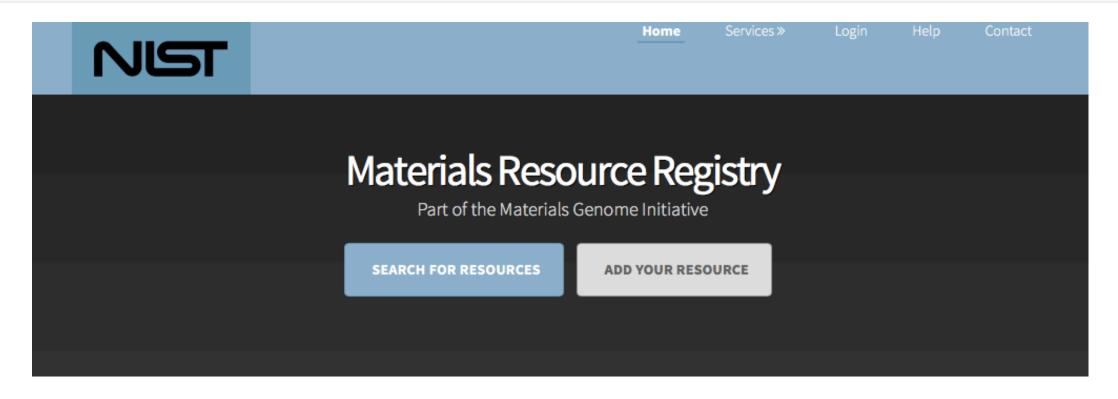


Further vocabulary work

- Further feedback still being taken; welcome contributions
 - Please respond to WG mailing list with comments by 1 May 2017
- Issues of granularity will affect future evolution (Later this session: discussion of granularity)

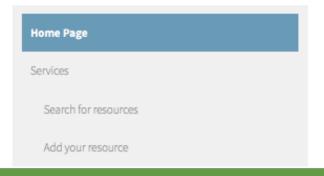


Materials Resource Registry Application



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.

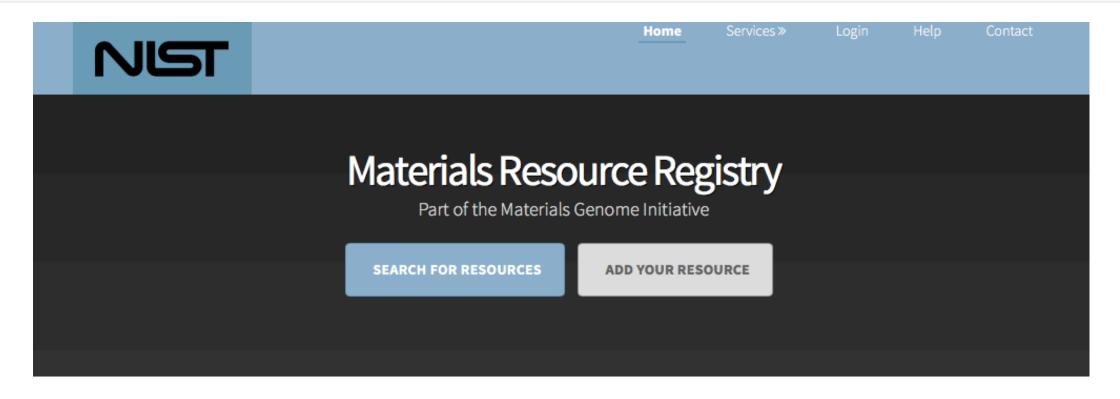


Deployment Status

- Long-term deployment at NIST (nist.gov)
 - Currently finishing security review
 - User accounts will be transferred from NDS instance
 - Available for community use
- Created provider's guide to the metadata (Andrea Medina-Smith)
- Second instance at Materials Data Facility
 - Will support the CHiMaD* project
 *Center for Hierarchical Materials Design
- Software available for deployment at other facilities
 - Available from GitHub
 - NIST can assist with software deployment



Demo



Find Materials Data

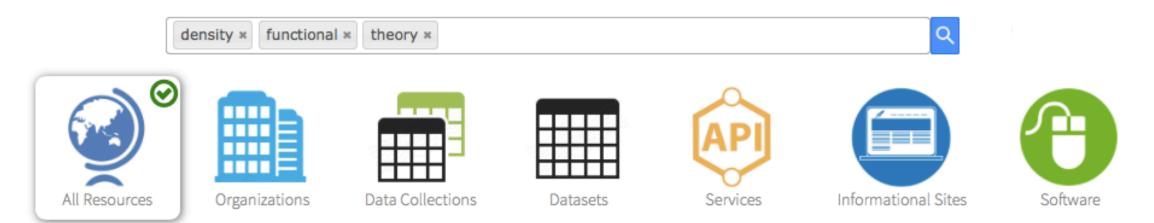
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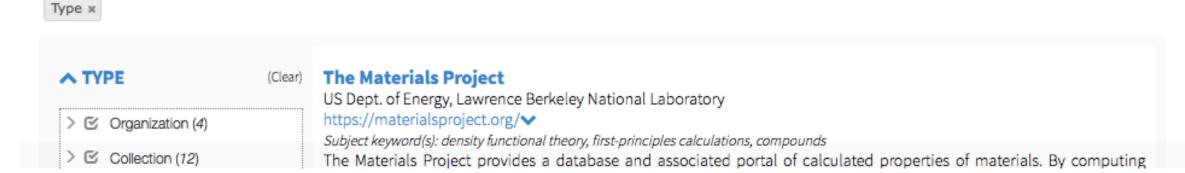




Search for Resources



Search criteria used (Clear all): 55 results



Search criteria used (Clear all): 73 results

Type ×

∧ TYPE > ☑ Organization (21) > Collection (25) Dataset (12) > **☑** Service (0) Software (2) > Web Site (14) **✓ MATERIAL TYPE**

▲ STRUCTURAL FEATURE

composites (6)



- unspecified defects (0)
- cracks (0)
- dislocations (2)

See detailed metadata

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Read full description

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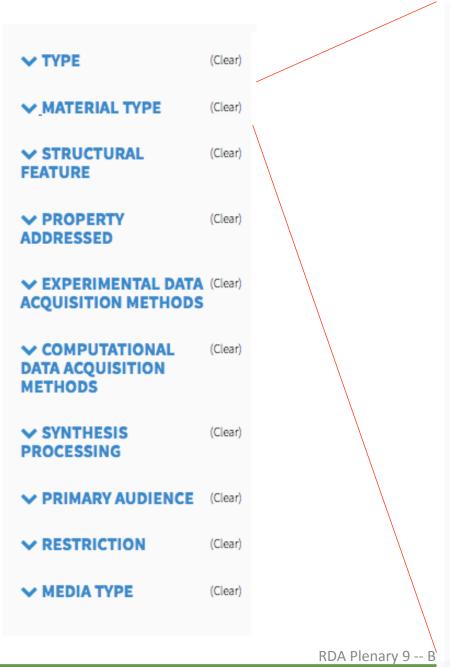
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Subject knowned/eli DOE engagered public data collections



∧ MATERIAL TYPE (Clear) biological (0) biomaterials (4) 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 prov Engineering) approac selection. Microstruct thermodynamics softv **Elasticity Data DS** National Institute of St https://materialsdata. Subject keyword(s): elasti This collection contain CALPHAD Assessn National Institute of St http://hdl.handle.net/ Subject keyword(s): CALP CALPHAD-based asse thermodynamics, diffu Materials Design ' Shengyen Li - Nationa https://mgi.nist.gov/g Subject keyword(s): struc-System (MDCS) This framework prov Engineering) approac selection. Microstruct thermodynamics softv

> **Thermodynamics** National Institute of S

> http://trc.nist.gov✓

Materials Resource Registry

Select a Resource type to add











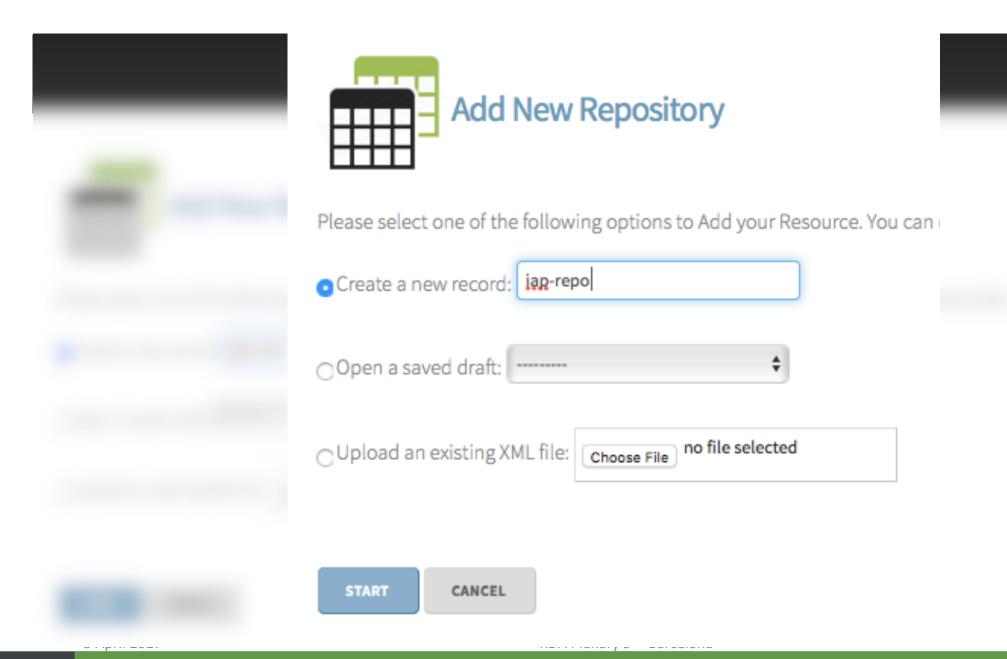


Organization - a group of people that come together to contribute to or participate in a federated data operation. Organizations can be hierarchical: an organization can contain or sponsor other organizations. Organizations can also aggregate or participate with other organizations in broader collaborations.

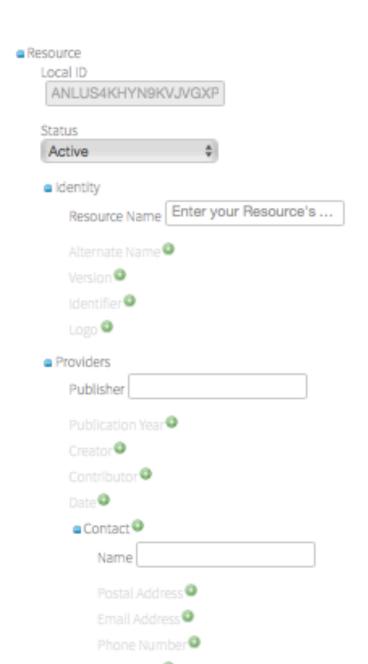
Data Collection - An aggregation of one or more datasets, possibly spanning many research projects or teams.

- 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.



Add New Resource



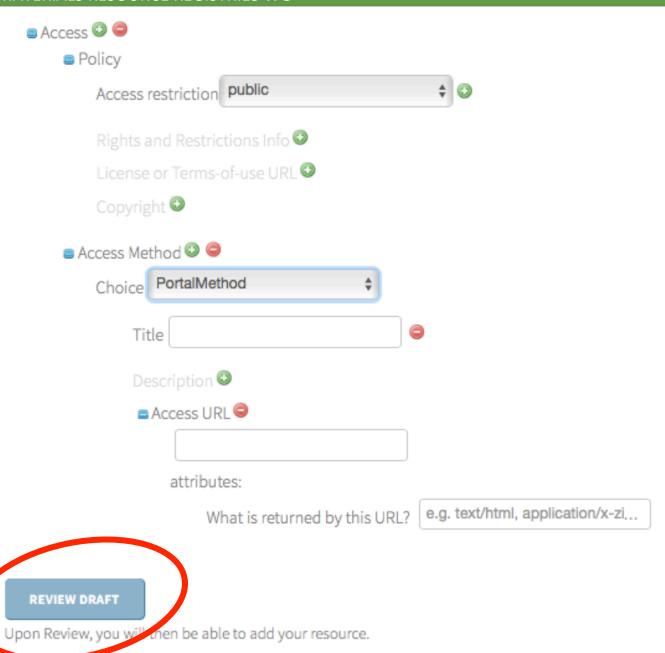
My Resources

5 April 2017

■ Applicab	illity to	Material Science			
Orig	gin of D	ata [©]			
	0	experiments			
	0	informatics and data science			
	0	simulations			
	0	theory			
Mate	erial T	уре [©]			
	0	biological			
	0	biomaterials			
`	~ 0	ceramics carbides			
		nitrides			
		 perovskites 			
		□ silicates			
	> ©	metals and alloys			
	0	metamaterials			
	\mathbb{S}	molecular fluids			
	> 0	organic compounds			
	0	organometallics			
,	> 0	polymers			
	> 0	semiconductors			
■ Stru	ıctural	Feature 🕯			
	> 0	composites			
,	> 0	defects			
	0	engineered structures			
,	> 0	Interfacial			

> O microstructures

MATERIALS RESOURCE REGISTRIES WG

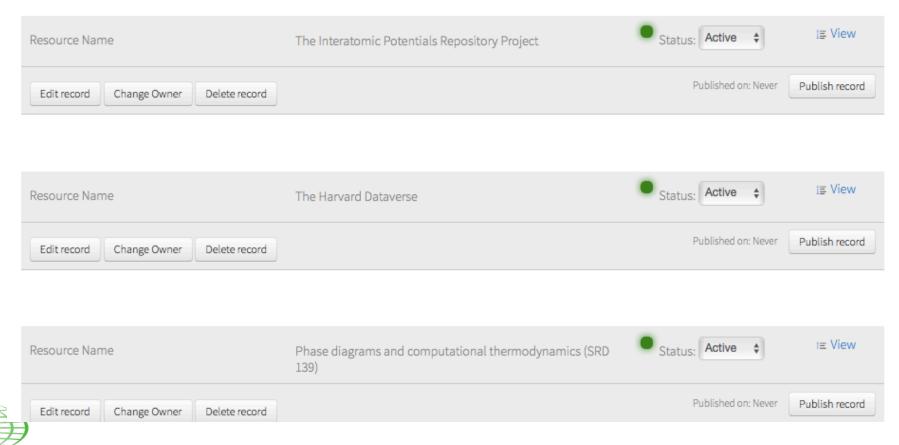


31

RESEARCH DATA ALLIANCE

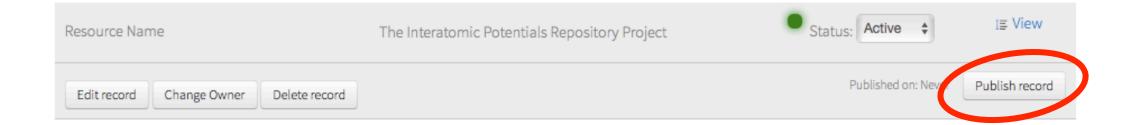
Check results through the browser

Browse your unpublished records through the Dashboard
 My Resources



Click "Publish"

My Resources



Goals for this meeting

- Get input from participants about changes to improve the vocabulary BY 01 MAY 2017
- Get feedback on MRR software experience BY 01 SEPTEMBER 2017
- Recruit & Identify
 - Registrants of materials resources at NIST registry
 - Organizations interested in operating instance of Registry for Federation (Asia, Australia, Europe...)
 - Contributors to Best Practices & Final Report documents

