

CHiMaD Data Schema Working Group

Report

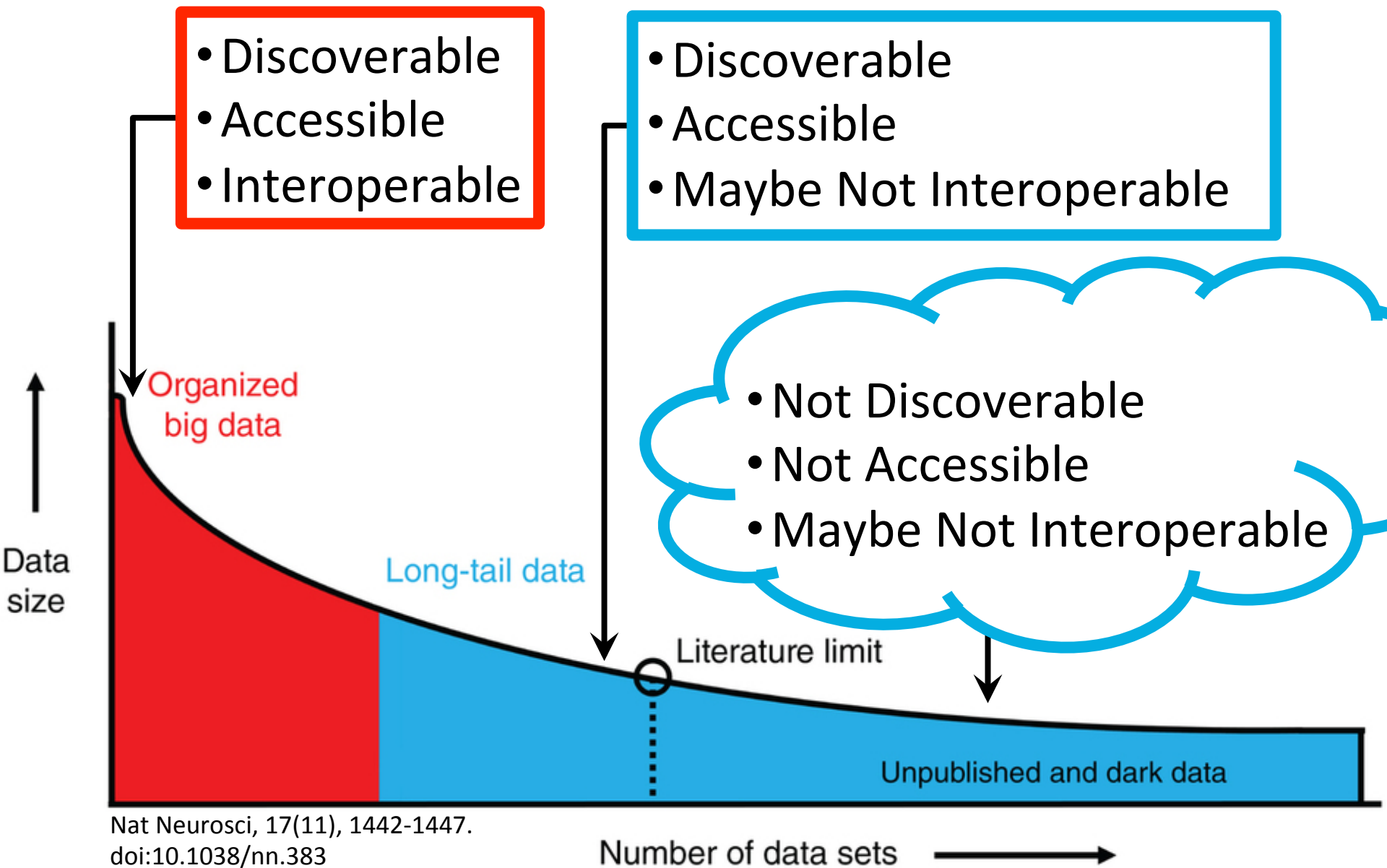
Topics of Today's Discussion

- Thermomechanical Processing History
- Hardness Testing
- Nanomine
- CALPHAD Protodata
- Workflow tool integration
- NoMaD Repository
- ASM Taxonomy

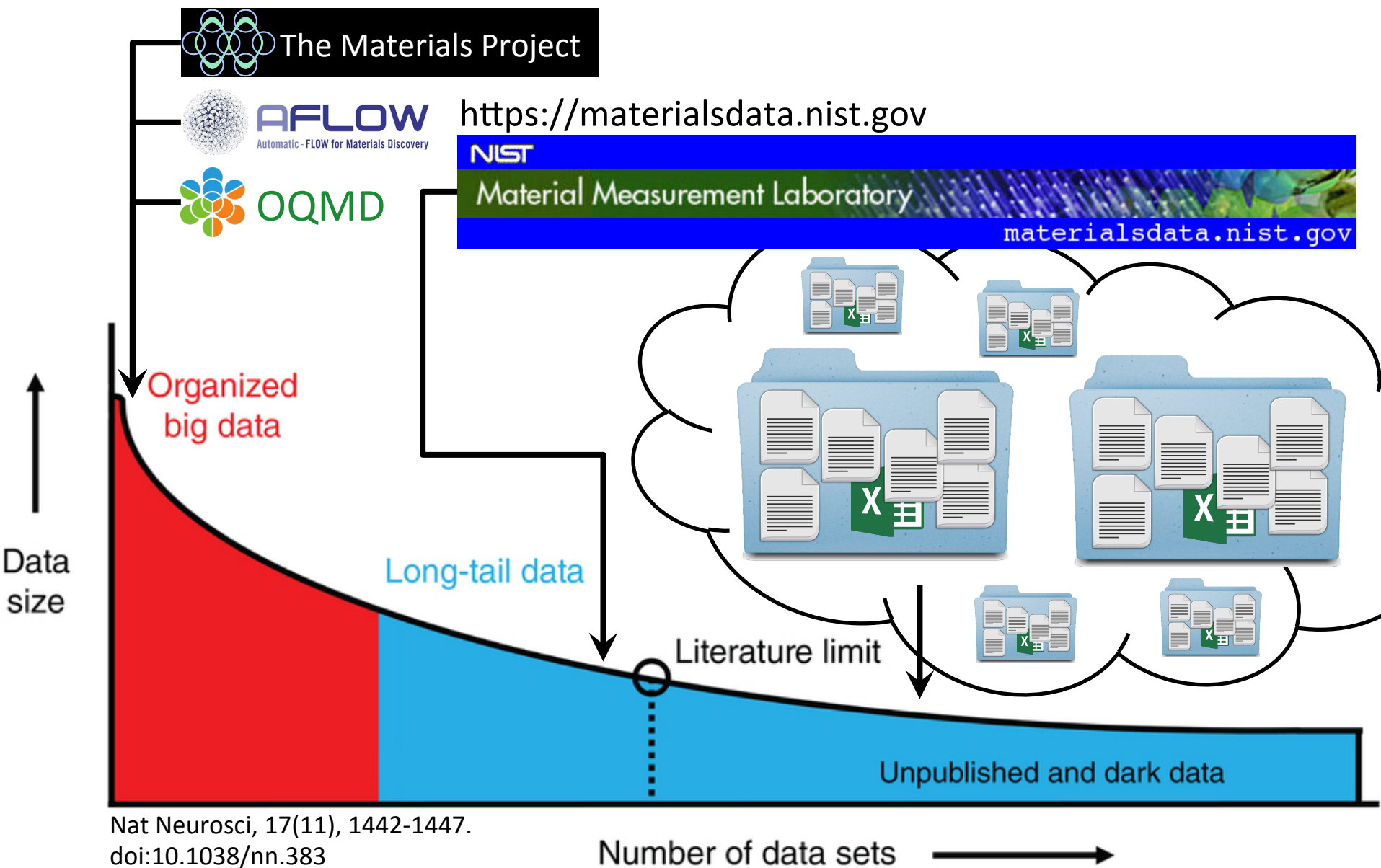
Goals of 3 Month Project

- Identify dataset(s) for curation in MDCS
- Discuss and agree on shared terminology for
 - metadata (e.g., strain rate)
 - data (e.g., load vs. displacement)
 - derived data (e.g., modulus of elasticity)
- Create reusable XML schema types
- Create scripts for data transformation
- Curate dataset(s) in MDCS

Materials Data



Materials Data



A Configurable Data Curation System

Configurable Interface

Data Management & Search Engine



Structured
Data

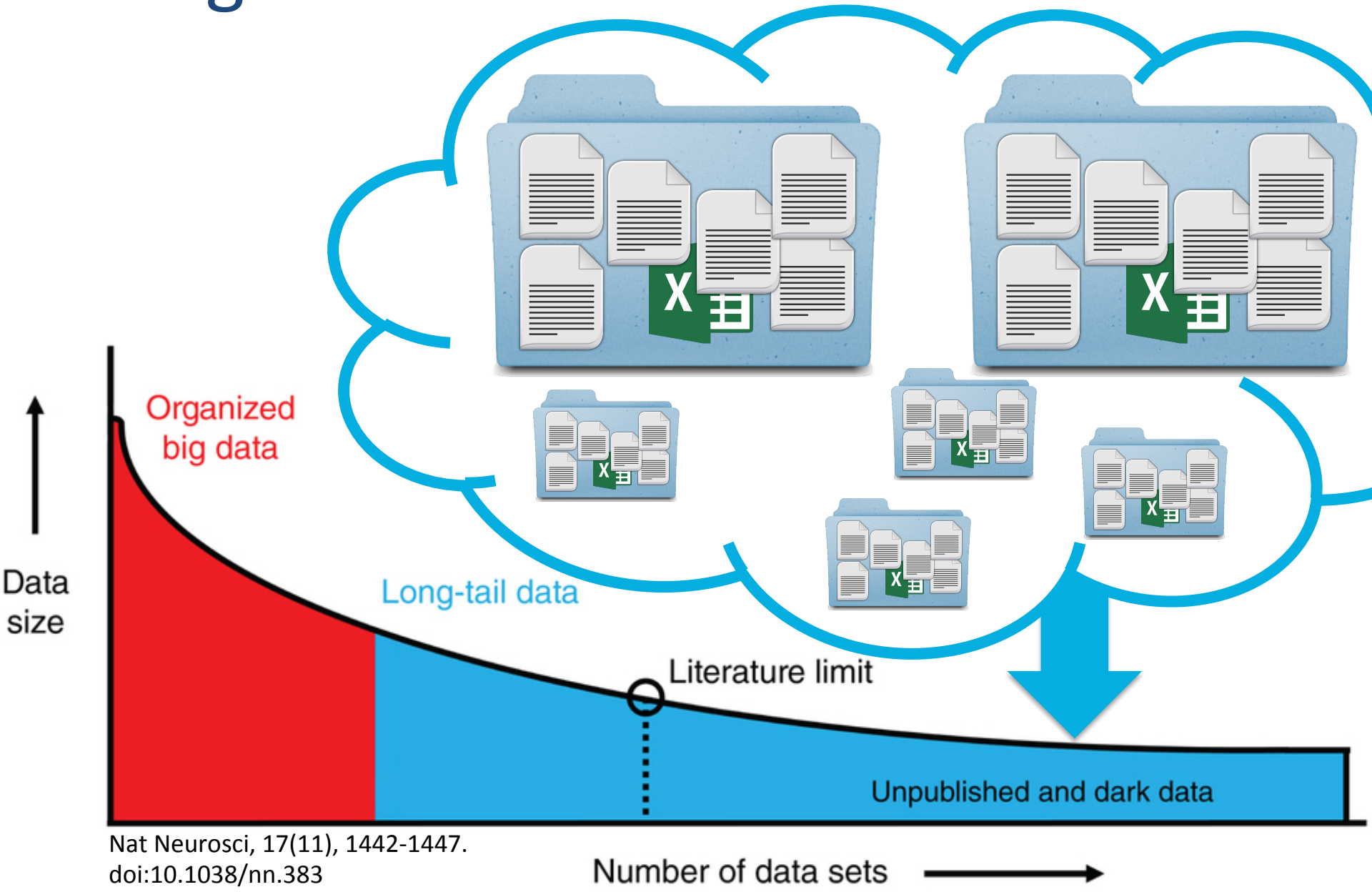


Large/Binary
Files



Your Data Repository or
Your Resource Registry

Long Tail

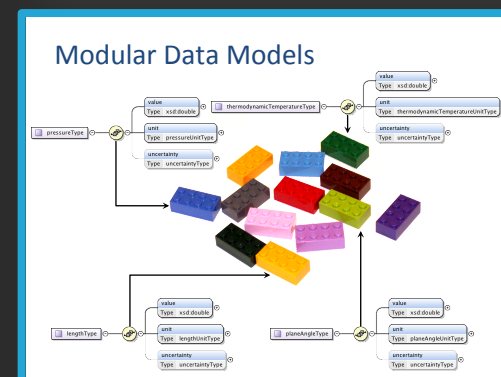
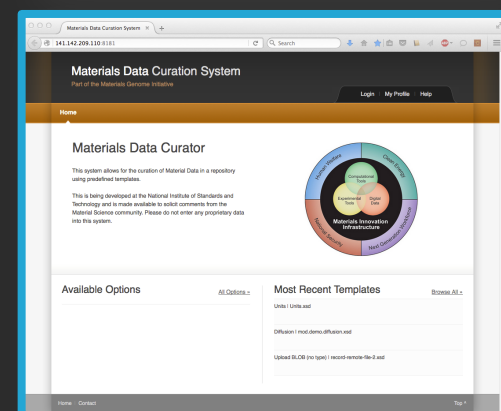
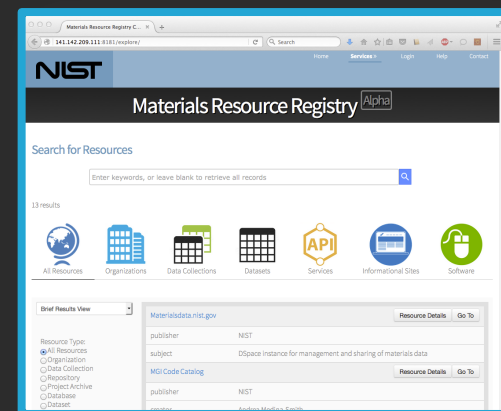


NIST MGI APPROACH TO LONG TAIL DATA

► Discoverable
(via the Registry)
<https://mgi.nist.gov/Zkp>

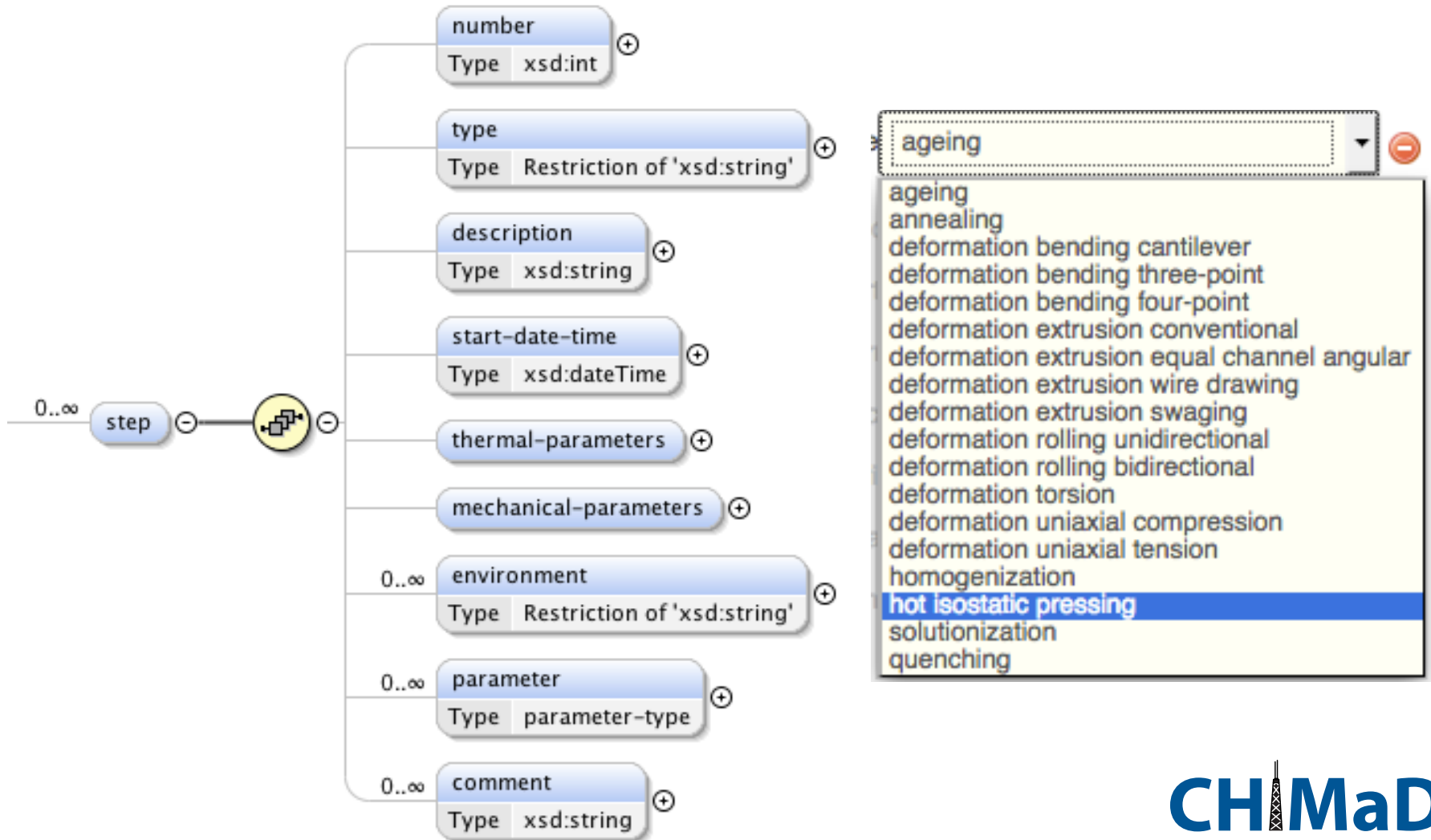
► Accessible
(via the Curator)
<https://mgi.nist.gov/ZkS>

► Interoperable
(via Community Data Standards)
<https://mgi.nist.gov/ZkG>

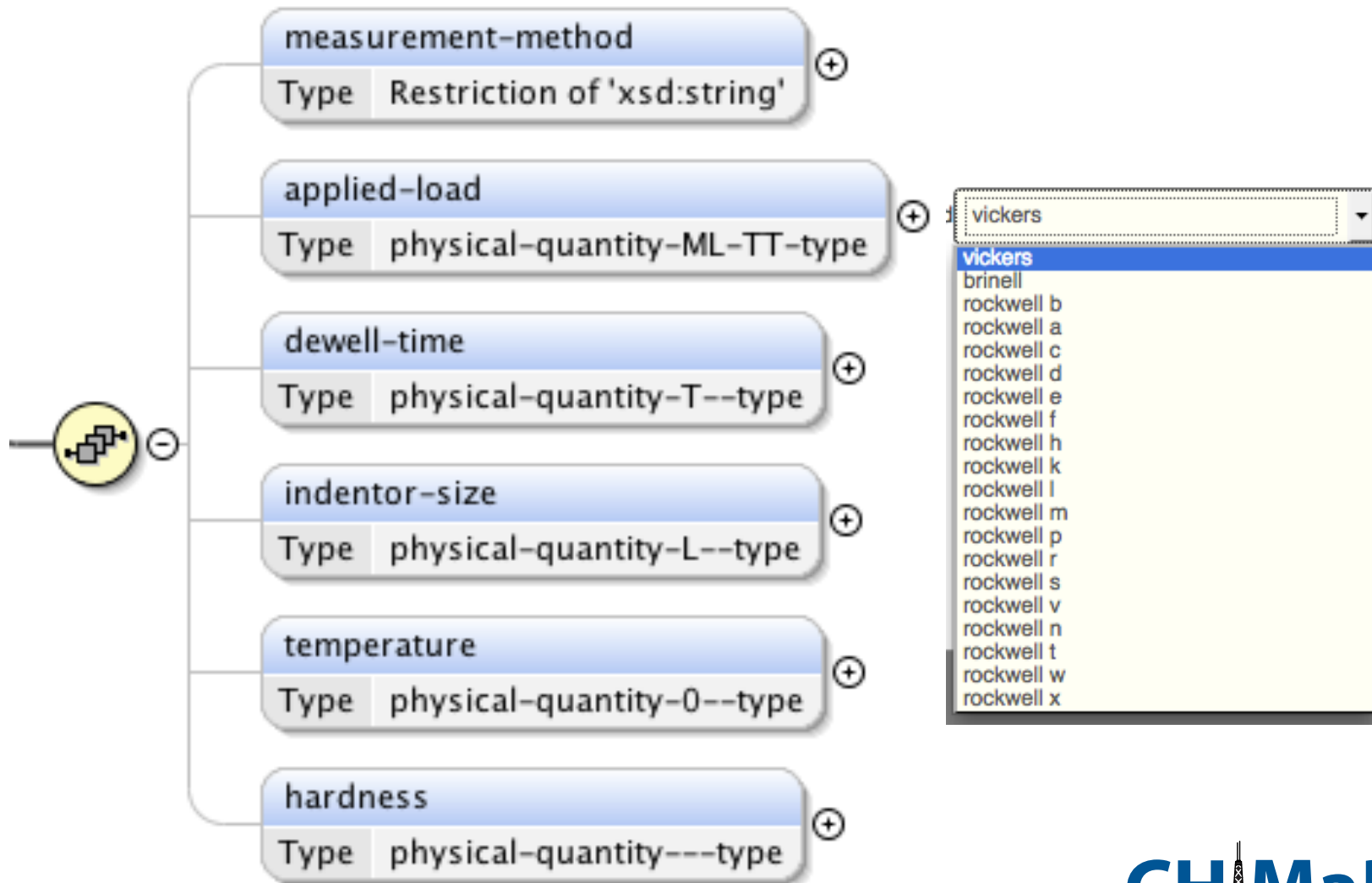


Group Activities/Discussion

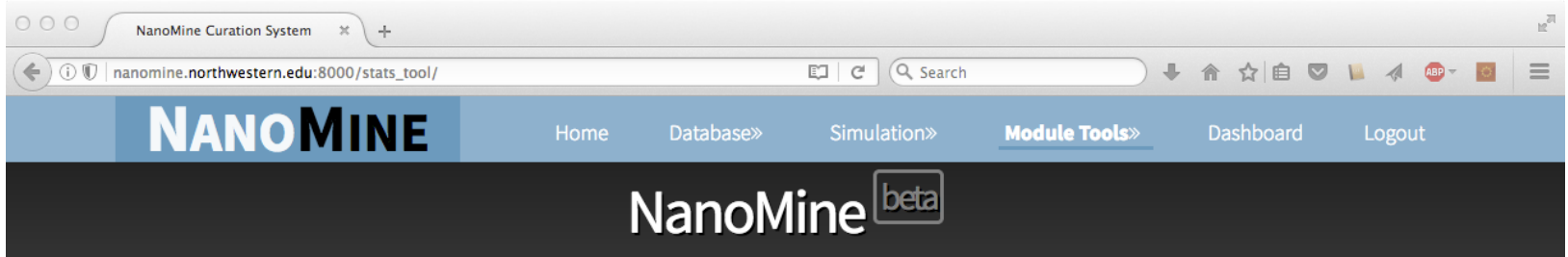
Draft Thermomechanical Processing History Schema



Draft Hardness Testing Schema

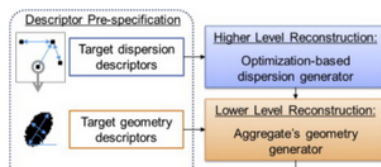
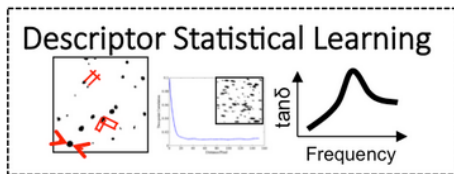


Nanomine



Statistical Learning and Analysis Module Tools

Statistical learning and analysis modules include web and downloadable packages that can be used to pre-process and analyze structure and material property data. Each of the modules will specify required format of input and output data, and provide a brief introduction of mechanism of the algorithm.



NIBLACK BINARIZATION

Descriptor Characterization is a modular tool that takes input from a micrograph image of a microstructure of material and generate statistical descriptors that can characterize the structure information. More details to follow.

DESCRIPTOR CHARACTERIZATION

Descriptor Characterization is a modular tool that takes input from a micrograph image of a microstructure of material and generate statistical descriptors that can

Nanomine

207 results

- L180_S6_Maillard_2012** polymer nanocomposite
 - PolymerNanocomposite**
 - ID : L180_S6_Maillard_2012
 - DATA_SOURCE**
 - Citation
 - MATERIALS**
 - Polymer
 - Particle
 - PROCESSING**
 - SolutionProcessing
 - CHARACTERIZATION**
 - Transmission_Electron_Microscopy
 - Atomic_Force_Microscopy
 - PROPERTIES**
 - Mechanical
 - Tensile
 - TensileModulus
 - ElongationAtBreak
- L180_S5_Maillard_2012** polymer nanocomposite
- L180_S4_Maillard_2012** polymer nanocomposite
- L180_S3_Maillard_2012** polymer nanocomposite
- L180_S2_Maillard_2012** polymer nanocomposite
- L180_S1_Maillard_2012** polymer nanocomposite

CALPHAD Protodata

Curating Diffusion Data

Sample Information

- Sample Id,
- Owner
- Date of Experiment

End Member Material Information

- Phase name
- Crystal structure
- Phase Fraction
- Composition
- Processing

Experimental Procedures

Diffusion Annealing Conditions

Collected Data

- Spreadsheet
- Micrograph

The screenshot displays the 'Materials Data Curation System' interface. The header includes 'Welcome, admin. Thanks for logging in.' and navigation links for 'Logout', 'Dashboard', and 'Help'. The main navigation bar contains 'Home', 'Data Curation', 'Data Exploration', and 'Composer'. Below this, there are tabs for 'Select Template', 'Enter Data', and 'View Data'. The 'Enter Data' tab is active, showing a 'Data Entry' form. The form includes a 'Data Curation' sidebar with steps: 1. Select Template, 2. Enter Data, and 3. View Data. The main content area contains instructions: 'Here you can fill in the Materials Data form. Once it is completed, you can go to "View Data" to review what you have entered. You won't be able to reach the review page before the document is valid according to the selected template. From the review page, you will be able to curate the data. The "Save Form" button allows you to save partial data that you may want to edit later. This will only save a temporary document and won't actually curate data. All grayed elements are optional. Thus, all elements written in black are required. The document may still be valid with empty elements. There are no validation on empty fields if no such constraint is defined in the template. Thus, an empty string of characters may not raise a validation error, but an empty number will.' Below the instructions are buttons for 'Clear Fields', 'Save Form', and 'Download'. The form fields are organized into a tree structure: 'DiffusionCouple' (expanded) contains 'SampleId' (expanded) with fields for 'Id' and 'SampleOwner', and 'Date'. 'Material' (expanded) contains 'MaterialName', 'NominalComposition', 'Phase', and 'AlloyForm'. A second 'Material' (expanded) contains 'MaterialName', 'NominalComposition', 'Phase', and 'AlloyForm'.

CALPHAD Protodata

Self Diffusion Resource

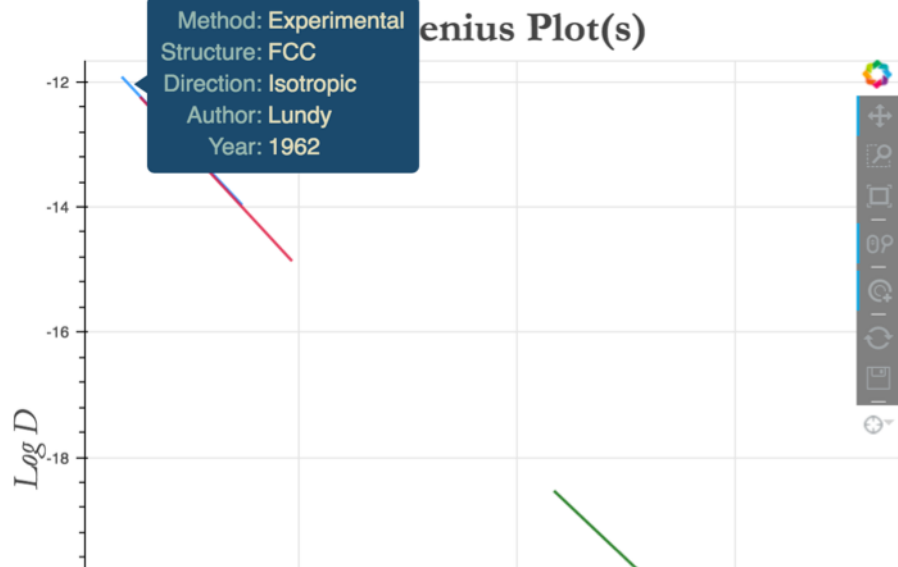
<http://www.ctcms.nist.gov/~gkl/selfdiffusion.html>

The screenshot shows a web browser window with the URL www.ctcms.nist.gov/~gkl/selfdiffusion.html. The page has a navigation bar with "OVERVIEW", "SELF-DIFFUSION", and "CONTACT". The main content is titled "Self-Diffusion Data" and features a periodic table where each element's cell contains its symbol, name, and a numerical value representing self-diffusion data. The values are color-coded: blue for alkali and alkaline earth metals, green for transition metals, orange for post-transition metals, and purple for lanthanides and actinides. Below the table is a header for a data table with columns: Method, Structure, Diffusion Direction, Frequency Factor D0 (m2/s), Activation Energy Q (kJ/mole), Temperature (K), Details, Reference, and Raw data.

Method	Structure	Diffusion Direction	Frequency Factor D0 (m2/s)	Activation Energy Q (kJ/mole)	Temperature (K)	Details	Reference	Raw data
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CALPHAD Protodata

Method	Structure	Diffusion Direction	Frequency Factor D0 (m ² /s)	Activation Energy Q (kJ/mole)	Temperature (K)	Details	Reference	Raw data
Experime...	fcc	isotropic	1.710e-04	142.4	729 - 916	26Al. Diffusion coup...	T.S. Lundy, J.F. Mur...	MDCS
Experime...	fcc	isotropic	2.200e-04	144.4	673 - 883	26Al. Dried-on from...	M. Beveler, Y. Adda...	MDCS
Experime...	fcc	isotropic	1.760e-05	126.5	358 - 482	Al. Void shrinkage (...)	T.E. Volin, R.W. Ball...	MDCS
Experime...	fcc	isotropic	1.370e-05	123.6	515 - 770	Al. NMR. SLRT (27A...	R. Messer et al.: Pr...	MDCS
First-prin...	fcc	isotropic	8.510e-04	131.2	654 - 934	DFT (PBEsol) + qua...	S.-L. Shang et al.: ...	not available
Experime...	fcc	isotropic	1.000e-05; 9.00e-04*	121.7; 172.8*	515 - 916	Al. NMR. SLRT (27A...	S. Dais, R. Messer. ...	not available
CALPHAD	fcc	isotropic	1.080e-05	126.7	300 - 900	Diffusion mobility m...	Y.W. Cui et al.: J. P...	not available
CALPHAD	fcc	isotropic	1.710e-04	142.0	300 - 900	Based on assessme...	A. Engstrom, J. Aqre...	not available
CALPHAD	fcc	isotropic	8.233e-05	123.1	300 - 900	No details available	L. Zhang, Y. Du: NI...	not available
CALPHAD	hcp	⊥ c axis	2.380e-05	79.79	300 - 900	Estimation using th...	Y.W. Cui et al.: J. P...	not available



$$D = D_0 \exp\left(\frac{-Q}{RT}\right)$$

$$^*D = D_0^1 \exp\left(\frac{-Q^1}{RT}\right) + D_0^2 \exp\left(\frac{-Q^2}{RT}\right)$$

$$^{**}D = D_0 \exp\left(\frac{-Q}{RT}\right) \exp\left(\Omega \frac{(T_M)^2}{T^2}\right)$$

Workflow Tool Integration

Experimental Analysis Groups



NAIVE

Proprietary Software
e.g: TA SW v2.0



INTERMEDIATE

Excel formulas
and charts



EXPERT

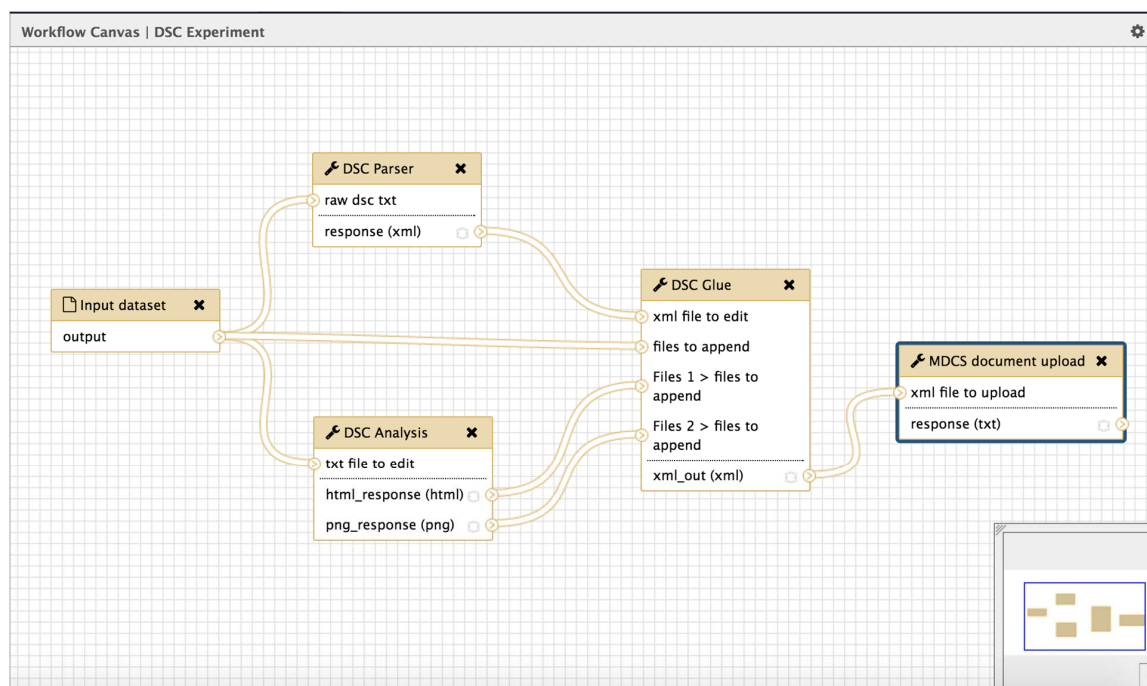
Python Scripting
and Matlab

Difficulties in sharing



Workflow Tool Integration

Reproducibility: MS Galaxy workflow



Workflow Tool Integration

Capabilities for MS-Galaxy users

How different levels of user can take advantage of galaxy



NAIVE

Store data and
perform analysis



INTERMEDIATE

Design
workflows



EXPERT

Create custom
tools for MS
galaxy



NoMaD Repository

The screenshot shows the NoMaD Lab Meta Info web application. The browser address bar displays the URL: `https://nomad-dev.rz-berlin.mpg.de/nomadmetainfo_public/index.html#/public/settings_molec`. The page header includes the NOMAD logo and the text "NOMAD Meta Info". Below the header, there are four search filters: "Search by name or description" (containing "molec"), "Select Parent Section" (set to "Any Section"), "Select Abstract Type" (set to "Any Abstract Type"), and "Select Type" (set to "Any Meta Info Type").

A legend below the filters identifies the colors used in the diagram: a red circle for "Section", a teal circle for "Abstract Type", a black circle for "Concrete Value", and a pink circle for "Dimension". There are also two buttons: "Disable zoom and panning" and "Reset view".

The main content area displays a hierarchical diagram of metadata sections. It shows three red circles representing sections: "section_run", "section_sampling_method", and "settings_molecular_dynamics". A blue double-headed arrow connects "section_run" and "section_sampling_method". A blue arrow points from "section_sampling_method" to "settings_molecular_dynamics". A teal star is placed next to "settings_molecular_dynamics".

Below the diagram, the text "settings_molecular_dynamics direct children:" is followed by three teal circles representing abstract types: "settings_barostat", "settings_integrator", and "settings_thermostat".

On the left side of the interface, a list of metadata fields is visible: `frame_sequence_external_url`, `frame_sequence_local_frames_ref`, `section_frame_sequence`, `section_method`, `settings_molecular_dynamics`, `stress_tensor`, `stress_tensor_kind`, `stress_tensor_method`, and `stress_tensor_value`.

NoMaD Repository

http://nomad...D8BFCF36D2AD

nomad-repository.eu:8080/search/index.zul;jsessionid=FC27B711A78FD628B569D8BFCF36D2AD

To display entries of the NoMaD Repository, select Items below and press Search.

SEARCH Reset search options DOIs and references

Compiled 8th September 2016

Home Layout Register

Garhain Installation

Login

Selected items are listed and can be deselected here:

[x] Al [x] Ni [x] Cu

Structure

System type	Crystal system
<input type="text"/>	<input type="text"/>

Methodology

Code	Basis set type	xc treatment
<input type="text"/>	<input type="text"/>	<input type="text"/>

Chemical Elements

Selected elements only

H																	He				
Li	Be															B	C	N	O	F	Ne
Na	Mg															Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr				
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe				
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn				
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo				
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu							
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr							

Authors and Comments

Type an author's name or choose from the list:

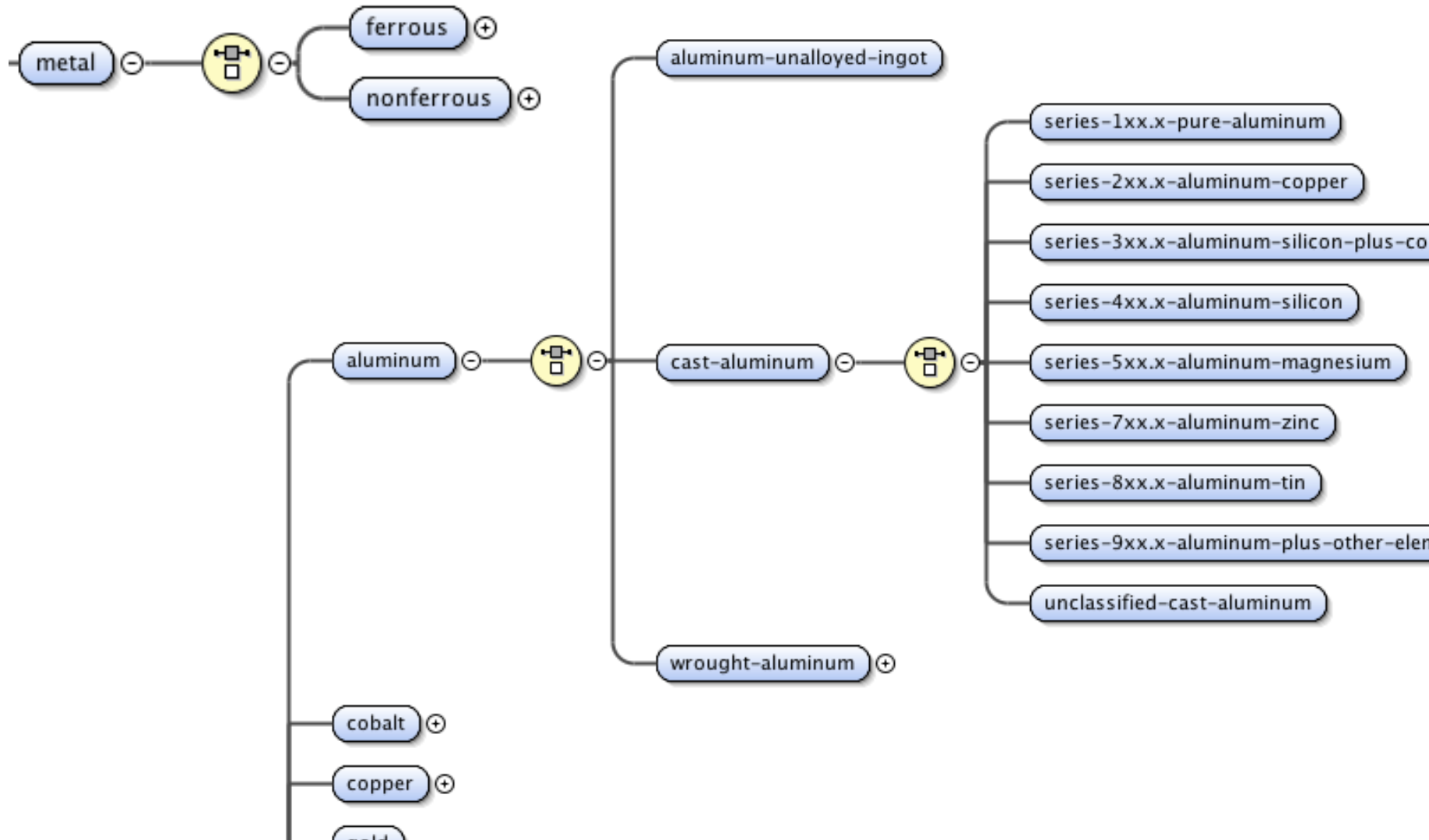
Search in comments:

Data access

Restricted

Open access

ASM Taxonomy



Closing Remarks

- New Schemas
- Integration