



Materials Science Data Management Initiatives at NIST

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Data and NIST

- NIST is a national and world resource for fundamental data
- Access should be easy and open
 - With regard to IP and privacy issues
- As our nation's standards organization...
 - NIST should be a leader in national and international standards efforts for data discovery and access
 - Discovery is fundamental
 - Discovery is enabled by metadata standards
- Key research at NIST should engage in data sharing strategies from the onset
- NIST should provide an infrastructure that makes data and information sharing as easy as possible

Office of Data and Informatics

SRD

- continue existing SRD distribution
- Quality Framework
- SRD Modes
- assess external need
- new product ideas
 - SRMDS
 - data streams
 - alternative delivery methods
- Open Data Initiative
- Open Govt Directive
- Data.gov

Research Data

- deal w/ data deluge
- provide advice to MML bench staff
- gather best practices
- interpret external rules & regulations
- reduce redundancy
- promote cooperation and coherent action
- manage changes in scholarly publishing
- coordinate with
 - WERB
 - Library
 - JResNIST

Lead/Liaison

- partner with ITL
- represent MML
 - NIST committees
 - NSTC & IWGs
 - NIH, NSF, DOE
 - other Fed Govt
 - Research Data Alliance (RDA)
- data standards
- champion proposals
 - budget initiatives
 - IMS
 - inter-agency, RDA

Data Science

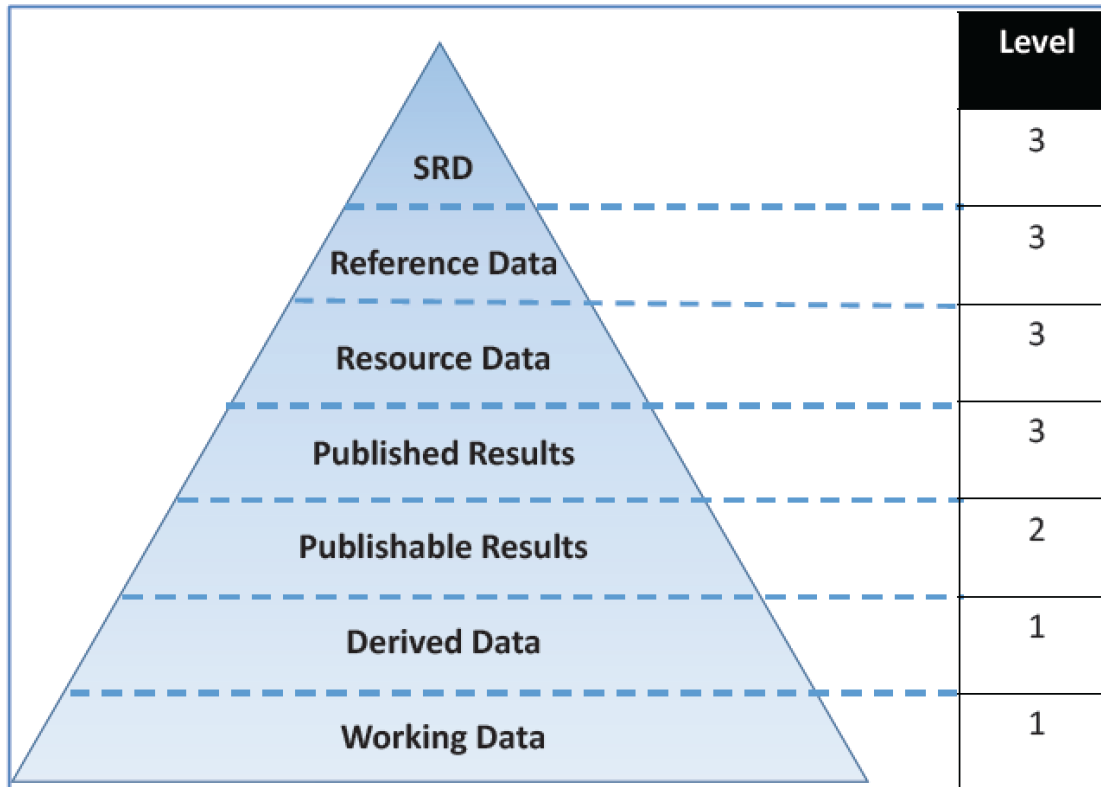
The 4th paradigm?

- will it stand next to
 - theoretical
 - experimental
 - computational
- Cloud
- Statistical Learning
- Big Data
- Knowledge Discovery
- very fast growing
- *many* new jobs
- new degrees/depts

Key ODI Activities

- Implementation of Open Data policies
- Support and modernization of Standard Reference Data
- Collaboration in design and implementation of improved data infrastructure
- Help improve data management practices for MML research staff
- Participate in national and international initiatives around open data, data discovery, access, and interoperability
- Consultancy to MML staff in informatics and analytics
- Support Materials Genome Initiative data management and sharing infrastructure, informatics initiatives

NIST Public Data Access Policy



Metadata values in NIST EDI are made publicly available

Metadata goes to NIST EDI and PID minted

No requirements

NIST Public Data Access Policy

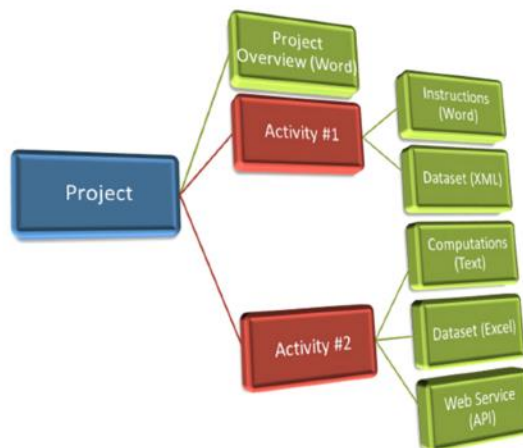
- Establish NIST's commitment to providing public access to scientific research results
- Support governance of and best practices for managing peer-reviewed scholarly publications and digital scientific data across NIST
- *How do we make this a benefit to staff rather than a burden?*
- Enhance innovation and competitiveness by maximizing the potential to create new business opportunities

<http://www.nist.gov/data/upload/NIST-Plan-for-Public-Access.pdf>

Implementation

- Data management plans
- Enterprise Data Inventory
- data.gov

MML Data Management Planning Tool



Project Plans for Hanisch, Robert

Projects plans are used for a top-level view of an entire project. Activities can then be defined as part of a project, and they will have their own activity-specific plans. Activities related to a project will be shown under their project, while standalone activities will be shown in the activities table. Click the "Create New Project DMP" button to define a project.

[+ Create New Project DMP](#)

Thanks to

- Chandler Becker
- Arlin Stoltzfus
- Craig Vogel
- Angela Lee
- Adam Morey

About the site

This website provides the tools that enable MML staff and associates to create and update Data Management Plans (DMPs). A DMP describes the nature of a project producing data such as the project goals, specific areas of research, and types of instrumentation being used and samples being studied. These tools are also used to identify and locate the datasets that result from the research described in the DMP. Information gathered through this website is used to populate the NIST Enterprise Data Inventory and the national data inventory at data.gov.

These tools will guide you through the DMP construction process, collecting both general descriptive information and specific information about data discoverability, access, and preservation.

Data Management Plans can be entered at the project level (blue icons in image), or at the activity level (red icons). Each project can have one or many activities. An activity may or may not be associated with a project. Each DMP (at either the project or activity level) can have one or many associated file locations (green icons) associated with it, which will allow linking to results, instructions, or other supporting documentation.

Data Management Plans

Listing Data Management Plans for Projects

Primary investigator	Title	Description	Category	Tags	Data category		
Linstrom, Peter	The NIST Chemistry Webbook	The NIST Chemistry WebBook provides users with easy access to chemical and physical property data for chemical species through the internet. The data provided in the site are from collections maintained	Energy, Environment and Climate, Manufacturing, Safety, Security and Forensics	chemical data, thermochemical data, thermodynamic data, thermophysical data, enthalpy, entropy, heat capacity, heat of formation, chemical structure, ionization potential, thermochemistry, boiling point, vapor pressure, IR spectrum, mass spectrum, UV/Vis spectrum, retention index, InChI, InChIKey	Standard Reference Data (SRD)	Show	Edit
Scott, John Henry J.	Accelerated Discovery to Delivery -- SEM Data Formatting/Capture for DoD	As part of this project, I will assemble a collection of example SEM data files from different instrument manufacturers that will serve as exemplars of file formats and metadata. The data files will co	Advanced Materials	materials genome initiative, MGI, Army, Navy, Air Force, schema, metadata capture	Working Data	Show	Edit
Shen, Vincent K.	Molecular simulation of complex fluids	Simulation results related to research on complex fluids.	Advanced Materials, Biosciences and Health, Energy, Environment and Climate, Manufacturing	molecular dynamics, monte carlo, thermophysical fluid properties	Published Results	Show	Edit

Data Management Plans

Data Management Plan for "NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials"

Summary of Activities

Title of Project: NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials

Principal Investigator: Siderius, Daniel

Category: Advanced Materials, Energy, Environment and Climate, Manufacturing

Tags: adsorbate, adsorbent, adsorption, isotherm, metal organic Framework, porous Material, surface science

Organizational Code: 646.04 -- Chemical Informatics Research Group

Data Description (Data.gov): The NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials (NIST SRD-205) is a free, web-based catalog of adsorbent materials and measured adsorption properties of numerous materials obtained from article entries from the scientific literature. Search fields for the database include adsorbent material, adsorbate gas, experimental conditions (pressure, temperature), and bibliographic information (author, title, journal), and results from queries are provided as a list of articles matching the search parameters. The database also contains adsorption isotherms digitized from the cataloged articles, which can be compared visually online in the web application or exported for offline analysis.

Process description (internal use): Data collection occurs through a sequence of steps: 1. PI compiles a list of articles from which to extract adsorption metadata and adsorption isotherms. Master list of articles abstracted or to-be-abstracted is maintained in an EndNote Library. 2. Students, interns, or NIST staff extract the correct adsorption metadata from articles, digitize adsorption isotherms, then input data into CSV flat files. 3. PI runs error checking software on CSV flat files, requests corrections. Steps 2 and 3 are repeated until CSV files pass error checks. 4. PI merges bibliographic information into metadata CSV file. 5. PI converts isotherm CSV files into JSON format. 6. PI uploads new dataset into MySQL database using administration panel (internal only) of web application. 7. Internal web server automatically send database updates to external web server once per week.

Release Date: 2014-10-28

Last updated: 2014-10-28

References: <http://adsorbents.nist.gov>, http://reaction.nist.gov/NISTOnly/adsorption_db/

Data Management Plans

Data Types and Classification

Data category (Preservation Level): Standard Reference Data (SRD)

All File Formats: json, csv, xls

Data dictionary url:

Data dictionary type:

Data standard:

Data types description: Bibliographic data and article metadata is contained in CSV flat files. Isotherm data from articles are stored in JSON files will certain reserved attribute fields (DOI, source description [table or figure number], temperature, material name, gas name, pressure units, adsorption units, isotherm pressure/adsorption pairs). Other attribute fields may be added without breaking file functionality for SRD-205. No standard for this file format exists as of 02/23/2015.

Preservation

Backup method: File server, Other

Preservation description: Local backup - Dataset (raw and processed) and web application are stored on PI's desktop computer, which is automatically mirrored 3x/week to NAS fileserver <http://h178112.nist.gov>. Weekly backups (if data has changed) of processed SQL database on internal web server (<http://reaction.nist.gov>). SQL dumps are backed up 3x/week to NAS fileserver <http://h178112.nist.gov>. Web application code managed through private git repository (http://github.com/usnistgov/adsorption_db). Local version of web application code is backed up 3x/week to NAS fileserver <http://h178112.nist.gov>.

The following distributions are covered under this project:







Distribution Details	Download url	Media type	Version	
NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials () The NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials (NIST SRD-205) is a free, web-based catalog of adsorbent materials and measured adso...			1.0	Show Edit Remove

[+ Describe New Distribution](#)

Data Management Plans

Discoverability and Access

Publisher: 646.04 -- Chemical Informatics Research Group

Relationship	Name	Organization		
Creator	Siderius, Daniel	Chemical Sciences Division	 Edit	 Remove
Contributor	Shen, Vincent K.	Chemical Sciences Division	 Edit	 Remove
Creator	van Zee, Roger D.	Chemical Sciences Division	 Edit	 Remove

 Add NIST Staff

 Add External Staff

Homepage url: <http://adsorbents.nist.gov>

Language: en-US

Public access level: public

Rights: Dataset is Standard Reference Data and is covered by copyright under the Standard Reference Data Act. Data are freely available through interface website or via request to PI. Dataset (not database or application) may be licensed to Springer Publishing for use in Landolt-Bornstein Database.

License: TBD - depends on licensing agreement with Springer Publishing. The data are Standard Reference Data and are copyright by the U.S. Secretary of Commerce.

Discoverability access description: This SRD product exists as two parts: 1) the actual dataset (described in detail above) and 2) the PHP-based web application that is the interface to the MySQL database. The full web application, with administrative panel, resides on <http://reaction.nist.gov>, and is subject to version control using a private git repository on github.com. Currently, updates to the web application are manually pushed to the external server, <http://adsorbents.nist.gov>, by the PI. This could be improved by automating the update through a git pull that also deletes the administrative panel.

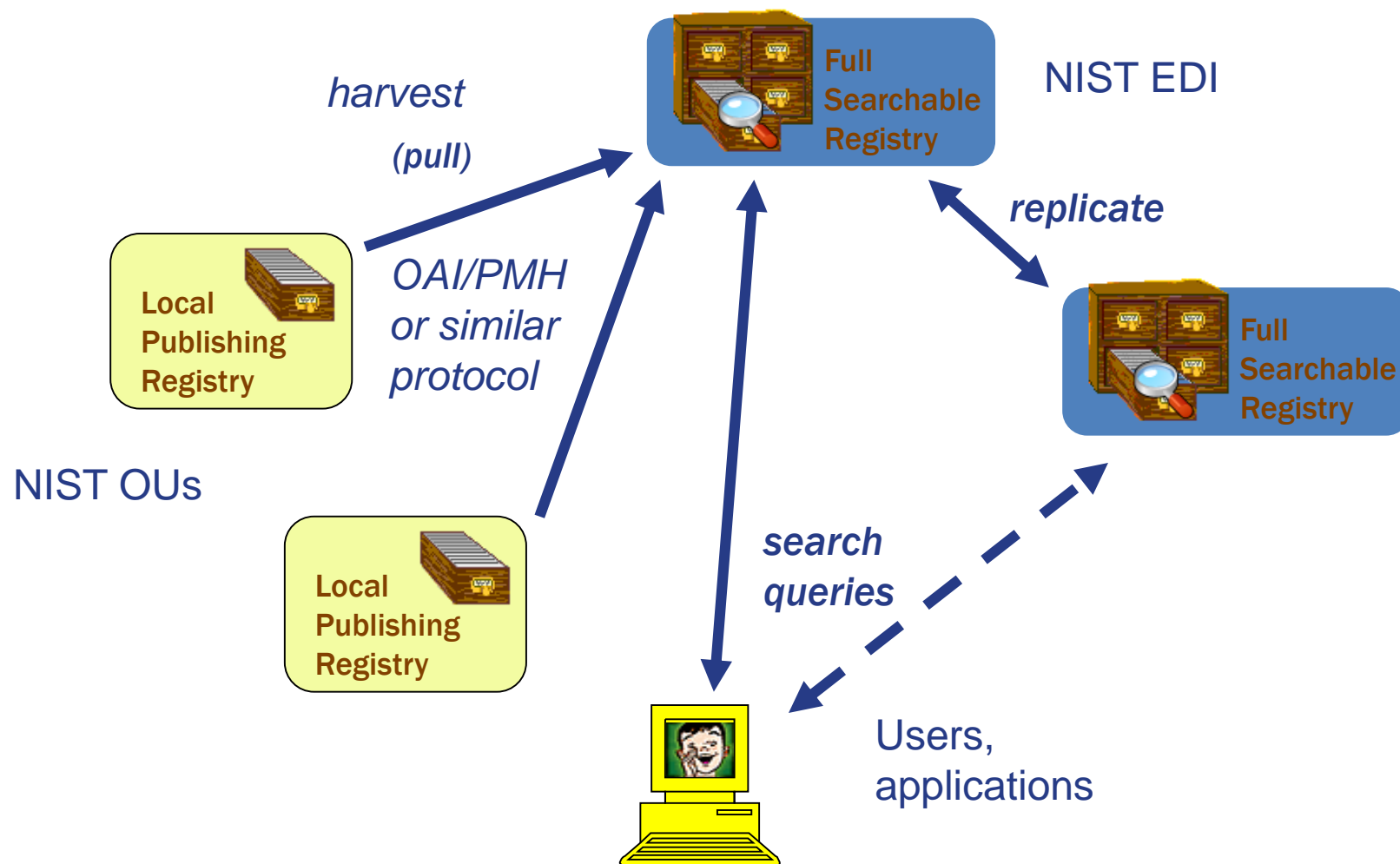
JSON Export to EDI, data.gov

```

{
  "title": "Cation substitution in thermochromic vanadium dioxide for smart windows",
  "identifier": "",
  "description": "This dataset includes infrared reflectances for thin film V_{1-x}M_{x}O_{2}, for M = Nb, Mo, W, Hf,
and x < 0.2, at temperatures of 5 \u00b0C to 85 \u00b0C, transition temperatures derived from the infrared reflectance
measurements, and x-ray diffraction spectra at 23 +/- 3 \u00b0C. It also includes Matlab codes for analysis and presentation
of the data. The dataset supports a study of the depression of transition temperatures in lightly substituted vanadium
dioxide (VO_2) for smart energy-efficient building windows. While unsubstituted VO_2 undergoes a phase transition at 68
\u00b0C with concomitant changes in the infrared reflectances, the temperature of transition can be depressed by low level
cation substitution.",
  "modified": "2015-02-19T11:32:35-05:00",
  "publisher": {
    "@type": "org:Organization",
    "name": "643.04 -- Functional Properties Group",
    "subOrganizationOf": {
      "@type": "org:Organization",
      "name": "National Institute of Standards and Technology",
      "subOrganizationOf": {
        "@type": "org:Organization",
        "name": "Department of Commerce",
        "subOrganizationOf": {
          "@type": "org:Organization",
          "name": "U.S. Government"
        }
      }
    }
  }
},
  "isPartOf": "",
  "accessLevel": "public",
  "keyword": [],
  "bureauCode": ["006:55"],
  "programCode": ["006:045"],
  "spatial": "NIST Gaithersburg",
  "theme": ["Advanced Materials", "Energy", "Environment and Climate"],
  "dataQuality": "true",
  "distribution": [
  ],
  "accrualPeriodicity": "",
  "landingPage": "",
  "language": ["en-US"]
},

```

Federated Architecture



Standard Reference Data

- SRD Act of 1968 authorized NIST to create Standard Reference Data
 - Copyright
 - Cost recovery
- ~100 databases, most are free to use
- Also Special Databases (most from ITL)



Public Law 90-396
90th Congress, H. R. 6279
July 11, 1968

An Act

To provide for the collection, compilation, critical evaluation, publication, and sale of standard reference data.

Be it enacted by the Senate and House of Representatives of the United States of America in Congress assembled,

Standard Reference
Data Act.

DECLARATION OF POLICY

SECTION 1. The Congress hereby finds and declares that reliable standardized scientific and technical reference data are of vital importance to the progress of the Nation's science and technology. It is therefore the policy of the Congress to make critically evaluated reference data readily available to scientists, engineers, and the general public. It is the purpose of this Act to strengthen and enhance this policy.

82 STAT. 339
82 STAT. 340

DEFINITIONS

SEC. 2. For the purposes of this Act—

(a) The term "standard reference data" means quantitative information, related to a measurable physical or chemical property of a substance or system of substances of known composition and structure, which is critically evaluated as to its reliability under section 3 of this Act.

(b) The term "Secretary" means the Secretary of Commerce.

SEC. 3. The Secretary is authorized and directed to provide or arrange for the collection, compilation, critical evaluation, publication, and dissemination of standard reference data. In carrying out this program, the Secretary shall, to the maximum extent practicable, utilize the reference data services and facilities of other agencies and instrumentalities of the Federal Government and of State and local governments, persons, firms, institutions, and associations, with their consent and in such a manner as to avoid duplication of those services and facilities. All agencies and instrumentalities of the Federal Government are encouraged to exercise their duties and functions in such manner as will assist in carrying out the purpose of this Act. This section shall be deemed complementary to existing authority, and nothing herein is intended to repeal, supersede, or diminish existing authority or responsibility of any agency or instrumentality of the Federal Government.

Collection and
publication of
standard refer-
ence data.

SEC. 4. To provide for more effective integration and coordination of standard reference data activities, the Secretary, in consultation with other interested Federal agencies, shall prescribe and publish in the Federal Register such standards, criteria, and procedures for the preparation and publication of standard reference data as may be necessary to carry out the provisions of this Act.

Standards, etc.
Publication in
Federal Register.

SEC. 5. Standard reference data conforming to standards established by the Secretary may be made available and sold by the Secretary or by a person or agency designated by him. To the extent practicable and appropriate, the prices established for such data may reflect the cost of collection, compilation, evaluation, publication, and dissemination of the data, including administrative expenses; and the amounts received shall be subject to the Act of March 3, 1901, as amended (15 U.S.C. 271-278e).

Sale of refer-
ence data.
Cost recovery.

SEC. 6. (a) Notwithstanding the limitations contained in section 8 of title 17 of the United States Code, the Secretary may secure copyright and renewal thereof on behalf of the United States as author or proprietor in all or any part of any standard reference data which

31 Stat. 1449;
Acte. P. 34,
U. S. copyright
and renewal
rights.
61 Stat. 655;
76 Stat. 446.

NIST Data Gateway - provides easy access to many (currently over 90) of the NIST scientific and technical databases. These databases cover a broad range of substances and properties from many different scientific disciplines. The Gateway includes links to free online NIST data systems as well as to information on NIST PC databases available for purchase.

SRD Examples



Element/Compound/Mixture Selection

In this database, it is possible to obtain photon cross section data for a single element, compound, or mixture (a combination of elements and compounds). Please fill out the following information:

[Help](#)

Identify material by:

Element
 Compound
 Mixture

Method of entering additional energies: (optional)

Enter additional energies by hand
 Additional energies from file (Note: Your browser must be file-upload compatible)

NIST Chemical Kinetics Database

Kinetics
Database
Resources

Simple Reaction
Search

Standard Reference Database 17, Version 7.0 (Web Version), Release 1.6.8
 Data Version 2013.03

Search Reaction
Database

A compilation of kinetics data on gas-phase reactions

Search
Bibliographic
Database

Notice: We are now accepting requests for abstracting kinetics data from journal articles and other references. Please use the "Submit an Article" link at the left if you find an article that has been missed in the database. You may request abstracting of a newer publication as well.

Set Unit
Preferences

Reaction Database Quick Search Form

Feedback

Enter the reactant(s) and/or product(s) in the fields below. Fields may be left blank.

Submit an Article

If you would like more search options, try...
 advanced reaction search form
 bibliographic search form

Rate Our
Products and

View Tables:

Please note that you can select only **ONE** table at a time of thermoelectric voltages of each type by temperature range, of the coefficients, or of the inverse coefficients.

Type	Temperature Range	Coefficients
B	Select Temperature Range ▾	Select Coefficients Table ▾
E	Select Temperature Range ▾	Select Coefficients Table ▾
J	Select Temperature Range ▾	Select Coefficients Table ▾
K	Select Temperature Range ▾	Select Coefficients Table ▾
N	Select Temperature Range ▾	Select Coefficients Table ▾
R	Select Temperature Range ▾	Select Coefficients Table ▾
S	Select Temperature Range ▾	Select Coefficients Table ▾
T	Select Temperature Range ▾	Select Coefficients Table ▾

[Download Tables of Thermoelectric Voltages and Coefficients](#)

[View Thermocouple Types Definitions](#)

[View Corrections to Coefficients Tables](#)

NIST Atomic Spectra Database Lines Form

Best viewed with the latest versions of Web browsers and JavaScript enabled

Spectrum

Lower Wavelength: or Upper Wavenumber (in cm⁻¹):

Upper Wavelength: or Lower Wavenumber (in cm⁻¹):

Units:

Dynamic Plots

Line Identification Plot:

Saha-LTE Spectrum:

Electron Temperature T_e(eV): Doppler-broadened spectrum

Electron Density N_e(cm⁻³): Ion Temperature T_i(eV): (if T_e ≠ T_i)

Grotian Diagram

Java subwindow size
 640 x 640 800 x 640 1024 x 768 1280 x 1024

Group by configurations | Term multiplicity

Show only radiatively linked levels

Make Criterion Diagram (requires Java2)

Java Security Error should be Medium. For Java 8 Update 25, add http://physics.nist.gov to the Java Control Panel exception site list.

Output Options

Format output: ▾

No JavaScript

Energy Level Units: ▾

Display output: ▾

Page size:

Output ordering: Wavelength
 Multiplet

Additional Criteria

Loss: All
 Only with transition probabilities
 Only with energy level classifications
 Only with observed wavelengths

Bibliographic Information: TP references, Line references

Wavelength Data: Observed
 Ritz
 Observed - Ritz (difference)
 Wavenumber (in cm⁻¹)

Material Measurement Laboratory Repository Server

This is the NIST Material Measurement Laboratory data repository server.

Use of this server is subject to [terms of service](#)

The repository itself is [here](#).

To get an account on this system (required for uploading), send a message to the [administrator](#). Please include your requested username, e-mail address, and first and last name.

View the [Repository](#) itself.

[Manage](#) your credentials.

The National Institute of Standards and Technology (NIST) is an agency of the U.S. Department of Commerce.

[Privacy Policy](#) / [Security Notice](#) / [Accessibility Statement](#) / [Disclaimer](#) / [Freedom of Information Act](#) / [Environmental Policy Statement](#) / [No Fear Act Policy](#) / [NIST Information Quality Standards](#) / [Scientific Integrity Summary](#)

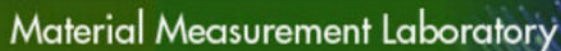
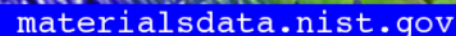
Date created: October 29, 2013 | Last updated: October 29, 2013 Contact: **Webmaster**

DSpace back-end

Thanks to

- Andrew Reid
- Carrie Campbell
- Ursula Kattner
- Ben Burton
- Casey Hume

[Login](#)

NIST Repositories

Communities in NIST Repositories

Select a community to browse its collections.

- [ASM Structural Materials Data Demonstration Project](#)
- [CHIMaD Data Collections](#)
- [Computational File Repository](#)
- [Experimental Data Repository](#)
- [Genome in a Bottle](#)
- [Heusler Phases: First Principles Simulations](#)
- [ICME Approach to Development of Lightweight 3GAHSS Vehicle Assembly](#)
- [ICME of Carbon Fiber Composites for Lightweight Vehicles](#)
- [MGI Catalogs](#)
- [NanoRelease](#)
- [NIST/DOE-EERE Advanced Automotive Cast Magnesium Alloys](#)
- [NIST Thermodynamics and Kinetics Test Space](#)
- [RDA Demonstration Project: DTR/PID & MGI Infrastructure](#)
- [Synchrotron Studies of Slot Die Coated Films](#)
- [Thermal Conductivity of CVD Diamond - DARPA Round Robin](#)
- [TMS Springer Integrating Materials and Manufacturing Innovation \(IMMI\)](#)

Recently Added

[Al-Cu Symmetric/Asymmetric Tilt Grain Boundary Dataset](#)

Tschopp, Mark A.; Coleman, Shawn P.; McDowell, David L.

Symmetric and asymmetric tilt grain boundaries in Cu and Al were generated using molecular statics energy minimization in LAMMPS with in-plane grain boundary translations and an atom deletion criterion. The following ...

[Interaction Between Oxygen Interstitials and Deformation Twins in alpha-Titanium](#)

Joost, William J.; Ankem, Sreeramamurthy; Kuklja, Maija M.

These data files provide input/output VASP and LAMMPS data along with spreadsheets containing data used to produce graphs in our above-reference article. The article abstract is: Twinning is an important deformation mechanism ...

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Author

[Du, Y.](#) (10)
[Burton, Benjamin P.](#) (7)
[Xu, Honghui](#) (7)
[Zhang, L.](#) (7)
[Liu, Shuhong](#) (6)
[Li, Changrong](#) (5)
[Du, Zhenmin](#) (4)
[Guo, Cuiqing](#) (4)
[Liu, Z.-K.](#) (4)
[van de Walle, Axel](#) (4)
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[PROPERTY CLASSES](#) (11)
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[Self-Diffusion](#) (8)
[Cr](#) (7)
[self-diffusion](#) (7)

Sample Entry

(repositories, disciplines, industries) (data, models, integration, etc.)
NIST File Repositories → NIST Data File Repositories → CALPHAD Assessments

CALPHAD Assessments

Search D Space

NIST File Repositories → NIST Data File Repositories → CALPHAD Assessments → View Item

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- Titles
- Subjects

Search within this collector

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Recent Submissions

AI-Cr-Ni Diffusion Mobilities
Campbell, C.E. (2013-02-11)
This work presents the assessed phases in the Ni-Al-Cr system. Available experimental ...

Ni-Al-Cr system Thermodynamics
Dupin, N.; Ansara, I.; Sundman B. A re-assessment of the ternary energy function for the gamma experimental liquidus tempera

Aq-Al Functional Descriptor
Du, Zeting; Jing, Zhan-Peng; L The energy expressions for G ones, are established by con energy and the ...

Data Citation:
AI-Cr-Ni Diffusion Mobilities in Gamma Prime and B2
Campbell, C.E.
<http://hdl.handle.net/11115/51>
Affiliation: Metallurgy Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-6555, USA
Contact Email: carelyn.campbell@nist.gov

Publication Citation:
Campbell, C.E. "Assessment of the diffusion mobilities in the gamma prime and B2 phases of the Ni-Al-Cr system," *Acta Mater.* 2008;56:4277.
<http://dx.doi.org/10.1016/j.actamat.2008.04.051>

Related Work:
Dupin, N., Ansara, I., Sundman B. "Thermodynamic Re-Assessment of the Ternary System Ni-Al-Cr," *CALPHAD* 2001;25:279. Publication: [http://dx.doi.org/10.1016/S0364-5916\(01\)00049-9](http://dx.doi.org/10.1016/S0364-5916(01)00049-9)
<http://hdl.handle.net/11115/10088>

Similar Work:
Zhang, L., Du, Y., Chen, Q., Steinbach, I., "Atomic mobilities and diffusivities in the fcc, L12 and B2 phases of the Ni-Al system," *International Journal of Materials Research*, 2010;146:1. <http://dx.doi.org/10.1464.110428>

Abstract:
This work presents the assessment of the diffusion mobilities in both the γ' (Ni₃Al-L12) and B2 phases in the Ni-Al-Cr system utilizing the phenomenological model developed by Helander and Available experimental tracer diffusivity, interdiffusion coefficients and activation energies evaluated and then used to optimize the composition- and temperature-dependent diffusion models. For both the B2 and γ' phases, the assessed diffusion mobility descriptions reproduce the Arrhenius temperature dependence for the Ni, Al and Cr tracer diffusivities and interdiffusion coefficient. The assessment reproduces the strong composition dependence of the diffusivities in the B2 phase observed experimentally. The measured composition dependences of the diffusivities in the γ' phase are also replicated by the present mobility descriptions. The assessed mobility descriptions are validated by comparing calculated and measured composition profiles for a variety of Ni-Al and Ni-Al-Cr diffusion couples, including B2/B2, γ (fcc)/ γ' and γ /B2 couples.

Digital Identifier

Related Work

Similar Work

Files in this item

	Name: exp-b2.zip Size: 9.374Kb Format: application/zip Description: Experimental data for NiAl B2 phase	View/Open
	Name: exp-ni3al.zip Size: 9.619Kb Format: application/zip Description: Experimental diffusion data files for NiAl	View/Open
	Name: alcrni-mob-NIST-0 ... Size: 57.23Kb Format: application/tdb Description: Diffusion mobility description for Ni-Al-Cr using N. Dupin thermodynamics (CALPHAD 2001)	View/Open
	Name: Re-... Size: 237.1... Format: PDF Description: Explanation of rev... mobility description	View/Open

The following license files are:

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This item appears in the following:

- [CALPHAD Assessments](#)

Data files

Offer licenses with attribution 3.0

Research Data Alliance



<http://rd-alliance.org/>

Home

About



Research Data Alliance

The Research Data Alliance (RDA) builds the social and technical bridges that enable open sharing of data Cross-border & cross-disciplinary challenges

The current global research data landscape is highly fragmented, by disciplines or by domains, from oceanography, life sciences and health, to agriculture, space and climate. When it comes to cross-disciplinary activities, the notions of "building blocks" of common data infrastructures and building specific "data bridges" are becoming accepted metaphors for approaching the data complexity and enable data sharing. The Research Data Alliance enables data to be shared across barriers through focused **Working Groups and Interest Groups**, formed of experts from around the world – from academia, industry and government. Participation in RDA is open to anyone who agrees to its **guiding principles** of openness, consensus, balance, harmonisation, community driven and non-profit approach. It was started in 2013 by a core group of interested agencies – the European Commission, the US National Science Foundation and National Institute of Standards and Technology, and the Australian Government's Department of Innovation. Other agencies, countries, companies, associations and institutes are due to join. RDA also has a broad, committed

RDA/CODATA Materials Data, Infrastructure & Interoperability IG



Status: Recognised & Endorsed

The development of advanced materials inherently rests on access to a distributed materials infrastructure and materials research data to fuel discovery and innovation. Given the complementary missions the RDA IG and the CODATA TG will work together under the following statement in support of the exchange of material data.

Co-chairs

- Jim Warren
- Laura Bartolo

Hanisch, NCI Nano WG, 12/17/2015

Materials Science Resource Registry

NIST[Home](#)[Services »](#)[Dashboard](#)[Help](#)[Contact](#)[API](#)

Materials Resource Registry

Search for Resources

General Keyword search:

Results view: Simple Detailed

Access Policy

**SEARCH****CLEAR****ADD MORE SEARCH FIELDS**

Thanks to

- Sharief Youssef
- Alden Dima
- Mary Brady
- Chandler Becker
- Ray Plante

© 2014-2015 NIST Materials Resource Registry | [Privacy Policy](#) | [Registration](#)

Materials Science Resource Registry

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Materials Resource Registry

Search Results for 'compound'

[Edit Search Criteria](#)
[New Search](#)


All Resources



Organizations



Data Collections



Datasets



Services



Informational Sites



Software

Detailed Results View

Resource Type:

- All Resources
- Organization
- Data Collection
- Repository
- Project Archive
- Database

AFLOW

Resource Details

Go To

Publisher

AFLOW Consortium

Resource Type

Repository

Material Science

Material Types: Metal, Semiconductor, Organic
Morphology/Structures: Crystalline, Bulk

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Materials Resource Registry



Add New Repository

[My Repositories](#)
[My Resources](#)

Repository Name

(required)

Short Name

(recommended)

Description

The Materials Project provides a database and associated portal of calculated properties of materials. By computing properties of all known materials, the Materials Project aims to remove guesswork from materials design in a variety of applications. Experimental research can be targeted to the most promising compounds from

(required)

Subjects

Reference URI

We would register resources like

- nanomaterialregistry.org
- nanohub.org
- ...

Materials Science Resource Registry

Material Types	<input type="checkbox"/> Metal <input type="checkbox"/> Semiconductor <input type="checkbox"/> Ceramic <input type="checkbox"/> Polymer <input type="checkbox"/> Biomaterial	<input type="checkbox"/> Organic <input type="checkbox"/> Inorganic <input type="checkbox"/> Oxide <input type="checkbox"/> Composite <input type="checkbox"/> Nanomaterials	<input type="checkbox"/> Superconductor <input type="checkbox"/> Non-Specific <input type="checkbox"/> Other	<input type="checkbox"/> ? (recommended)
Morphology/Structures	<input type="checkbox"/> Crystalline <input type="checkbox"/> Amorphous <input type="checkbox"/> Fluid <input type="checkbox"/> Quasi-periodic <input type="checkbox"/> Bulk <input type="checkbox"/> 2-Dimensional	<input type="checkbox"/> 1-Dimensional <input type="checkbox"/> Film <input type="checkbox"/> Nanotube <input type="checkbox"/> Fiber <input type="checkbox"/> Composite <input type="checkbox"/> Interfacial	<input type="checkbox"/> Interphase <input type="checkbox"/> Line Defect <input type="checkbox"/> Point Defect <input type="checkbox"/> Non-Specific <input type="checkbox"/> Other	<input type="checkbox"/> ? (recommended)
Material Property Classes	<input type="checkbox"/> Optical <input type="checkbox"/> Mechanical <input type="checkbox"/> Thermodynamic	<input type="checkbox"/> Structural <input type="checkbox"/> Simulated <input type="checkbox"/> Interfacial	<input type="checkbox"/> Defect <input type="checkbox"/> Non-Specific <input type="checkbox"/> Other	<input type="checkbox"/> ? (recommended)
Experimental Data Acquisition Methods	<input type="checkbox"/> Electron Microscopy <input type="checkbox"/> Scattering/Diffraction <input type="checkbox"/> Calorimetry <input type="checkbox"/> Load Frame Testing	<input type="checkbox"/> Atomic Force Microscopy <input type="checkbox"/> Spectroscopy <input type="checkbox"/> Optical Microscopy <input type="checkbox"/> Impact Testing	<input type="checkbox"/> Indentation <input type="checkbox"/> Dilatometry <input type="checkbox"/> Other	<input type="checkbox"/> ? (recommended)
Computational Data Acquisition Methods	<input type="checkbox"/> Density Functional Theory <input type="checkbox"/> Molecular Dynamics Simulation <input type="checkbox"/> Numerical Simulations <input type="checkbox"/> Multiscale Modeling <input type="checkbox"/> Finite Element Analysis <input type="checkbox"/> Computational Thermodynamics	<input type="checkbox"/> Statistical Mechanics <input type="checkbox"/> Dislocation Dynamics <input type="checkbox"/> Phase Field <input type="checkbox"/> Crystal Plasticity <input type="checkbox"/> Other	<input type="checkbox"/> ? (recommended)	
Sample Processing Methods	<input type="checkbox"/> Casting <input type="checkbox"/> Annealing <input type="checkbox"/> Vapor Deposition <input type="checkbox"/> Milling	<input type="checkbox"/> Extrusion <input type="checkbox"/> Pressing <input type="checkbox"/> Exfoliation <input type="checkbox"/> Melt Blending	<input type="checkbox"/> Polymerization <input type="checkbox"/> Curing <input type="checkbox"/> Evaporation <input type="checkbox"/> Other	<input type="checkbox"/> ? (recommended)

Materials Data Curation System

Materials Data Curation System

Part of the Materials Genome Initiative

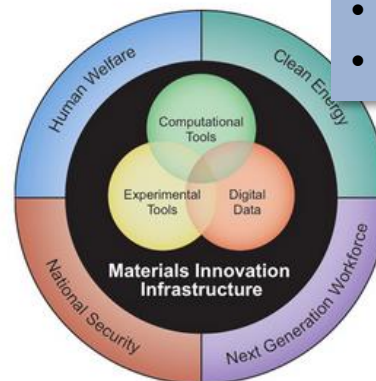
Login | My Pr

Home Data Curation Data Exploration

Materials Data Curator

This system allows for the curation of Material Data in a repository using predefined templates and a prototype ontology.

This is being developed at the National Institute of Standards and Technology and is made available to solicit comments from the Material Science community. Please do not enter any proprietary data into this system.



Credit to

- Alden Dima
- Sharief Youssef
- Guillaume Sousa-Amaral
- Mary Brady
- Carrie Campbell
- Zach Trautt

Available Options

[All Options »](#)



Curate your Materials Data

Click here to select a form template and then fill out the corresponding form.

Most Recent Templates

[Browse All »](#)

Demo Diffusion Data v2.0 | demoDiffusionData_v2.0.xsd

Demo Light | demo.light.xsd

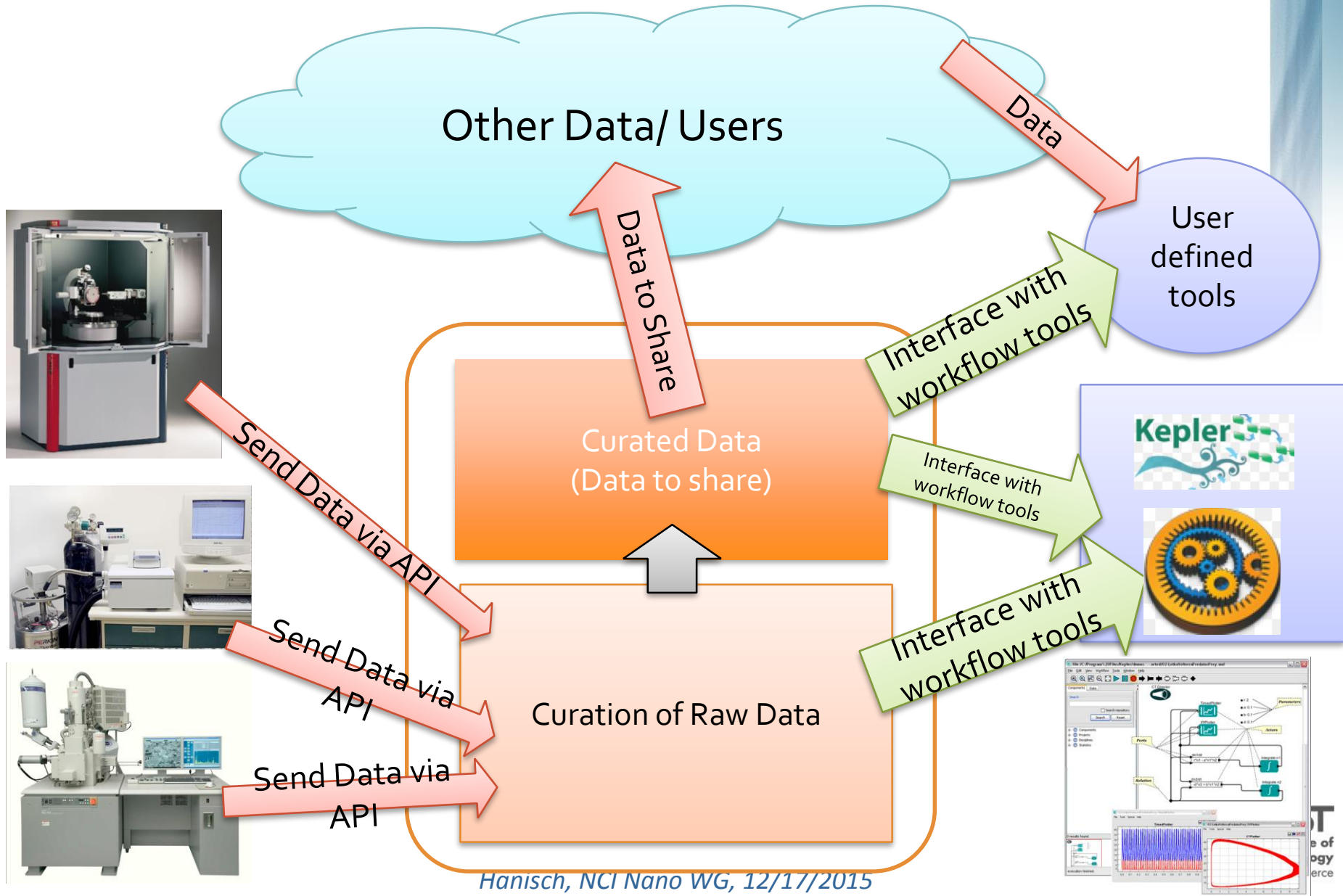
Demo Diffusion | demo.diffusion.xsd

Features:

- Ability to store templates
- Schema management tools
- REST API interface
- *Schema Composer*

- Written in python
- Backed by MongoDB
- SPARQL Query interface
- XML-based Schema
- Table input

Metadata Curation Schematic



National Data Service

The National DATA SERVICE

Home About ▾ Projects ▾ News Get Involved ▾

NDS LABS AND NDS SHARE

These new platforms allow the NDS community to try out new tools and explore new ideas for sharing data as we prototype key NDS capabilities.

[READ MORE ABOUT NDS LABS →](#)

[READ MORE ABOUT NDS SHARE →](#)

The National Data Service (NDS) is an emerging vision for how scientists and researchers across all disciplines can find, reuse, and publish data. It builds on the data archiving and sharing efforts already underway within specific communities and links them together with a common set of tools designed around the following capabilities:

Search

The NDS will allow users to easily search for data across disciplinary boundaries. As users hone in on data of interest, they can easily switch to discipline-specific tools.

Publish

The NDS will connect users to tools for building and sharing collections of data. It will help users find and deliver data to the best repository for data-publishing.

Link

The NDS will create robust connections between data and published articles. When researchers reference an article, they have ready access to the underlying data.

Reuse

The NDS will not only provide access to data for download, it will provide tools for transferring data to processing platforms or allow analysis to be attached to the data.

Hanisch, NCI Nano WG, 12/17/2015

NDS Materials Data Facility

Materials Data Facility

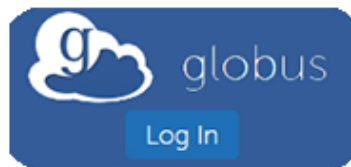
A National Data Service Pilot Program

MDF Home

User Home

Documentation ▾

About



Publish Data

Search Scopus at UIUC Library

Search Metadata at DataCite

Led by

- Ian Foster (U. Chicago, Argonne)


Supported by MGI, MML/ITL



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Font Awesome font licensed under [SIL OFL 1.1](#).

NDS Materials Data Facility


[Publish](#)
[Manage Data](#) ▾
[Groups](#)
[Support](#) ▾
[rplante](#) ▾

License
Describe
Describe
Globus Transfer
Verify
Complete

Submit: Describe this Item ?

Please fill in the requested information about this submission below. In most browsers, you can use the tab key to move the cursor to the next input box or button, to save you having to use the mouse each time.

Descriptive title of the dataset

Dataset Title *

Owner of the dataset

Owner * ➤

Institution * + Add More

Department * ▾

Curating Institution * ▾

Terms describing the dataset to facilitate searching

Keywords + Add More

NDS Materials Data Facility

Materials Data Facility Search

Search:

Article Matches - Scopus

2 Matches

1: **Erratum: Thermal conductivity measurement from 30 to 750 K. The 3ω method (Review of Scientific Inst...**

Cahill, D.G.

Review of Scientific Instruments. October 2002, Vol. 73 Issue 10, p3701.

 [Get Full-Text](#)

Datasets

2: **Thermal conductivity measurement from 30 to 750 K: The 3ω method**

Cahill, D.G.

Review of Scientific Instruments. 1990, Vol. 61 Issue 2, p802-808.

 [Get Full-Text](#)

Datasets

[See all 2 Matches](#)

National Metrology Institutes

Bureau
International des
Poids et
Mesures

– the intergovernmental organization through which Member States act together on matters related to measurement science and measurement standards.

Search facility:



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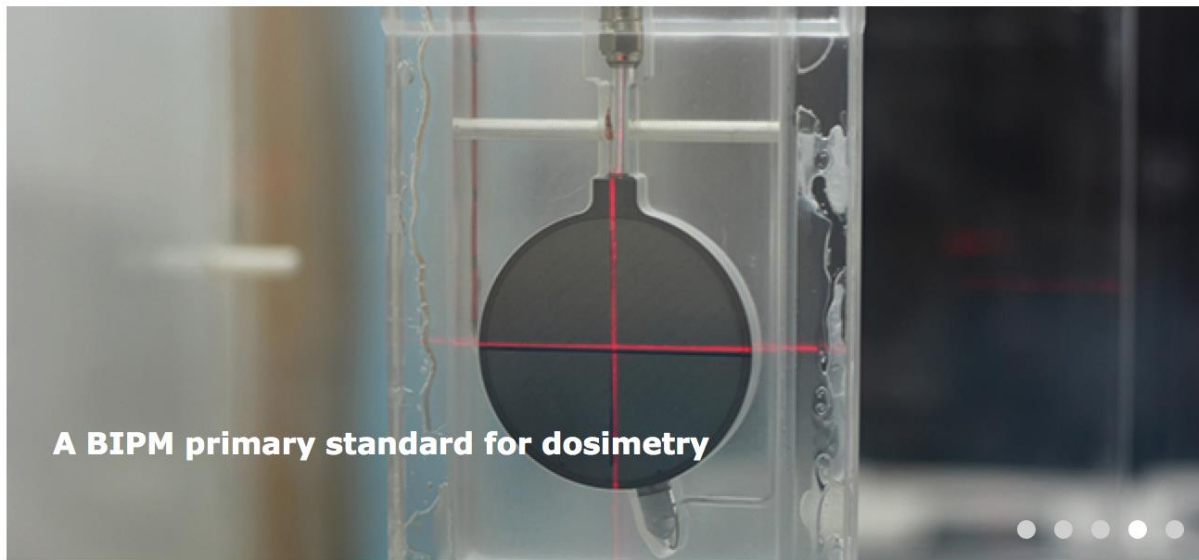
[MEASUREMENT UNITS](#)

[SERVICES](#)

[PUBLICATIONS](#)

[MEETINGS](#)

About the BIPM



A BIPM primary standard for dosimetry

Metrology area:

- ↘ Acoustics, Ultrasound and Vibration
- ↘ Chemistry and Biology
- ↘ Electricity and Magnetism
- ↘ Ionizing Radiation
- ↘ Length
- ↘ Mass and related quantities
- ↘ Photometry and Radiometry
- ↘ Thermometry
- ↘ Time and Frequency
- ↘ Units



UTC Date: Saturday 28 November

↘ [International time](#)

UTC 16:40:47

Your estimated transmission delay: 1.01 second(s)

National Metrology Institutes



– the intergovernmental organization through which Member States act together on matters related to measurement science and measurement standards.

Search facility:



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> You are here: [worldwide metrology](#) > [national metrology infrastructure](#)

National Metrology Institutes (NMIs)

Each State has its own metrology infrastructure. In most cases the BIPM interacts principally with one National Metrology Institute (NMI) per State, as nominated through the State's Foreign Affairs Department. That NMI is responsible for coordinating with any other institutes (NMIs or others) that make up that nation's metrology system.

→ The dropdown menu on the right-hand side of this page gives access to more details about the metrology infrastructure in individual Member States and Associates. In particular, these pages list all the institutes participating in the CIPM Mutual Recognition Arrangement (CIPM MRA), the international framework through which the NMIs demonstrate the equivalence of their measurement standards and the calibration and measurement certificates they issue.

The BIPM hosts (approximately annual) meetings of the Directors of NMIs, providing a unique occasion for discussion of metrological issues of world-wide concern, and of course for discussion of the BIPM's work programme. Such meetings sometimes also include governmental representatives from Member States, to allow discussion of the financial implications.

→ Hub for Member States and Associates:

- ✦ Directors of NMIs of Member States
- ✦ Directors of NMIs of Associates
- ✦ Representatives of States Parties

↘ Member State/ Associate:

↘ Related links:

- ✦ **DCMAS Network:**
Metrology, Accreditation and Standardization for Developing Countries
- ✦ **National Metrology Infrastructure in EURAMET Member Countries – An Analysis and Recommendations (EURAMET Guide 11 (2011))**



An International Resource Registry for National Metrology Institutes

Dr. Willie May

Director

National Institute of Standards and Technology

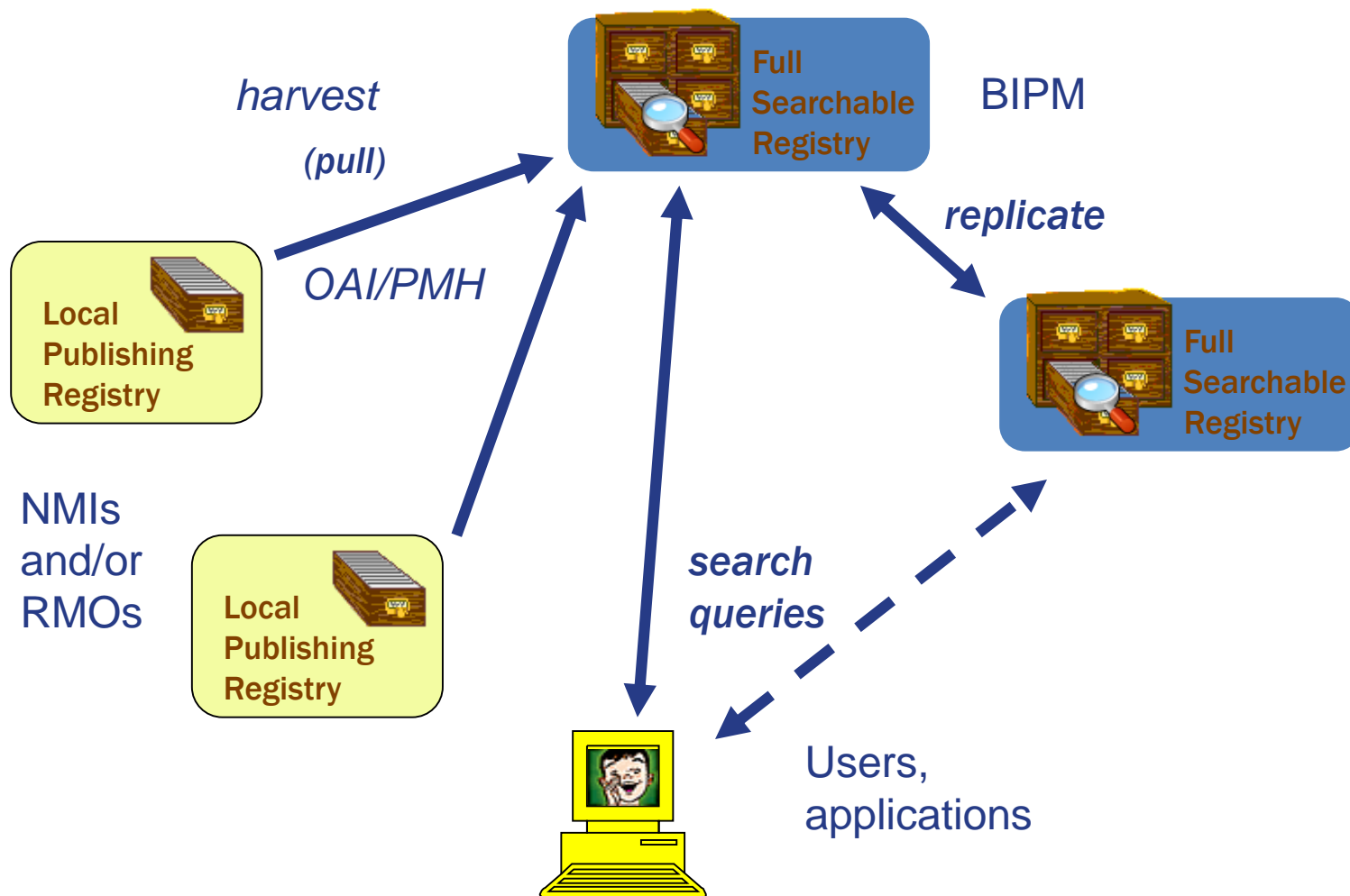
The Issue

- The network of National Metrology Institutes hold valuable collections of reference data and provide state-of-the-art metrology services
- How does one find out, across all NMIs, where particular data and data-related services are located?
 - Standard Reference Data
 - Reference Data
 - Data associated with publications
 - Data associated with Standard Reference Materials
 - Simulation data
- Need a data-focused analog to the Key Comparisons Database

Concept

- Build an international *registry* of NMI data resources
 - A *registry* is a simple database of metadata that describe data resources: where data collections are located, what kind of data they contain, how the data can be accessed, etc.
- Resource descriptions (metadata) would be provided by NMIs
- Metadata would be federated using existing, well-proven technology for metadata federation, the Open Archive Initiative – Protocol for Metadata Harvesting (OAI-PMH)
 - Has been in use in the research library community for more than 20 years
- Federated resource registry would be searchable through web page and via application programming interface (API)

Federated Architecture



Example from Astronomy



Search All Virtual Observatory Collections:

M101

Search criteria; instead of astronomical object name, could be "aluminum oxide" or "electron scattering"

[User Guide](#) | [Discovery Tool v1.5 \(6846\)...](#)

Examples: [M101](#), [14.03.12.6](#) + [54.20.56.7](#), [more...](#)

Start Page x M101 r=1m x

31 Total Rows 97.4% of resources searched

MESSIER 101 (RA: 14:03:12.545, Dec: +54:20:56.22), radius: 0.01667°

341 new rows received Refresh Table

Filters

Clear Filters Edit Facets... Help...

Filter All Record Fields

Type

- Catalog (14 of 14)
- Image (13 of 13)
- Spectra (4 of 4)

Waveband

- EUV (2 of 2)
- Gamma-ray (5 of 5)
- Infrared (7 of 7)
- Millimeter (4 of 4)
- Optical (12 of 12)
- Radio (3 of 3)
- UV (7 of 7)
- X-ray (8 of 8)

Publisher

- Canadian Astronomy Data Centre (2 of 2)
- CDS (4 of 4)
- Chandra X-ray Observatory (2 of 2)
- ESO (1 of 1)
- European Space Agency (1 of 1)
- (1 of 1)
- (3 of 3)
- (1 of 1)
- (2 of 2)
- (1 of 1)

Actions	Short Name	Type	Title
	CADC		CADC Image Search
	CADC/SIAv1		CADC Image Search (SIA)
	HLA [1]		Hubble Legacy Archive
	Simbad		The SIMBAD astronomical database
	ST-ECF/HST/SSA		ST-ECF Hubble Space Telescope Spectra
	NED(sources)		The NASA/IPAC Extragalactic Database
	ST-ECF/HST/SIA		ST-ECF Hubble Space Telescope Images
	ST-ECF/HLA/SIA		ST-ECF Hubble Legacy Archive Images
	CDA [1]		Chandra X-ray Observatory Data Archive
	NED/SED		The NASA/IPAC Extragalactic Database SED Data Discovery Service
	DSS ESO		Digitized Sky Survey
	GALEX		Galaxy Evolution Explorer
	hdap_siap [1]		HDAP -- Heidelberg Digitized Astronomical Plates
	CSC [1]		Chandra Source Catalog
	GALEX		Galaxy Evolution Explorer
	J/AJ/104/92		HII Regions Properties in M101 (Scowen+ 1992)
	SDSSDR5		Sloan Digital Sky Survey DR5 - Images
	ISSA		The IRAS Sky Survey Atlas

AstroView

14:02:25.380 +54:22:37.340
14:03:12.545 +54:20:56.220

RA DEC
hhmmss/deg

List of data resources with direct links

Facets or filters that permit easy refinement of search

NIST research data: ~10 year horizon

- Expand the Standard Reference Data collection.
 - Identify through internal and external inputs where new SRD are needed.
 - Prioritize, scope, and find resources for development work
- Establish NIST as an exemplar federal agency in data management.
 - Implement and share best practices for preservation, curation, discovery, re-use, and interoperability
 - Facilitate community-based development of metadata standards & data models
 - Participate in leadership of national and international data federation activities
 - Research Data Alliance, National Data Services Consortium, CODATA and World Data System
 - Contribute to solving the challenge of long-term sustainability of data repositories
 - Share NIST-developed technologies to assist other agencies in improving data access and data services
 - Collaborate with federal and non-federal organizations in developing and deploying common solutions
 - Establish a data-aware, data-savvy culture at NIST
 - Improve efficiency of experimentation and simulation
 - Improve reliability and reproducibility of research results
 - Increase value of NIST to the research and industrial communities

Some things to think/worry about

- Quality metadata is key for discovery, interoperability, re-use
 - Reproducibility
 - Integrity of the scientific process
 - Metadata curation is non-trivial, can be costly
- Address interoperability at the proper scale
 - Too wide: very expensive, difficult/impossible to reach consensus across disciplines; what is the scientific motivation?
 - Too narrow: Scientific stovepipes, missed opportunities for discovery at the intersections of complementary data collections

Some things to think/worry about

- Standards for metadata, data access protocols, etc., require community participation to assure take-up
 - Major research organizations
 - Professional societies (national, international)
 - Recognized standards organizations
 - RDA, CODATA, NDS, EUDAT, etc.

Some things to think/worry about

- Little national commitment to sustaining infrastructure for open data
 - Domain repositories often must (re)compete for basic resources, rely on complex business models
 - Federal funding agencies require Data Management Plans, but provide no common infrastructure and no consistent review process
 - Commercial academic publishers poised to take on data preservation roles; open data could move behind pay-walls

<http://tinyurl.com/domainrepositories25>

International Data Week

- September 12-16, 2016, Denver
- RDA Plenary, CODATA SciDataCon, ICSU World Data Service