



International Materials Resource Registries

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Summary of the Problem

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- As the wealth of digital data grows, it becomes increasingly difficult for researchers to learn what data exists.
 - National initiatives for materials science (e.g. Materials Genome Initiative) are driving that growth
 - Researchers want to search for data using concepts of their domain:
e.g. looking for simulations of semiconductors
 - Start with what high-level resources—repositories, databases, portals, software—exist.
 - A registry-based discovery system is a practical, extensible start
 - Looking for solution can be owned, shared by a community
 - Connect users to data providers' sites and tools
 - Enable data providers, experts to control curation of metadata
 - Robust against failure (including funding failure)
 - This discovery problem applies to all domains
 - Can we use materials science to pilot a solution that can be adapted to other domains?

Highlights of the Recommendation

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- A blueprint for a creating registry federation for data discovery
 - No central or primary registry
 - Each of the distributed registries collects resource descriptions for a sub-community
 - Registries trade resource descriptions via OAI Protocol for Metadata Harvesting
 - Enumeration of required standards
 - A materials science resource metadata XML schema
 - Generic + domain-specific extension
 - Materials Vocabulary
 - Basis for materials science-specific metadata
 - SKOS definition
 - Open-source registry software featuring APIs and plugin schemas
 - Working pilot: 2-node registry federation
 - Over 300 data resources described

NIST Materials Resource Registry

Part of the Materials Genome Initiative

SEARCH FOR RESOURCES

ADD YOUR RESOURCE

Search for Resources

electrical x properties x

All Resources Organizations Data Collections Datasets Services Informational Sites Software

Search criteria used (Clear all):
Type x Material Type x

5 results

TYPE (Clear)

- Organization (0)
- Collection (0)
- Dataset (2)
- Service (0)
- Software (0)
- Web Site (1)

ORIGIN OF DATA (Clear)

MATERIAL TYPE (Clear)

- biological (0)
- biomaterials (1)
- ceramics (2)
- metals and alloys (2)
- metamaterials (0)
- molecular fluids (0)
- organic compounds (1)
- organometallics (1)
- polymers (4)
- semiconductors (2)

STRUCTURAL FEATURE (Clear)

PROPERTY ADDRESSED (Clear)

MatWeb
MatWeb
<http://www.matweb.com/index.aspx>
Subject keywords: engineering, material properties, database, suppliers
"The heart of MatWeb's services is our searchable online database of engineering materials. We have over 115,000 data sheets in our collection and have many powerful search tools available to help our users find the materials information that they need. While we have a variety of services that we offer to companies in the engineering community, our ... show more

Microelectronics Packaging Materials Database
CINDAS LLC
<https://cindasdata.com/products/mpmimd>
Subject keywords: electronics packaging materials, material properties
"The MPMID contains data and information on thermal, mechanical, electrical and physical properties of electronics packaging materials, and it is available in a Web-based format. The database is continually updated and expanded. The MPMID contains over 1,025 materials, 388 properties, and contains approximately 22,500 data curves."

JARVIS - Joint Automated Repository for Various Integrated Simulations
Kamal Choudhary/National Institute of Standards and Technology, Faical Y. Congo/National Institute of Standards and Technology, Chandler A. Becker, Francesca M. Tavazza/National Institute of Standards and Technology - NIST
<http://www.ctcms.nist.gov/~kncb/periodic.html>
Subject keywords: Materials Science, Empirical Potentials, Density Functional Theory, Energetics properties, Elastic properties
JARVIS (Joint Automated Repository for Various Integrated Simulations) is a repository designed to automate materials discovery using classical force-field, density functional theory, machine learning calculations and experiments. The Force-field section of JARVIS (JARVIS-FF) consists of thousands of automated LAMMPS based force-field calculations... show more
↳ Harvested from CHIMaD MDF mrr.materialsdatafacility.org...

Elemental vacancy diffusion database from high-throughput first-principles calculations for fcc and hcp structures
Angsten, Thomas/University of Wisconsin-Madison, Mayeshiba, Tam/University of Wisconsin-Madison, Wu, Henry/University of Wisconsin-Madison, Morgan, Dane/University of Wisconsin-Madison - NIST
<http://hdl.handle.net/11256/76>
Subject keywords: Materials Science, Bulk Diffusion, Density Functional Theory
This work demonstrates how databases of diffusion-related properties can be developed from high-throughput ab initio calculations. The formation and migration energies for vacancies of all adequately stable pure elements in both the face-centered cubic (fcc) and hexagonal close packing (hcp) crystal structures were determined using ab initio calcul... show more
↳ Harvested from CHIMaD MDF mrr.materialsdatafacility.org...

Supplementary information for a study of DFT+U in the context of BifeO3
John Kane Shenton/University College London: London, London, United Kingdom - Github.com
<https://github.com/JohnKaneShenton/Supplementary-information-for-a-study-of-DFT+U-in-the-context-of-BifeO3>

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Materials Resource Registry

Add New Resource

My Resources

Resource

Local ID
JWTW3DURXLKF1JBV4WIT

Status
Active

Identity

Resource Name NIST Chemistry WebBook

Alternate Name

Version

Identifier

Logo

Providers

Publisher National Institute of Standards and Technology

Publication Year

Creator

Contributor

Date

Contact

Name NIST

Postal Address

Email Address webbook11@nist.gov

Phone Number

Time Zone

Content

Description

"This site provides thermochemical, thermophysical, and ion energetics data compiled by NIST under the Standard Reference Data Program."

Two nodes

- NIST: <https://materials.registry.nist.gov>
- Materials Data Facility: <http://registry.materialsdatafacility.org/>

Software available at

<https://github.com/usnistgov/MaterialsResourceRegistry>

Impact of the Recommendation

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- Scalable, sustainable network of registries for discovering materials science data
 - A recipe and toolset for establishing registries supporting other communities
 - Adaptable to other metadata formats, exchange protocols
 - A foundation for developing a variety of deep search capabilities
 - Leveraging archive-level search services
 - Integration of search services into third-party tools

Endorsements/ Adopters

- Sufficient take up in materials science to continue further development
 - Continue to encourage community to register resources
 - Fostering partnerships to establish additional registry nodes
 - Prototyping advanced searching capability
- Have adapted model and software to set up registries for other communities
 - International **Metrology** Resource Registry – <http://imrr.bipm.org/>
 - Greenhouse Gas research community