P9: Joint Session of Materials Data, Infrastructure, & Interoperability IG & Int’l Materials Resource Registries WG
Welcome & Introductions,
Laura Bartolo, Northwestern U. & Ray Plante, NIST
Other MDII IG, Co-Chairs:
James Warren & Chandler Becker, NIST

Round the Room - Brief Introductions (name & institution, pls)

Brief News from the Floor
- Breakout 6, 06 Apr 14:00 MR 8 Joint Session: Chem, Mat’ls, Photon/Neutron

Discussion:
- Review of WG Mission, Scope, & Timeline, Laura
- Vocabulary & Technical Issues, Ray
- Next Steps: Meeting Goals, All
  - 1 Yr Preliminary Recommendations, Adopters, & Outputs
  - 18 Mo Final Recommendations, Adopters, & Outputs
Goals for this meeting

- Present materials vocabulary & registry work to date
- 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
Review of P8 & 2/23/17 Teleconference
Materials Registry Working Group

Chandler Becker and Ray Plante
Sharief Youssef, Alden Dima, Zachary Trautt, Kimberly Tryka, Robert Hanisch, Jim Warren, Mary Brady

National Institute of Standards and Technology

Laura Bartolo
Northwestern University

RDA Plenary 8 & 23 February 2017 Teleconference
Materials Data, Infrastructure, & Interoperability (MDII) Interest Group

- Accelerate discovery, design, & development of advanced materials in ½ time & ½ cost.
  - Explore opportunities for fundamental research & public/private partnerships of data-based services, tools, & applications.

- Establish free & open data exchange mindful of intellectual property & national security.
  - Exchange computational & experimental materials data through shared online repositories, standardized formats/terminologies, & open programming interfaces.
RDA websites

- **Interest group**
  - [https://rd-alliance.org/groups/rdacodata-materials-data-infrastructure-interoperability-ig.html](https://rd-alliance.org/groups/rdacodata-materials-data-infrastructure-interoperability-ig.html)

- **Working group**
  - [https://www.rd-alliance.org/groups/working-group-international-materials-resource-registries.html](https://www.rd-alliance.org/groups/working-group-international-materials-resource-registries.html)

- **Case statement**
WG members (31 Dec 2016)

- **Brian Matthews**
  - Science and Technology Facilities Council
- **Chandler Becker**
  - National Institute of Standards and Technology
- **Charles Vardeman**
  - University of Notre Dame
- **Clare Paul**
  - Air Force Research Laboratory
- **Deborah Mies**
  - Granta Design, Ltd.
- **Haiqing Yin**
  - Beijing Univ. of Science and Tech.
- **James Warren**
  - National Institute of Standards and Technology
- **Kathleen Fontaine (TAB Liaison)**
  - Rochester Polytechnic Institute (RDA)
- **Laura Bartolo**
  - Northwestern University
- **Raphael Ritz**
  - Max Planck Society, Garching
- **Raymond Plante**
  - National Institute of Standards and Technology
- **Robert Hanisch**
  - National Institute of Standards and Technology
- **Sharief Youssef**
  - National Institute of Standards and Technology
- **Tobias Weigel (TAB Liaison)**
  - German Climate Computing Center (DKRZ)
- **Vasily Bunakov**
  - Science and Technology Facilities Council
- **Zachary Trautt**
  - National Institute of Standards and Technology
- **Yibin Xu**
  - National Institute for Materials Science

Any new people who haven’t joined yet?
A resource registry is a catalog containing descriptions of *resources* that are useful for (materials science) data-driven research

- Mainly datasets, databases, and data services
- Can also be portals, software, organizations, …

A starting point for *discovering* useful data and tools

- Make high level metadata descriptions searchable
- Direct users to the web sites that host the data
What does federation mean? **Think Globally, Act Locally**

- Comprised of a network of registries; there is no single Registry
  - Any registry can collect a globally-comprehensive collection of resource descriptions and make it searchable
- Resource metadata exchange
  - There a common mechanism(s) for sharing descriptions of available data resources
- Allow local metadata curation
  - Any organization can run registry of their own data resources and share it with the world

Why federate?

- Distribute metadata curation
  - Allow experts who provide/operate data resources to manage how they are described, update descriptions as they evolve
- No single point of failure (including funding failure)
- Allow innovation in providing search capabilities

How do we federate?

- Common metadata exchange mechanism
  - We propose starting with OAI-PMH
- Common metadata schema
Since the last meeting (Sept. 2016)

- Significant vocabulary development, helped greatly by VOCAMP in December 2016
  - Balance the need for specificity against not overwhelming users with options

- Further software development to support the new vocabulary and improve the user experience
  - Resources can have multiple types (organization, repository, software, etc.)
  - Streamlined user interface
  - Record harvesting has been enabled
The Draft Case Statement for the Working Group on International Materials Resource Registries (WG IMRR) requires a continuation of technical and political process. As an outgrowth to discussions held in MDII IG working sessions and based on knowledge of the materials community, MDII IG proposes core members for its Working Group. The core members would be comprised of "doers" in the materials and cognate communities to identify those in their organizations who need to be involved. More details are available in the draft Case Statement.

Link to the TAB Review

Recent Activity

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File Repository

- Materials Vocabulary Draft (31 Jan 2017)

Latest Webconference

- Plenary 9 Materials IG & WG Sessions & Latest Posting Of MatSci Vocab
Full timeline

- Month 1 (Jul ’16)
  - recruit domain specialists to participate in WG

- Month 2 (Aug/Sep ’16)
  - initiate discussions about conducting a survey of existing materials science data providers
  - develop 20 typical data discovery queries to inform metadata discussions

- Month 3 (Sep/Oct ’16)
  - hold meeting to draft 1st version of metadata extensions to Dublin Core

- Months 4-8 (Oct ‘16-Feb ’17)
  - disseminate draft to the materials science community, both within and external to RDA, and solicit feedback

- Month 8 (Feb ’17)
  - hold teleconference to refine metadata extensions and establish implementation pilot program

- Months 9-12 (Mar – Jun ’17)
  - Evaluate & give feedback on MatSci Vocabulary BY 01 May 2017
  - Implement pilot federated registry and recruit testers/evaluators
  - Write best practices guidelines document

- Months 13-15 (Jul – Sep ’17)
  - Adoption & Recommendations BY 01 SEPTEMBER 2017
  - Document metadata development process: what worked well, what didn’t
  - expand content of pilot registry

- Months 16-18 (Oct – Dec ’17)
  - Prepare final document for delivery to RDA