Materials Data Curation System

Alden Dima, Guillaume Sousa Amaral, Phillippe Dessauw, Marcus Newrock, Pierre-François Rigodiat, Xavier Schmitt, Sharief Youssef

Information Systems Group - Mary Brady, Group Leader

Software and Systems Division

Information Technology Laboratory

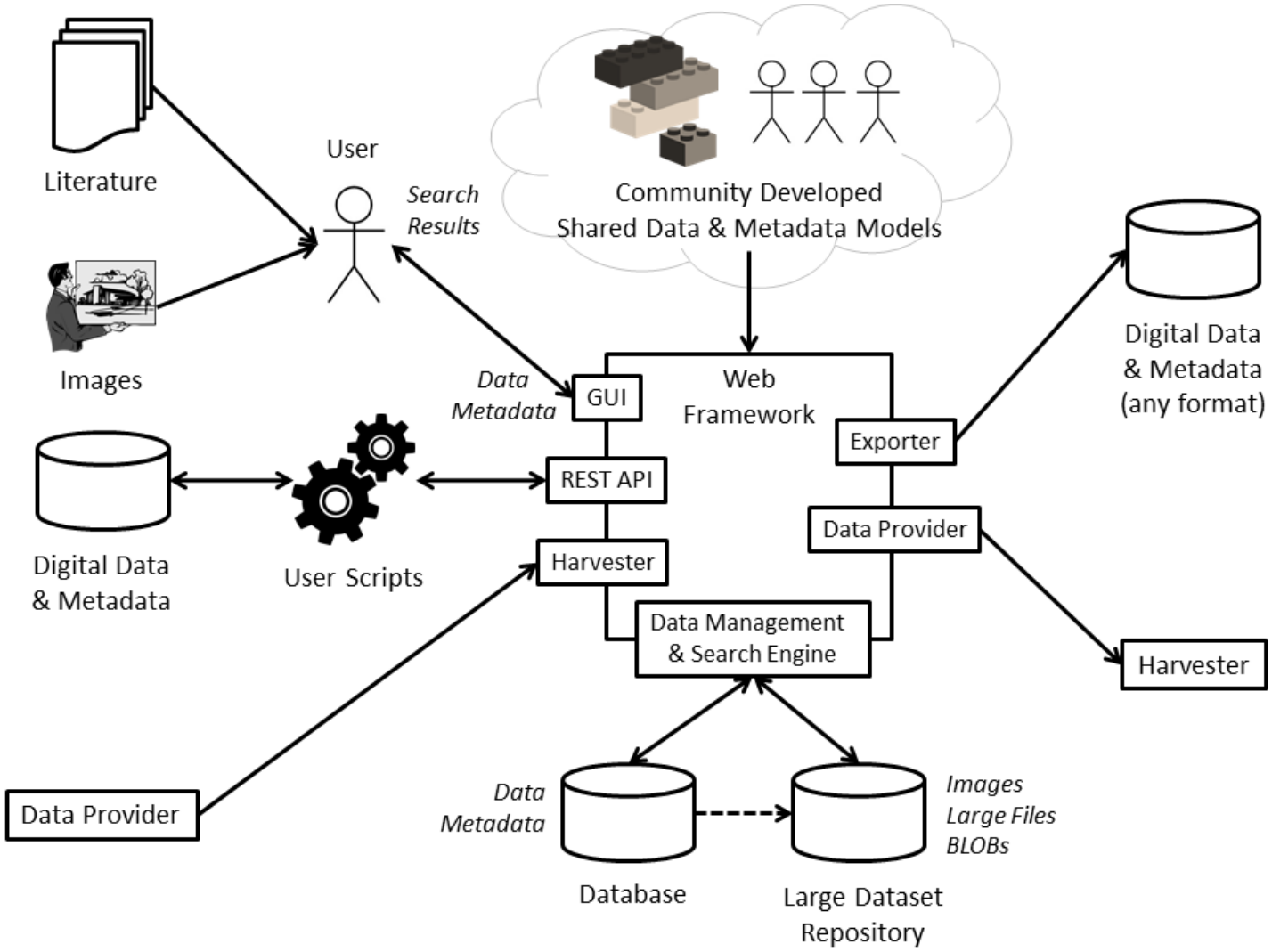
National Institute of Standards and Technology (NIST)

Materials Data Curation System

Components and Features:

- Data Curation (data markup)
- Data Exploration (search)
- Composer (Template builder)
- Exporter (any output desired)
- Module System (Rich GUI Widgets)
- RESTful Application Program Interface (API)
- Administrative Dashboard (for admins)
- New Features (1.4 release)

Materials Data Curation System



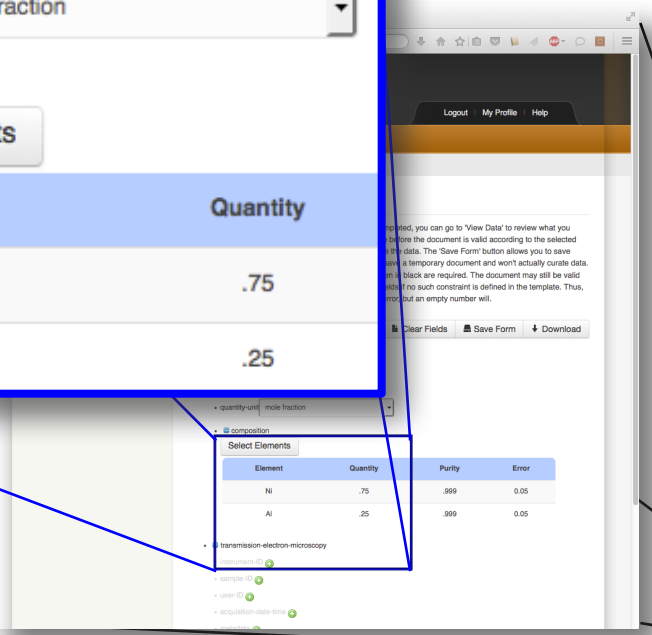
Data Curation

Summer Undergraduate Researcher

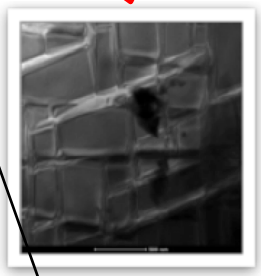
- quantity-unit: mole fraction
- composition

Select Elements

Element	Quantity
Ni	.75
Al	.25



Sample 3?

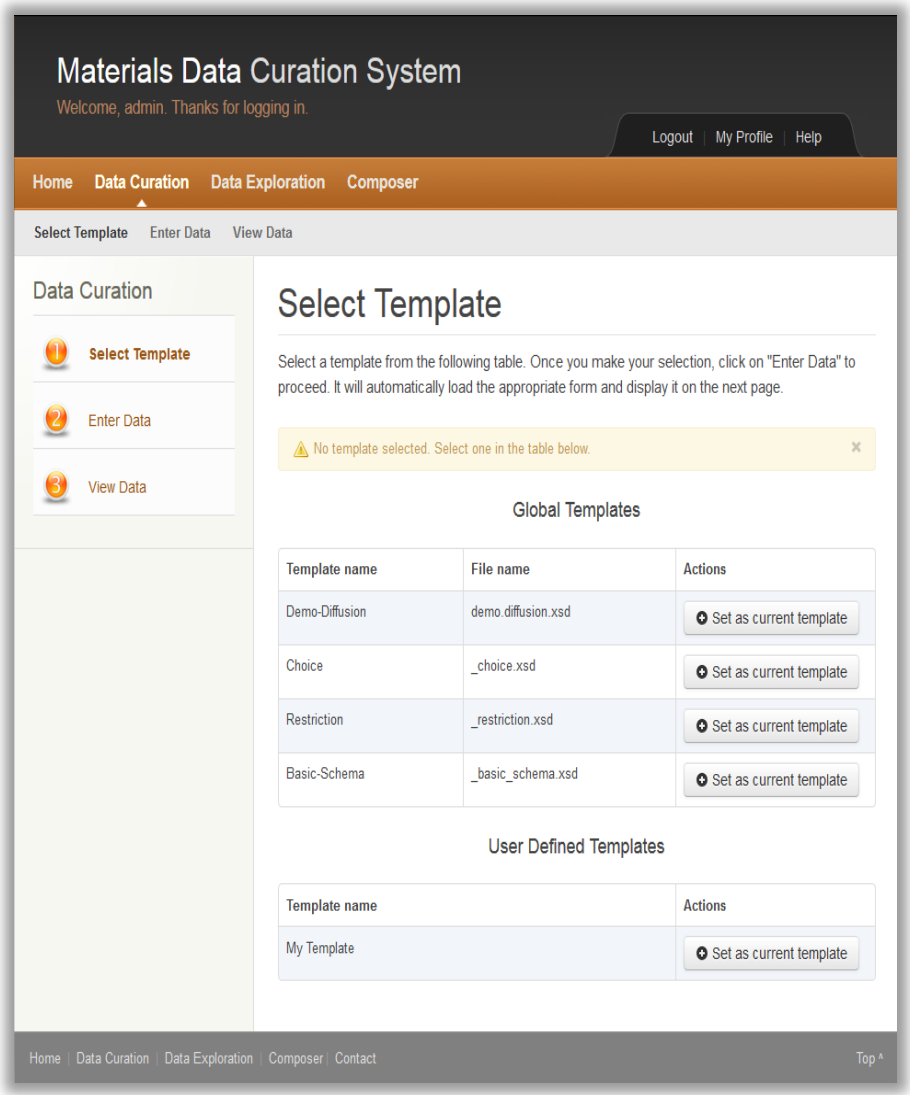


Sample-3.jpg

Data Curation

Three Steps to Curate

1. Select Template
   - Global Templates
   - User Defined Templates
2. Enter Data
   - HTML Generated
   - Based on Template
3. View Data
   - Requires Validation
   - Download in XML Format
   - Can save to Repository



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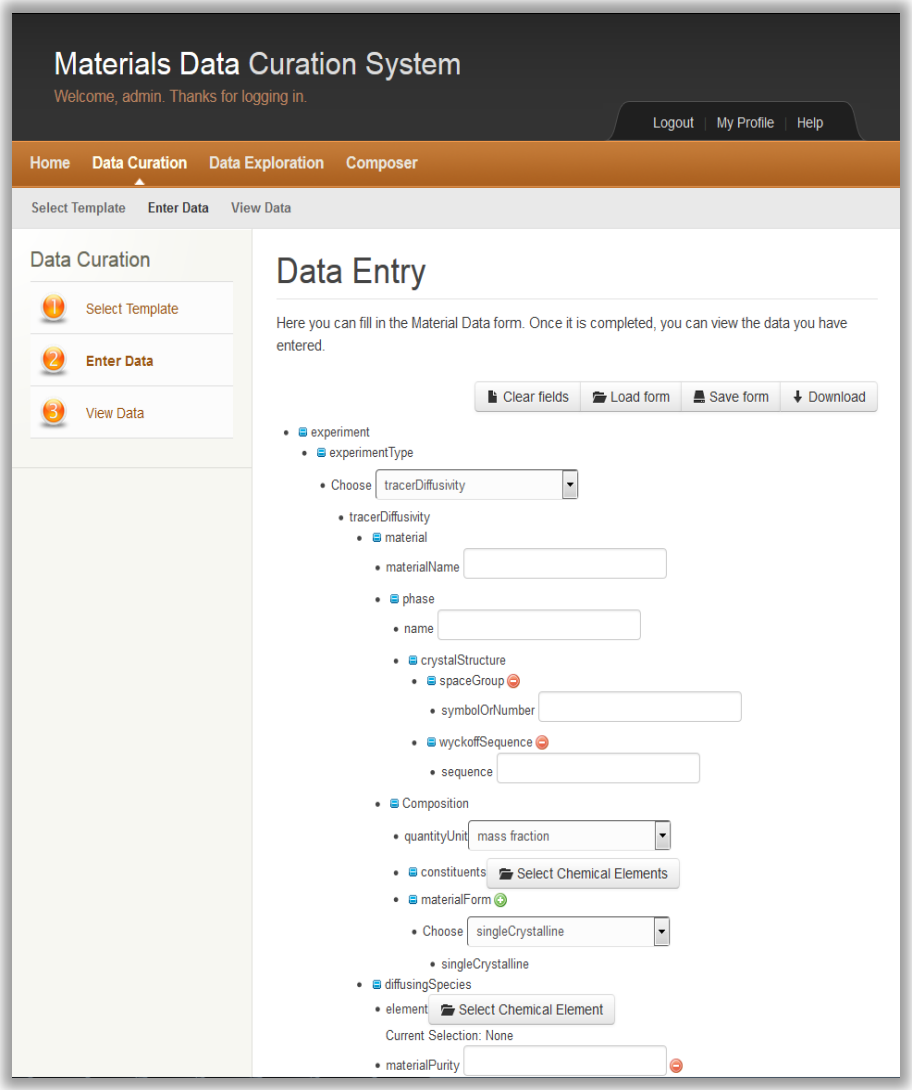

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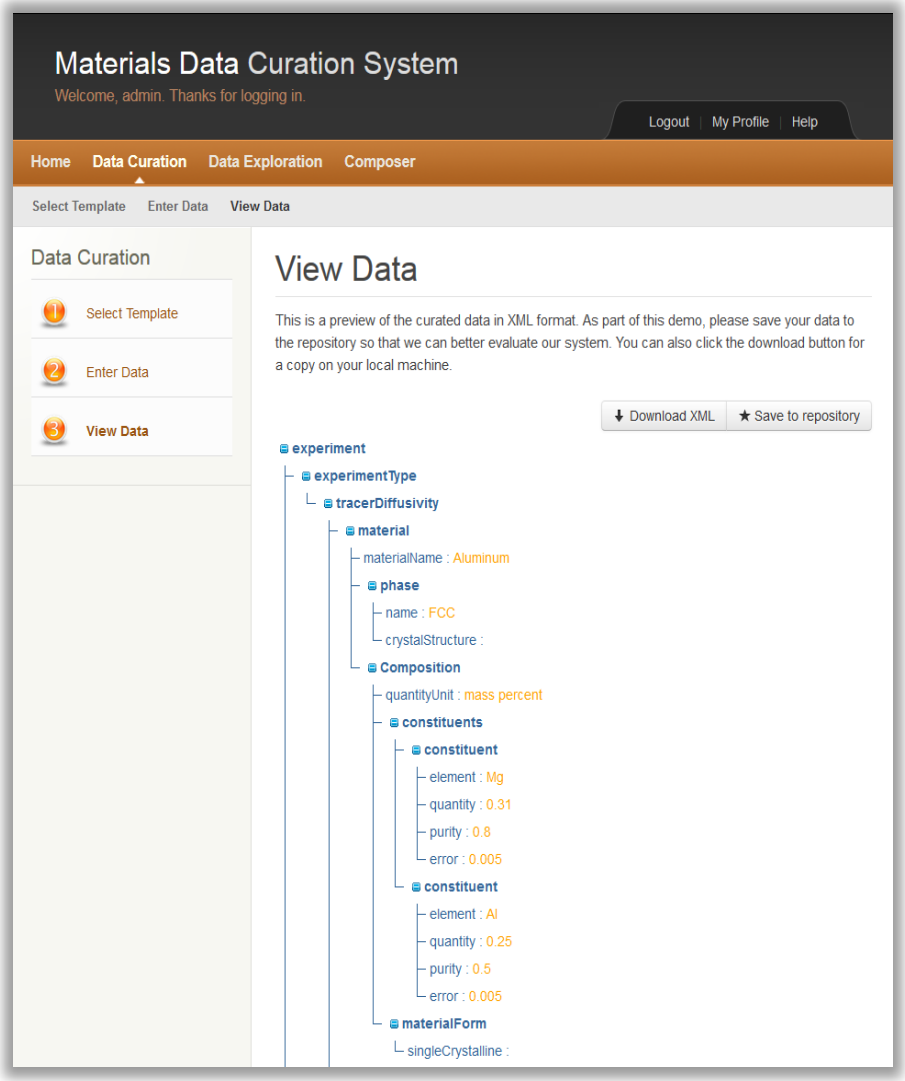
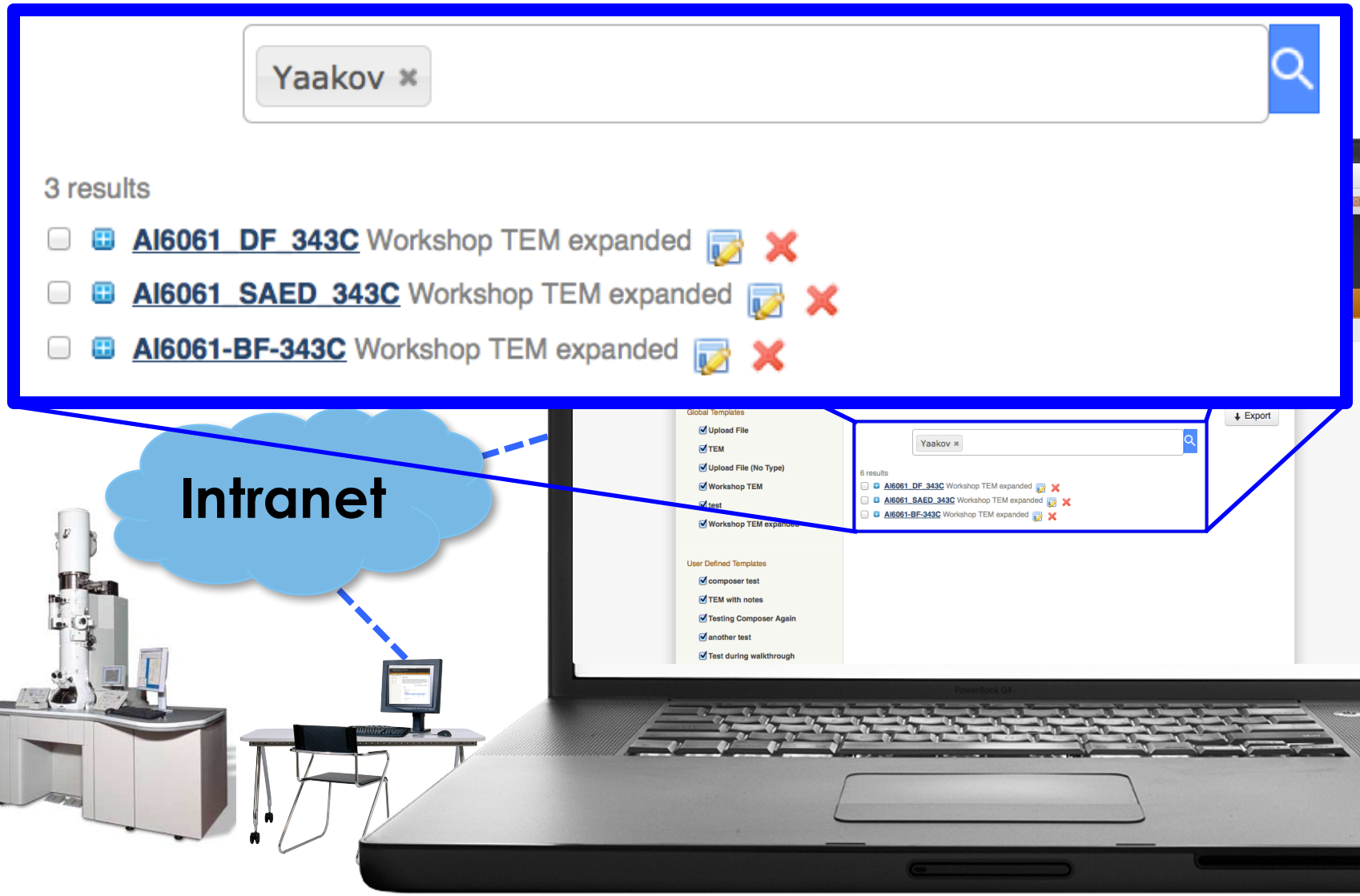


> One step when using REST API

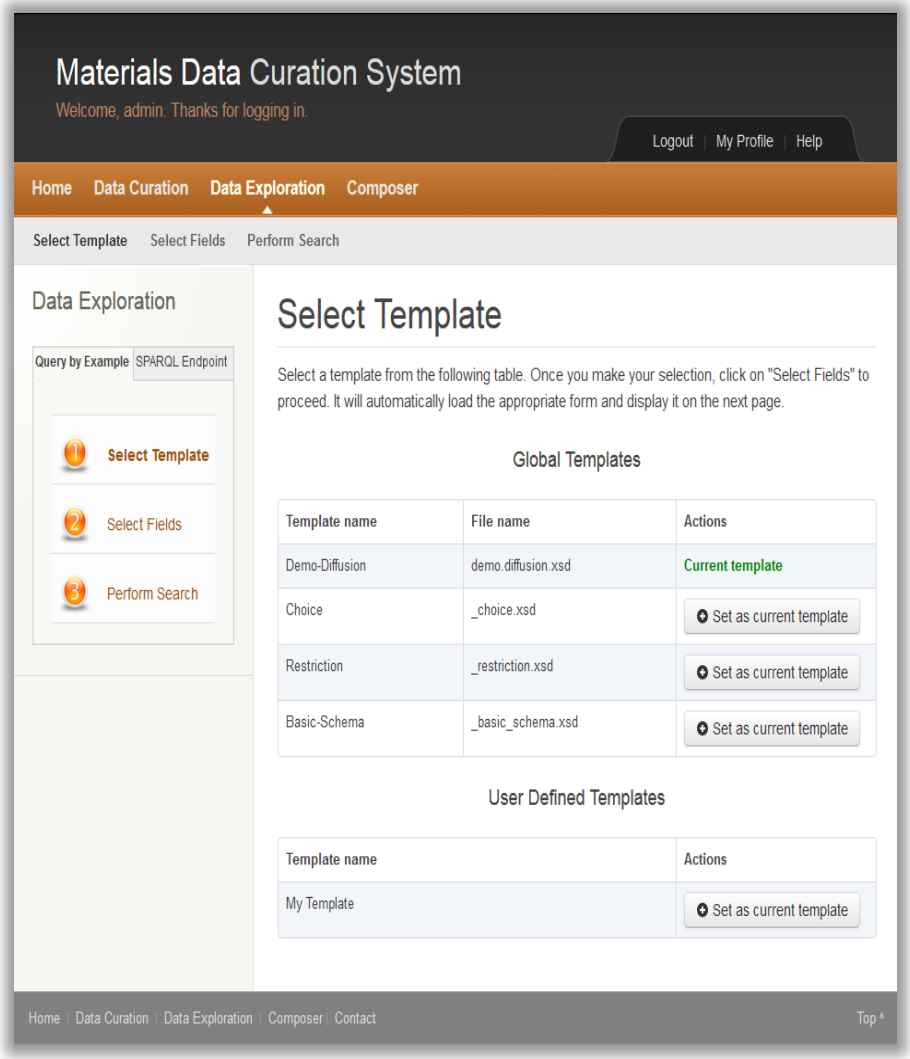
Data Exploration



Data Exploration

Three Steps to Explore:

1. Select Template
   - Global Templates
   - User Defined Templates
2. Select Fields
   - Specific fields to search against
3. Perform Search
   - Query By Example
   - Search by Keyword



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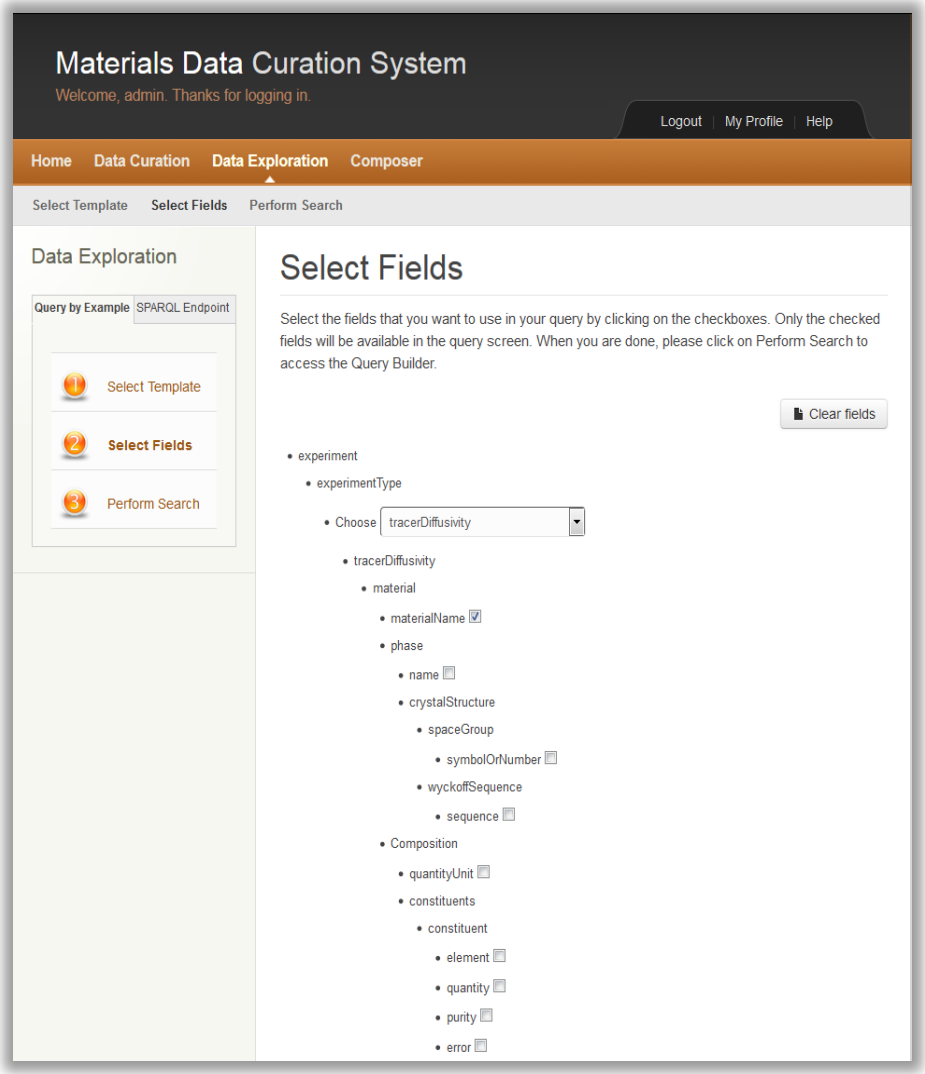

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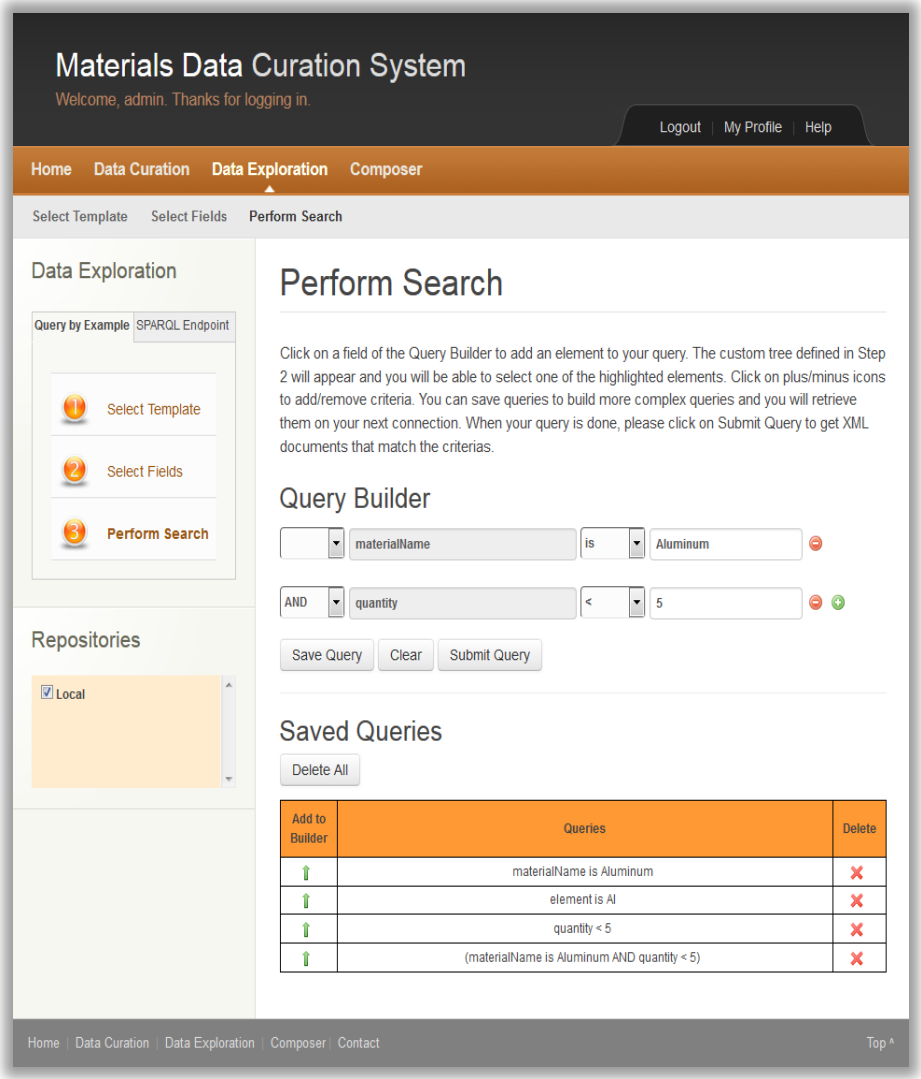
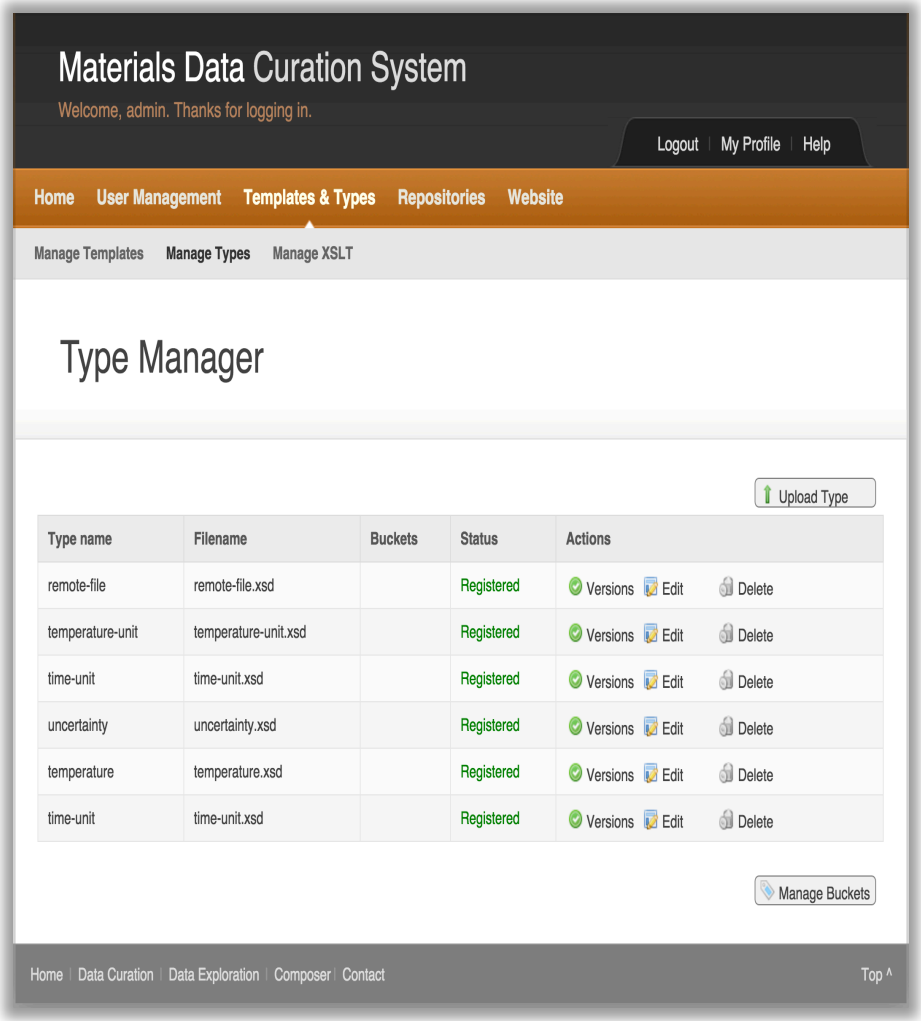


Composer

Begin with Types

Available functions for Type Manager:

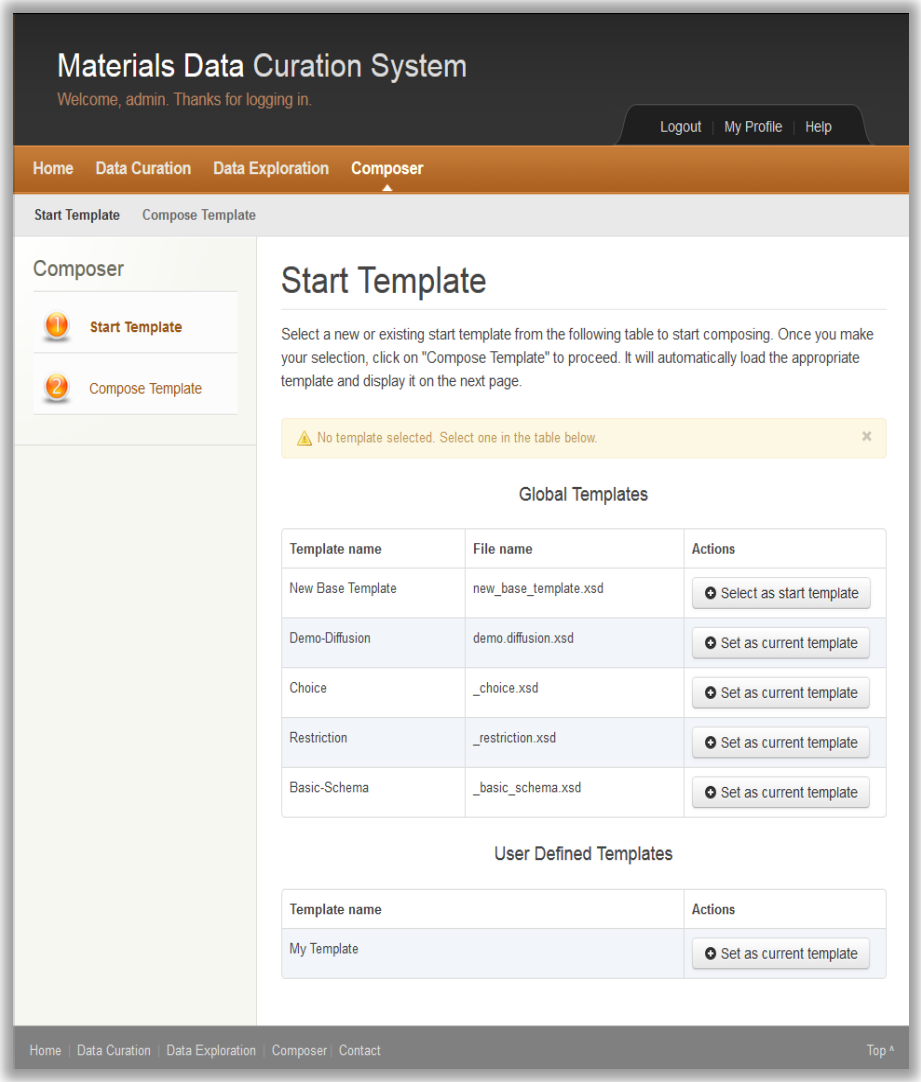
- Upload Types
- Manage Versions
- Edit Types
- Delete Types



Composer

Two Steps to Compose:

1. Start Template
   - Global Templates
   - User Defined Templates
2. Compose
   - Based on Selected Template
   - Add/Delete Elements and Attributes
   - Save to a new User Defined Template



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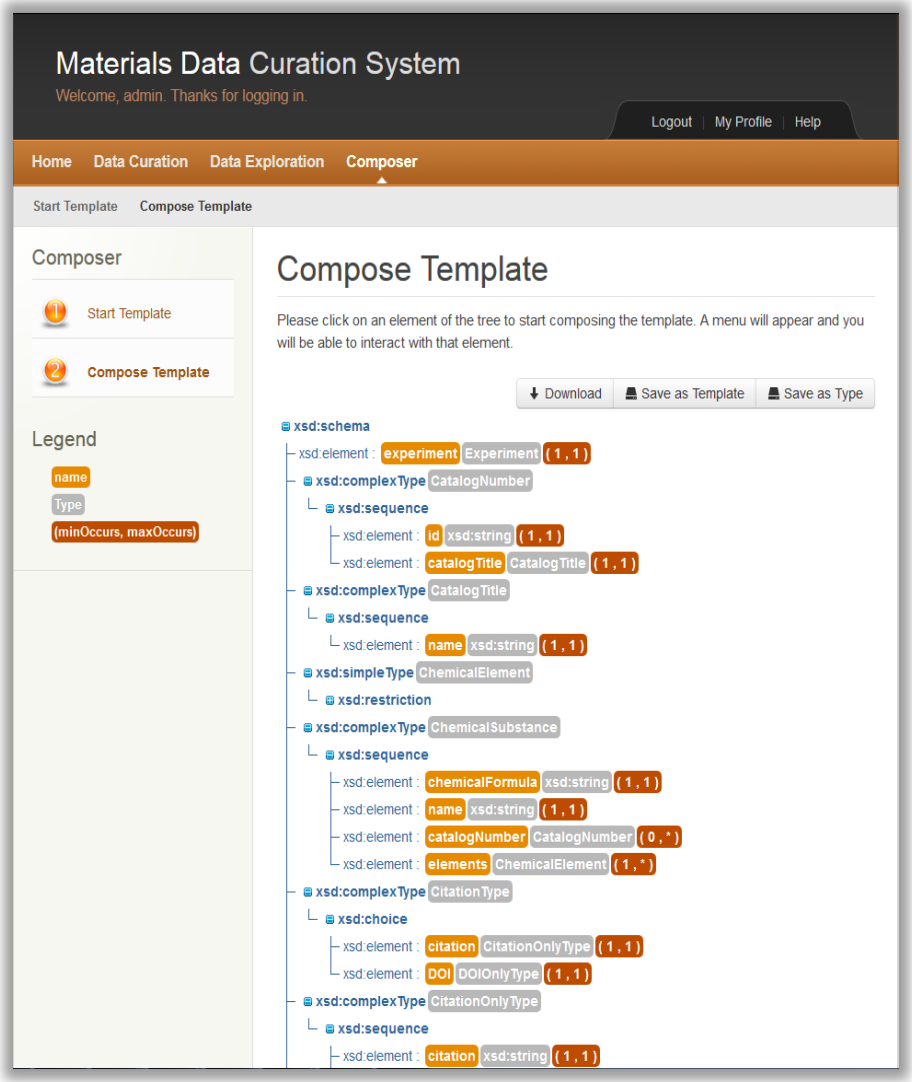
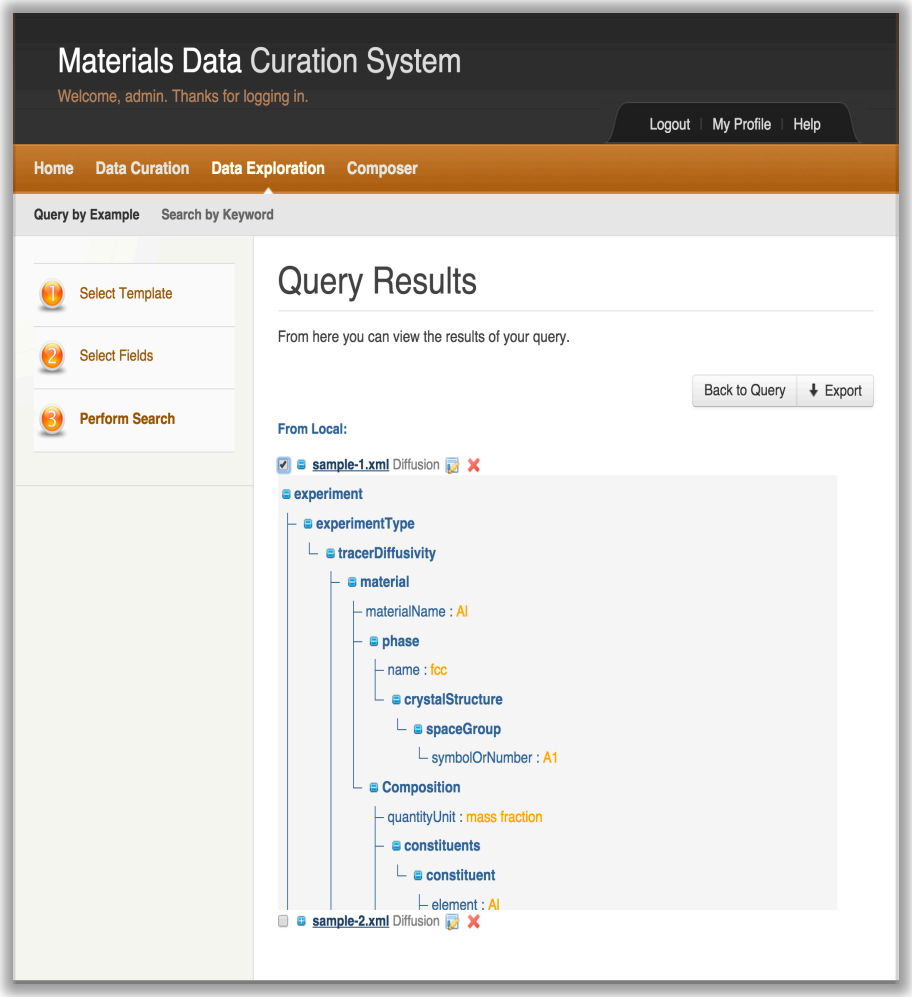


Exporter

Three Steps to Export:

1. Select search result to export from
   - One search result
   - Multiple search results
2. Select an Export format to export to
   - Web based
3. Export data into file type desired
   - POP, CSV, HTML, Script



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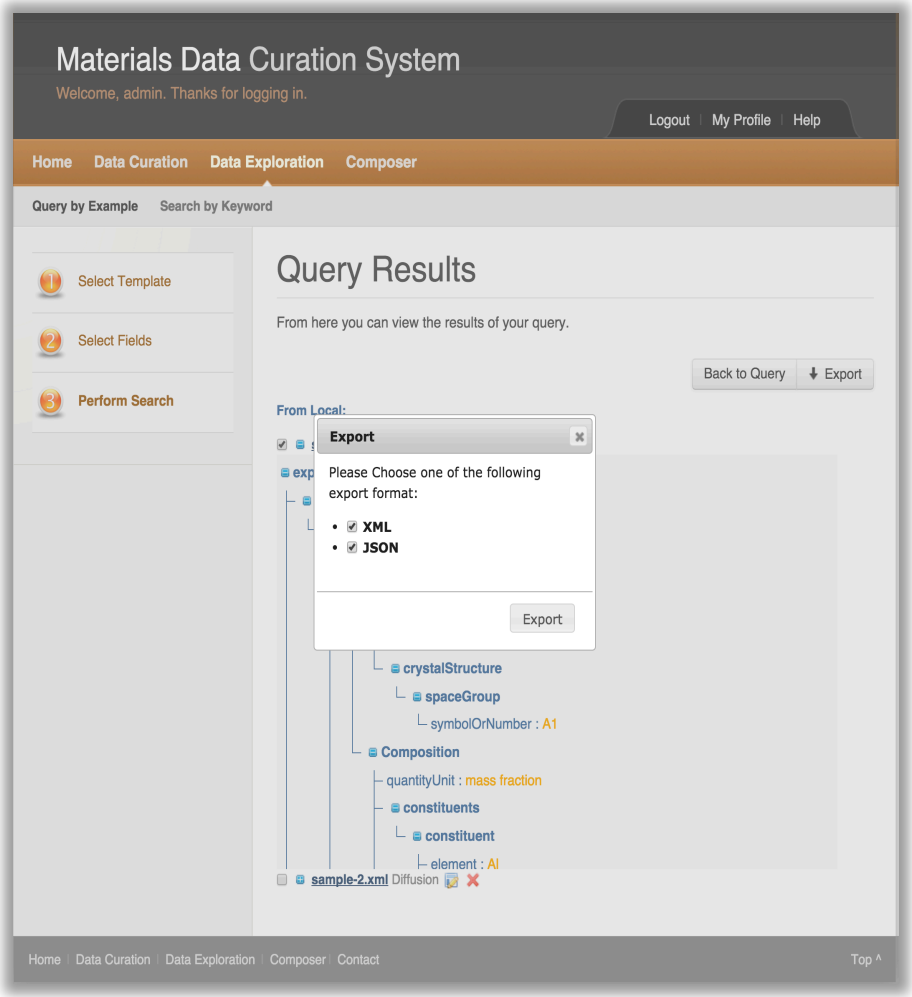

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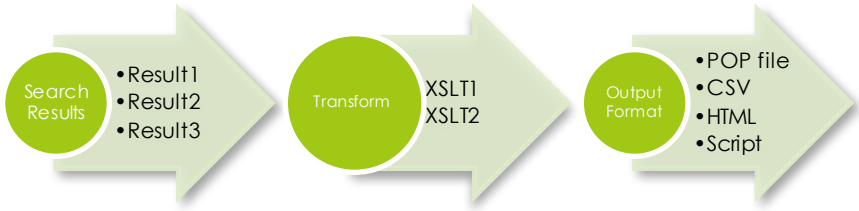
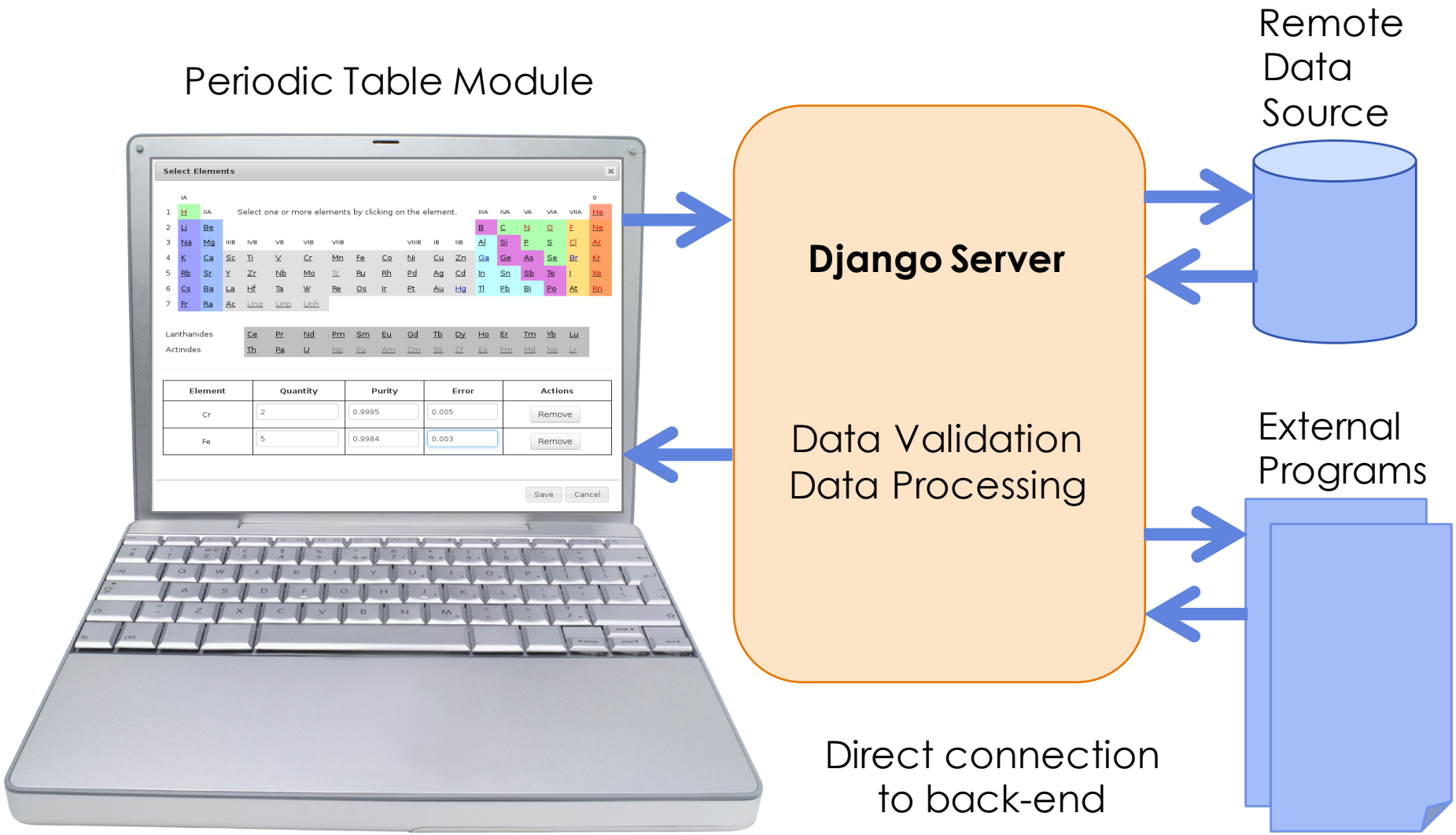


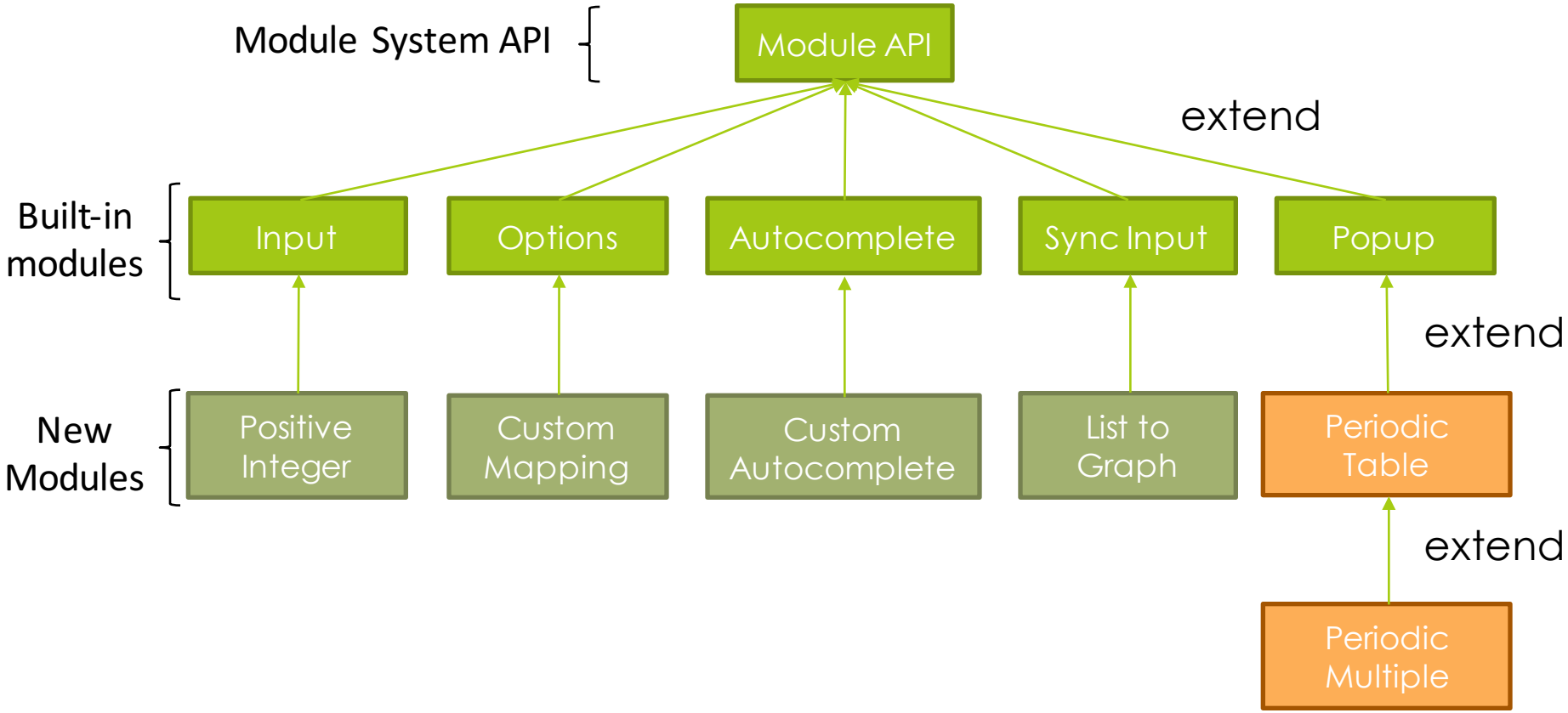

```
$$  POP File
$$ CREATED 10-28-2014
$$
$$

TABLE 10
CREATE_NEW_EQ @@,0
CHANGE_ST COMP Al,MG ENT
CHANGE_STATUS PHASE FCC =ENT 1
S-COND  N=1 P=101325
S-COND  w(al)=.1 w(cr)=.12
S-COND  T=@1
EXPERIMENT DT(FCC,Mg)=@4
TABLE_VALUES
$$ T ( C)    Time (s)         D(cm2/s)     D(m2/s)
655.1        3564             5.97E-08     5.97E-12
587.6        3390             1.46E-08     1.46E-12
530.5        12702            4.20E-09     4.20E-13
478.7        21342            1.05E-09     1.05E-13
433      67614            2.70E-10     2.70E-14
394      151740       8.12E-11     8.12E-15
TABLE_END
```

Module System API



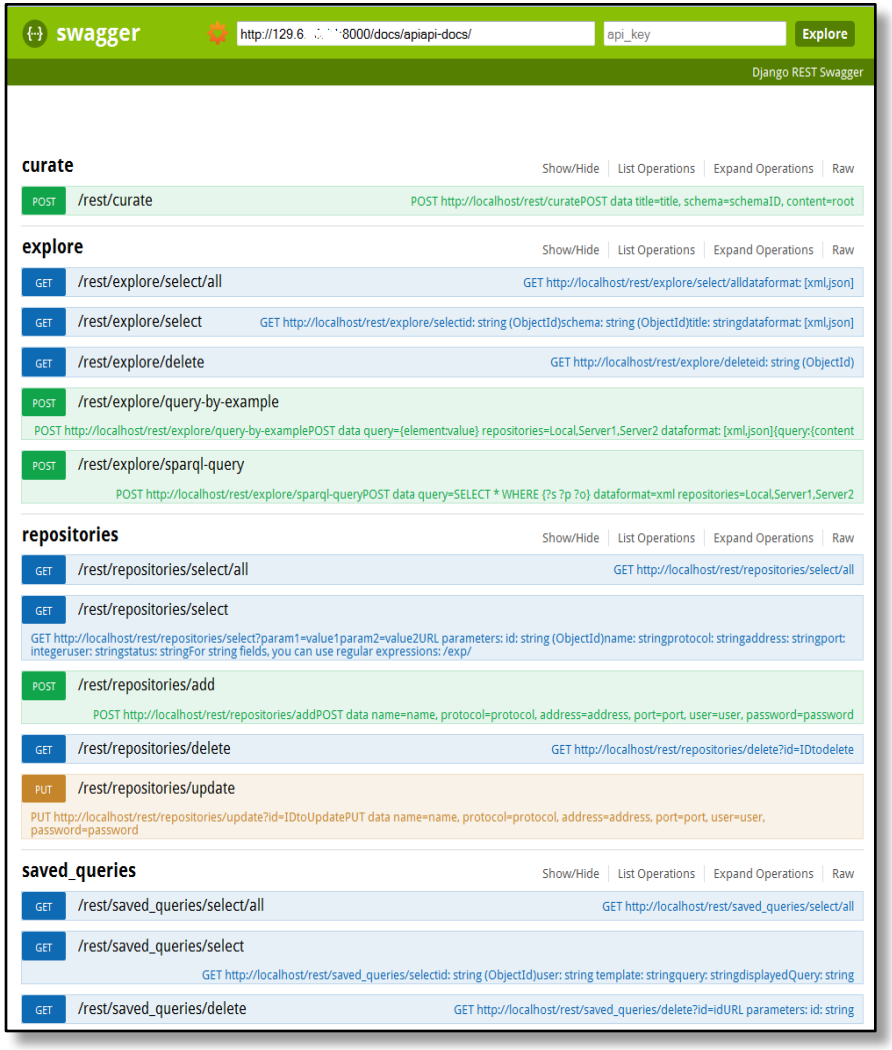
Module System



REST API

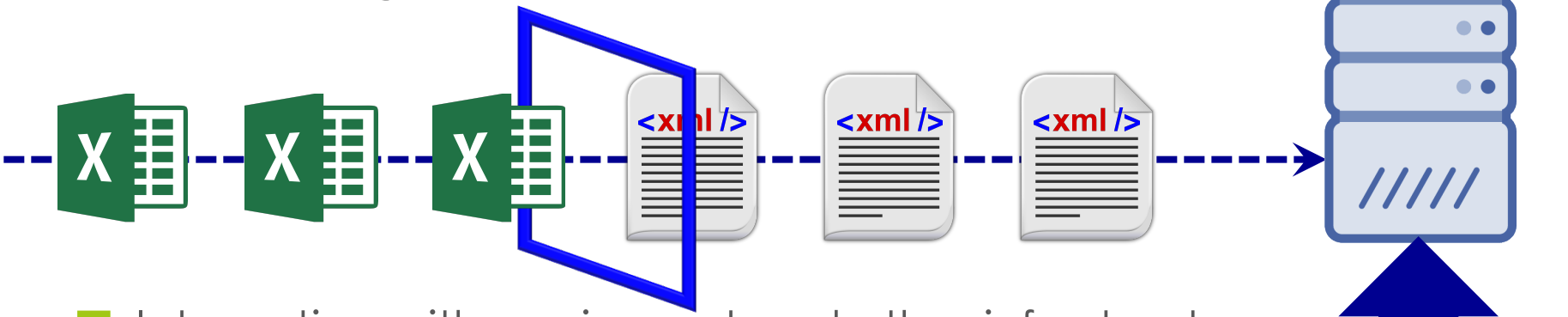
CRUD Operations for:
(create, read, update and delete)

- Curate
- Explore
  - Query by Example
  - Search by Keyword
- Templates
- Types
- Saved Queries
- Repositories
- Users and Groups

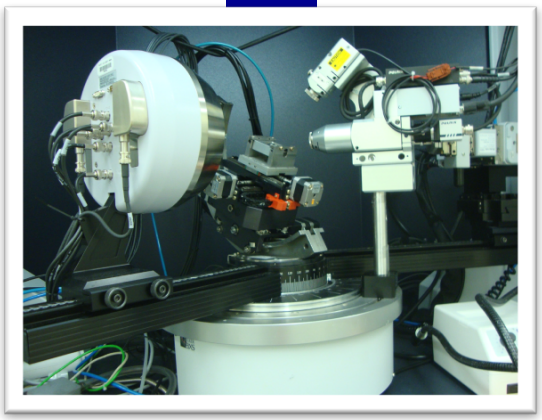


REST API

- Automating Repetitive tasks



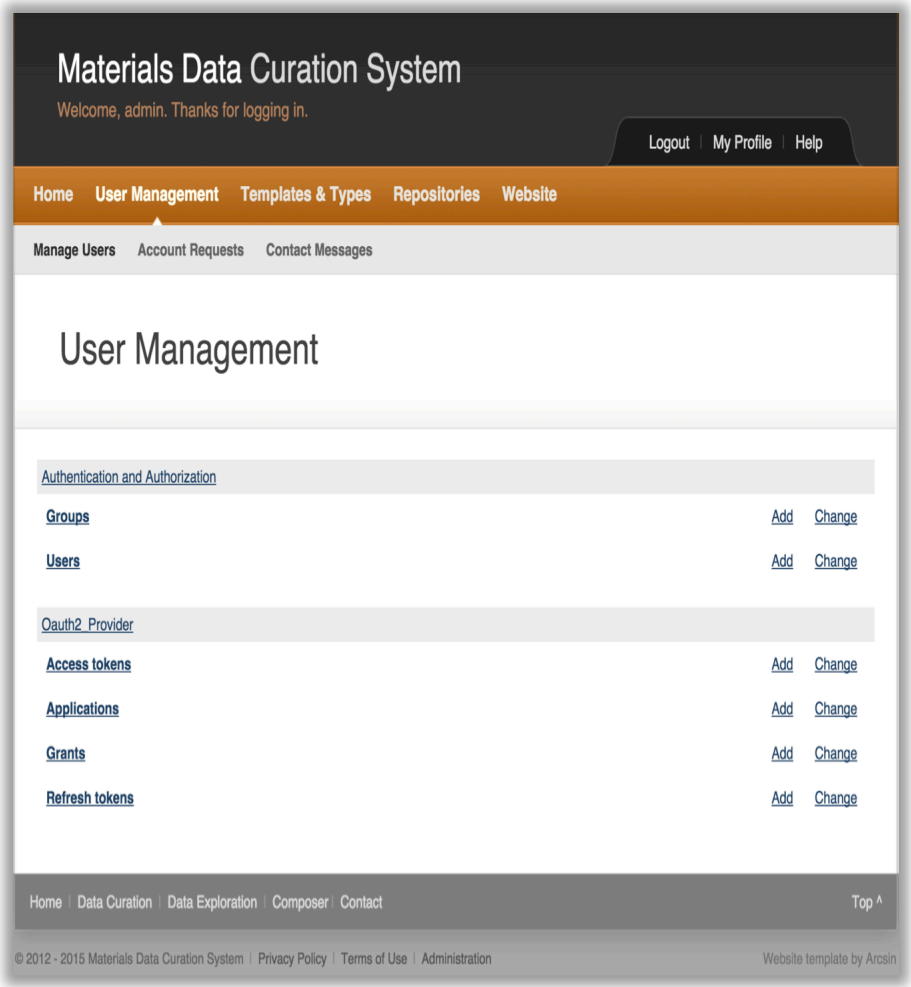
- Integration with equipment and other infrastructure



Administrative Dashboard

Main Features:

- User Management
  - Manage Users
  - Manage Groups
- Templates & Types
  - Manage Templates
  - Manage Types
  - Manage Modules
- Repositories
  - Federated Search
- Website Management



MDCS Releases (2015 to Present)

- Release 1.0 – circa February 12, 2015
- Release 1.1 – circa March 3, 2015
- Release 1.1.1 – circa May 7, 2015
- Release 1.2 – circa October 1, 2015
- Release 1.2.1 – circa November 3, 2015
- Release 1.3 – circa January 12, 2016
  - Exporter – using XSLT or Python
  - Access Control of MDCS components via User Permissions
  - Module System Improvements
  - General Improvements
  - More customizable User Interface
  - Search by Keywords and Dynamic Refinements
- Release 1.4 – circa June-July, 2016

New Features for 1.4

- User Dashboard
- OAI-PMH Support
- XML Schema elements and attributes
  - Extensions
  - Imports
  - Namespaces
  - Key/keyrefs
- Parser Decoupling
- Search by Keyword
- Common code base development

NIST Materials Resource Registry

Shares the same technology stack as MDCS

- Django Web Framework
- Python and Modules
- MongoDB and MySQL for persistence
- Support for XML Schemas parsing and rendering
- Module System (Rich GUI widgets)
- Administrative Dashboard
- User Dashboard
- OAI-PMH protocol support for sharing records

Thank You – Questions?

Materials Data Curation System

Download on GitHub:
https://github.com/usnistgov/MDCS

Presented at the CHiMaD Workshop in Evanston, IL.

Sharief Youssef (NIST)
Email: sharief.youssef@nist.gov