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

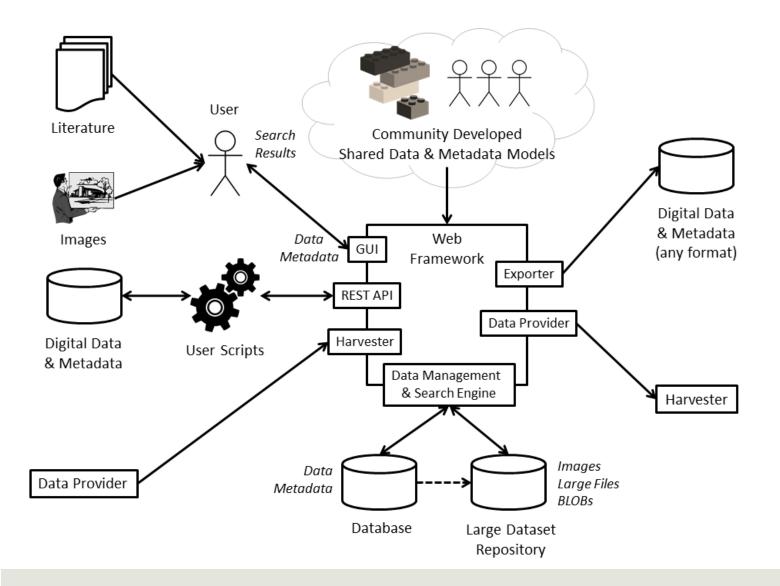
National Institute of Standards and Technology (NIST)

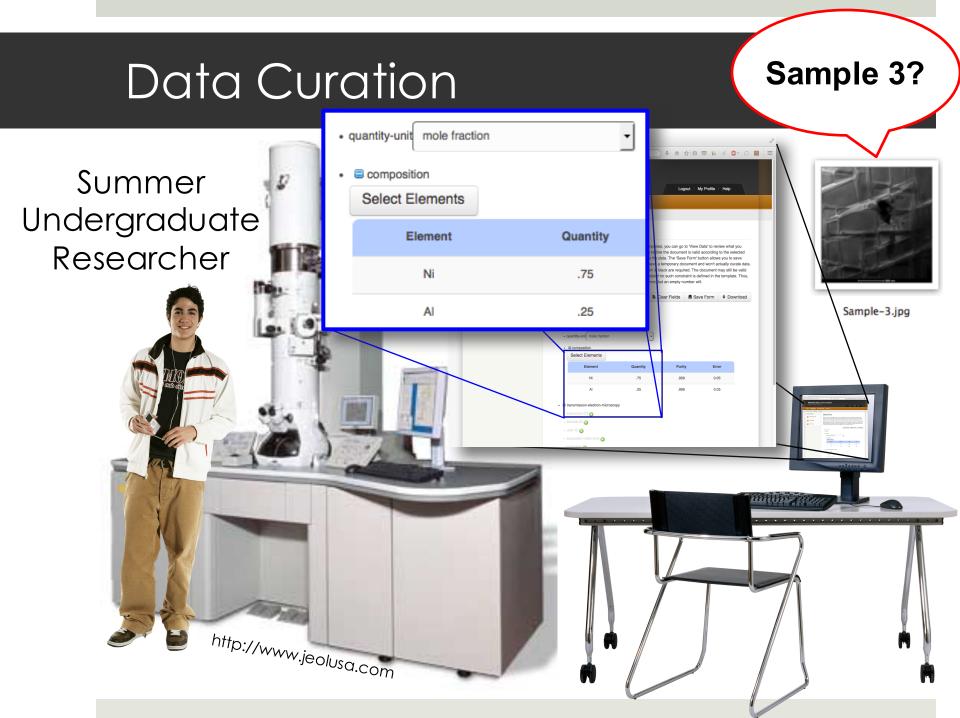
Materials Data Curation System

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

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 п Format
 - Can save to Repository

Materials Data C Welcome, admin. Thanks for log		iem	Logout My Profile Help			
Home Data Curation Data E	ploration Composer					
Select Template Enter Data View	r Data					
Data Curation	Select Ter	nplate				
0 Select Template			your selection, click on "Enter Data" to			
2 Enter Data	proceed. It will automati	proceed. It will automatically load the appropriate form and display it on the next page.				
	🛕 No template selecte	×				
Uiew Data	Global Templates					
	Template name	File name	Actions			
	Demo-Diffusion	demo.diffusion.xsd	• Set as current template			
	Choice	_choice.xsd	• Set as current template			
	Restriction	_restriction.xsd	• Set as current template			
	Basic-Schema	_basic_schema.xsd	• Set as current template			
		User Defined Templ	lates			
	Template name		Actions			
	My Template		• Set as current template			

Data Curation

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Materials Data (Welcome, admin. Thanks for log	Curation System
	Logout My Profile Help
Home Data Curation Data E	xploration Composer
Select Template Enter Data View	v Data
Data Curation	Data Entry
0 Select Template	Here you can fill in the Material Data form. Once it is completed, you can view the data you have
2 Enter Data	entered.
	Clear fields 🖆 Load form 🛔 Save form 🕴 Download
View Data	•
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	Constituents Select Chemical Elements
	• E materialForm 3
	Choose singleCrystalline
	 singleCrystalline ■ diffusingSpecies
	element
	Current Selection: None
	materialPurity

Data Curation

Three Steps to Curate

- 1. Select Template
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 - Download in XML Format
 - Can save to Repository

> One step when using REST API

Materials Data Co Welcome, admin. Thanks for loggi			
		Logout My	y Profile Help
Home Data Curation Data Exp	oration Composer		
Select Template Enter Data View D	ata		
Data Curation	View Data		
Select Template	This is a preview of the curated data in XML format. As	s part of this demo, ple	ease save your data to
2 Enter Data	the repository so that we can better evaluate our syste a copy on your local machine.	em. You can also click	the download button for
View Data		↓ Download XML	★ Save to repository

Yaakov ×		٩
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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

		J	Logout My Profile Help		
ome Data Curation Data	Exploration Composer				
elect Template Select Fields	Perform Search				
ata Exploration	Select Ten	nplate			
uery by Example SPARQL Endpoint		ne following table. Once you make ally load the appropriate form and	your selection, click on "Select Fields" to display it on the next page.		
0 Select Template		Global Templates			
2 Select Fields	Template name	File name	Actions		
	Demo-Diffusion	demo.diffusion.xsd	Current template		
9 Perform Search	Choice	_choice.xsd	• Set as current template		
	Restriction	_restriction.xsd	• Set as current template		
	Basic-Schema	_basic_schema.xsd	• Set as current template		
		User Defined Temp	lates		
	Template name		Actions		
	My Template		Set as current template		

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Materials Data (Welcome, admin. Thanks for lo	Curation System
	Logout My Profile Help
Home Data Curation Data E	xploration Composer
Select Template Select Fields P	erform Search
Data Exploration	Select Fields
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O Select Template	access the Query Builder.
2 Select Fields	• experiment
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	• error 📖

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Materials Data Welcome, admin. Thanks for Ic		elp
Home Data Curation Data E	xploration Composer	
Select Template Select Fields F	Perform Search	
Data Exploration	Perform Search	
Query by Example SPAROL Endpoint Image: Select Template Image: Select Fields Image: Select Fields Image: Select Fields Image: Select Fields Image: Select Fields		ninus icons etrieve
Repositories	Save Query Clear Submit Query	
V Local	Saved Queries Delete All Add to Queries	Delete
	Builder materialName is Aluminum	×
	1 element is Al	×
	¢ quantity < 5	×
	(materialName is Aluminum AND quantity < 5)	×

Composer

Begin with Types

Available functions for Type Manager:

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

				Logout	My Profile Help
ome User Mana	agement Templates & T	Types Reposit	tories Websi	te	
anage Templates	Manage Types Manage XS	LT			
Type M	anager				
1900 11	unugoi				
					1 Upload Type
Type name	Filename	Buckets	Status	Actions	
Type name remote-file	Filename remote-file.xsd	Buckets	Status Registered	Actions	分 Delete
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remote-file	remote-file.xsd	Buckets	Registered	🖉 Versions 😺 Edit	
remote-file temperature-unit	remote-file.xsd temperature-unit.xsd	Buckets	Registered Registered	 Versions Edit Versions Edit 	🗊 Delete
remote-file temperature-unit time-unit	remote-file.xsd temperature-unit.xsd time-unit.xsd	Buckets	Registered Registered Registered	 Versions Edit Versions Edit Versions Edit Versions Edit 	Delete

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

			Logout My Profile Help			
ome Data Curation Data	Exploration Composer					
art Template Compose Templa	te					
omposer	Start Temp	late				
0 Start Template	· · · · ·	Select a new or existing start template from the following table to start composing. Once you make				
2 Compose Template	your selection, click on "C template and display it on		ill automatically load the appropriate			
_	▲ No template selected. Select one in the table below. ×					
		Global Templates	5			
	Template name	File name	Actions			
	New Base Template	new_base_template.xsd	• Select as start template			
	Demo-Diffusion	demo.diffusion.xsd	• Set as current template			
	Choice	_choice.xsd	• Set as current template			
	Restriction	_restriction.xsd	• Set as current template			
	Basic-Schema	_basic_schema.xsd	• Set as current template			
		User Defined Templ	ates			

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

Curation System		
	Logout My Prof	ile Help
xploration Composer		
Compose Template		
Please click on an element of the tree to start composing the will be able to interact with that element.	e template. A menu w	ill appear and you
↓ Download	Save as Template	Save as Type
a xsd:complexType CatalogTitle sxd:sequence xsd:element i name xsd:string (1,1) a xsd:smpleType ChemicalElement a xsd:restriction a xsd:complexType ChemicalSubstance xsd:element : chemicalFormula xsd:string (1,1) xsd:element : chemicalFormula xsd:string (1,1) xsd:element : catalogNumber CatalogNumber xsd:element : elements ChemicalElement (1, a xsd:complexType CitationType xsd:element : catalogNumber (1,1) xsd:element : elements ChemicalElement (1, a xsd:complexType CitationType xsd:element : element : CitationOnlyType (1,1) xsd:element : 001 DOIONlyType (1,1) xsd:element Type CitationOnlyType	.1) (0.*) *)	
	sping in. xploration Composer Compose Template Please click on an element of the tree to start composing the will be able to interact with that element. Download xsd:schema xsd:element : experiment Experiment (1,1) a xsd:schema xsd:element : experiment Experiment (1,1) a xsd:sequence xsd:element : exatalogTitle CatalogTitle xsd:element : name xsd:string (1,1) xsd:element : name xsd:string (1,1) xsd:element : name xsd:string (1,1) xsd:element : chemicalElement xsd:element : chemicalSubstance xsd:element : chemicalFormula xsd:string (1 xsd:element : chemicalFormula xsd:string (1,1) xsd:element : chemicalFormula xsd:string (1,1) xsd:element : clatalogNumber CatalogNumber xsd:element : elements ChemicalElement (1 xsd:element : clatalogNumber CatalogNumber xsd:element : clatalogNumber xsd:element : clatal	gging in Logout My Prof xploration Composer Compose Template Please click on an element of the tree to start composing the template. A menu will be able to interact with that element. Download Save as Template xsd:schemat xsd:element: exsd:sequence xsd:element: exsd:sequence xsd:element: asd:sequence xsd:element: asd:sequence xsd:element: asd:sequence xsd:element: exsd:sequence xsd:element: exsd:element: element: <lic< th=""></lic<>

Exporter

Three Steps to Export:

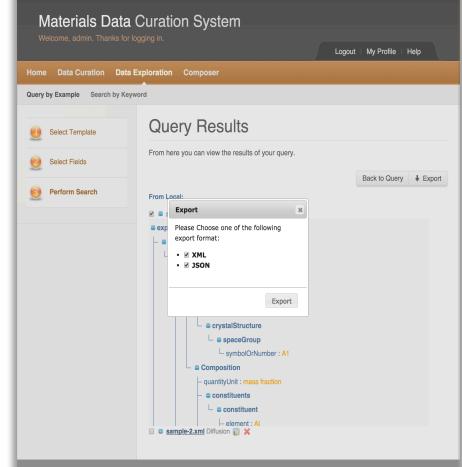
- 1. Select search result to export from
 - One search result
 - Multiple search results
- 2. Select an Export format to export to
 Web based
- 3. Export data into file type desired
 POP, CSV, HTML, Script

Home Data Curation Dat	a Exploration Composer	Logout My Profile Help
Home Data Curation Dat		
Query by Example Search by K	eyword	
Select Template	Query Results	
2 Select Fields	From here you can view the results of your query.	
Perform Search		Back to Query + Export
U	From Local:	
	✓ ■ sample-1.xml Diffusion	
	experiment	
	– ■ experimentType	
	- materialName : Al	
	- B phase	
	- name : fcc	
	■ crystalStructure	
	🖵 🛢 spaceGroup	
	L symbolOrNumber : A1	
	Composition	
	- quantityUnit : mass fraction	
	- Constituents	
	🖵 🛢 constituent	

Exporter

Three Steps to Export:

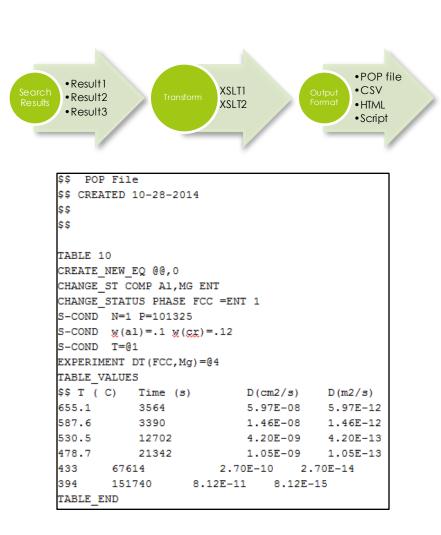
- Select search result to export from
 - One search result
 - Multiple search results
- 2. Select an Export format to export to
 Web based
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 POP, CSV, HTML, Script



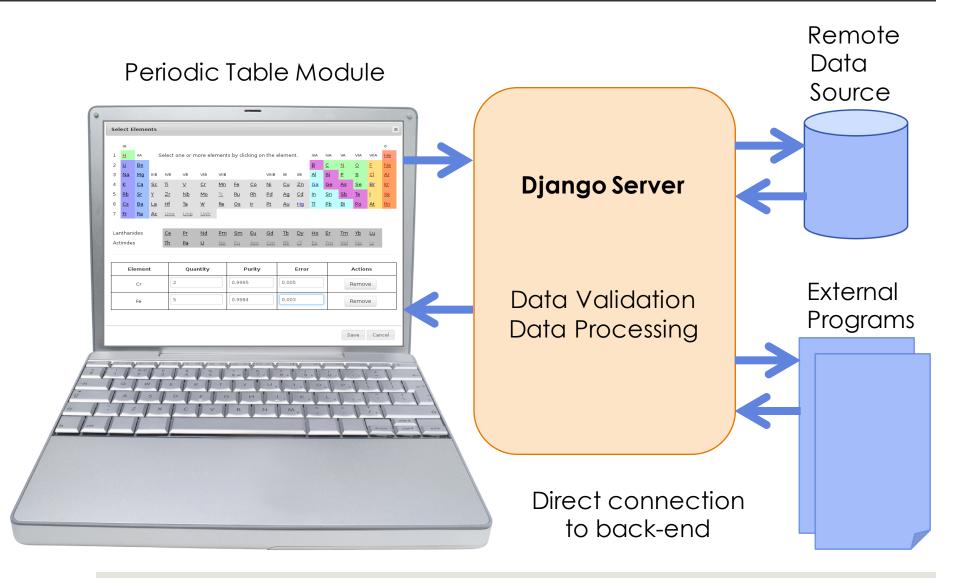
Exporter

Three Steps to Export:

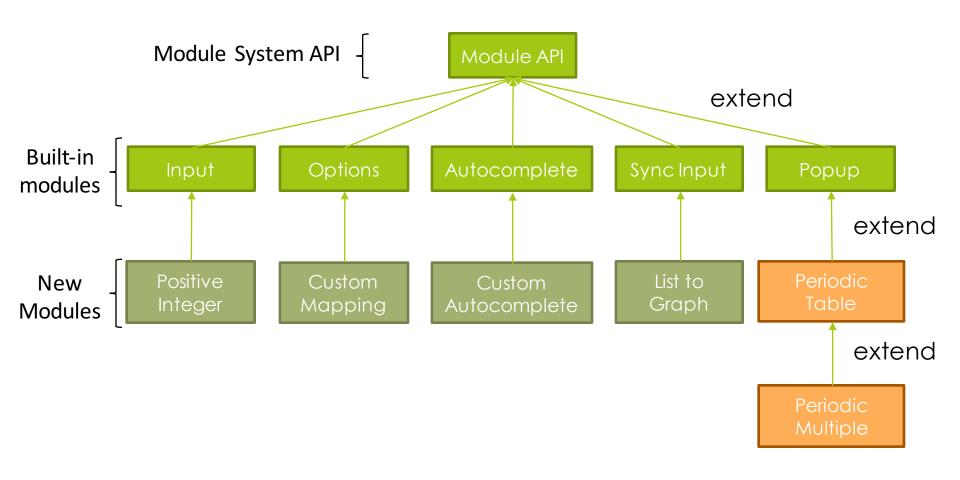
- 1. Select search result to export from
 - One search result
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Module System API



Module System



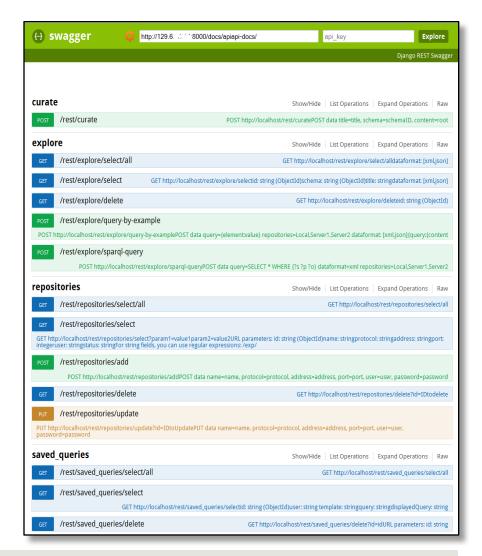
G. Sousa Amaral, P. Dessauw (NIST)

REST API

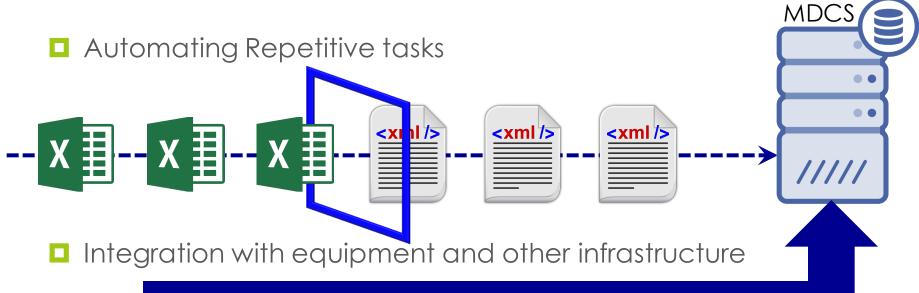
CRUD Operations for:

(create, read, update and delete)

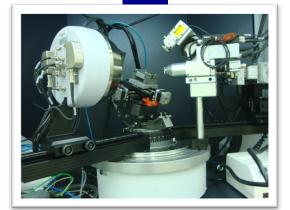
- Curate
- - Query by Example
 - Search by Keyword
- Templates
- Types
- Saved Queries
- Repositories
- Users and Groups







Automated Capture







Administrative Dashboard

Main Features:

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

Materials Data Curation S	ystem				
Welcome, admin. Thanks for logging in.			Logout	My Profile H	lelp
Home User Management Templates & Types	Repositories	Website			
Manage Users Account Requests Contact Messages					
User Management					
Authentication and Authorization					
Groups				Add	<u>Change</u>
Users				Add	<u>Change</u>
Oauth2 Provider					
Access tokens				Add	Change
Applications				Add	<u>Change</u>
Grants				Add	<u>Change</u>
Refresh tokens				Add	<u>Change</u>
Home Data Curation Data Exploration Composer Contact					Top ^
© 2012 - 2015 Materials Data Curation System Privacy Policy Terms of	Use Administration			Website	template by Arcsin

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: <u>sharief.youssef@nist.gov</u>

National Institute of Standards and Technology

