

# Data Curation: Diffusion Couple IN100-IN718

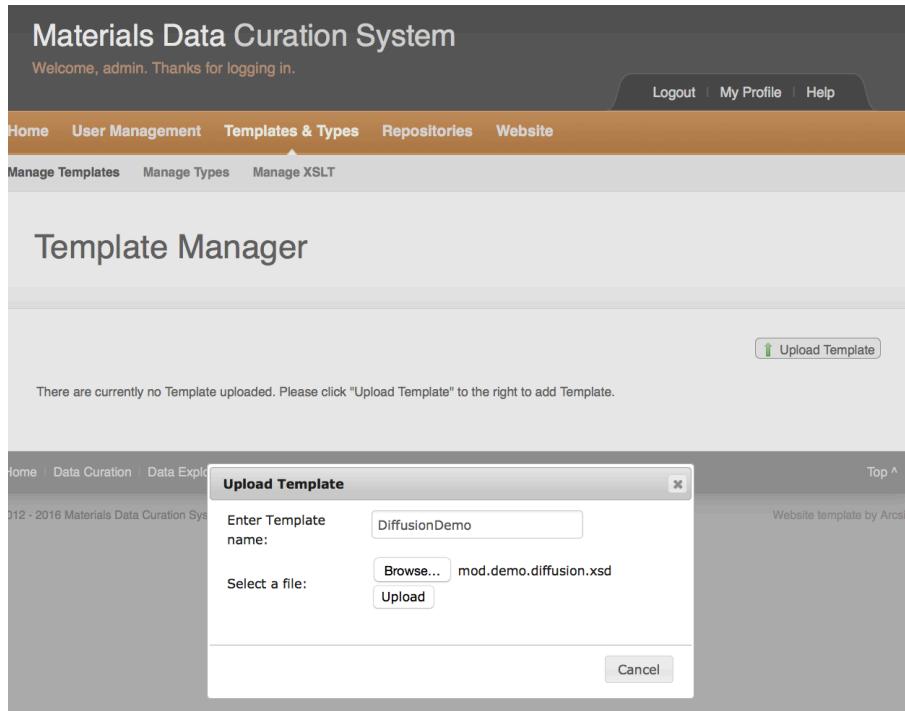
1. To start this tutorial, we first need to upload the “DemoDiffusion” template. So we start Administrator dashboard and “Templates & Types” menu.

The screenshot shows the Materials Data Curation System interface. At the top, there's a navigation bar with links for Home, Data Curation, Data Exploration, and Composer. Below the navigation is a banner titled "Materials Data Curator" with a brief description of the system's purpose. To the right of the banner is a circular diagram divided into segments: Human Welfare (blue), Clean Energy (green), Materials Innovation Infrastructure (center), Digital Data (red), Experimental Tools (yellow), Next Generation Workforce (purple), and National Security (orange). Below the banner, there are two sections: "Available Options" and "Most Recent Templates". The "Available Options" section contains three items: "Curate your Materials Data" (with a pencil icon), "Explore the repository" (with a magnifying glass icon), and "Compose a template" (with a document icon). The "Most Recent Templates" section has a "Browse All" link. At the bottom of the page, there's a footer with links for Home, Data Curation, Data Exploration, Composer, Contact, Logout, My Profile, Help, and Administration. The "Administration" link is circled in red.

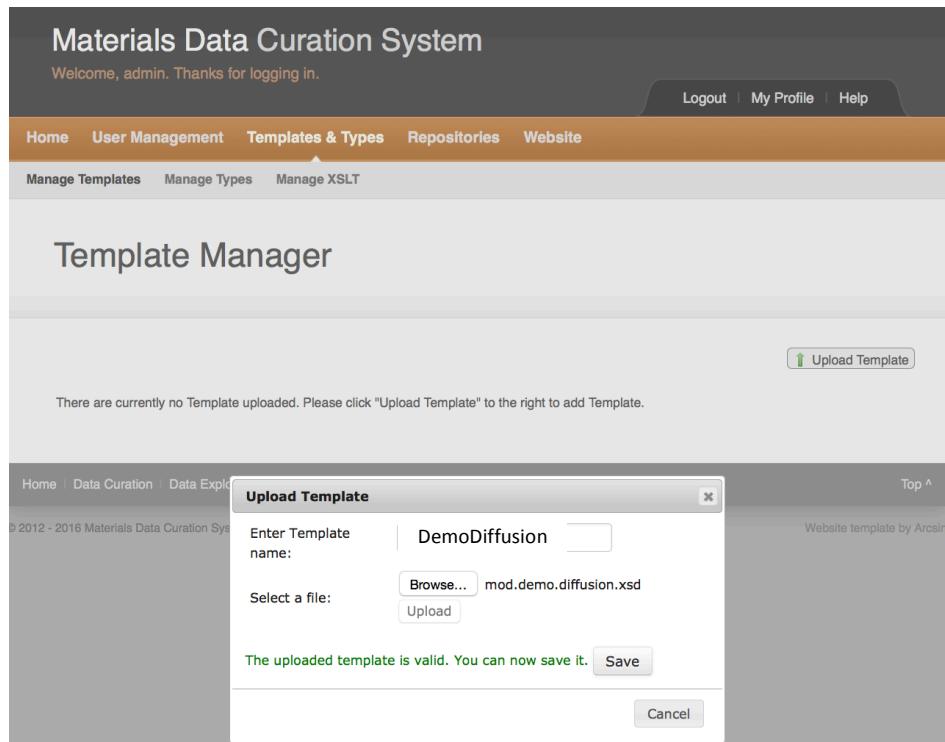
2. Under the “Template & Types” window, select upload template.

The screenshot shows the "Templates & Types" page of the Materials Data Curation System. The top navigation bar includes links for Home, User Management, Templates & Types, Repositories, and Website. Below the navigation, there are links for Manage Templates, Manage Types, and Manage XSLT. The main content area is titled "Template Manager" and displays a message: "There are currently no Template uploaded. Please click \"Upload Template\" to the right to add Template." On the right side of this message, there is a red circle around the "Upload Template" button. At the bottom of the page, there's a footer with links for Home, Data Curation, Data Exploration, Composer, Contact, Logout, My Profile, Help, and Administration. The "Administration" link is circled in red.

3. Upload the “mod.demo.diffusion.xsd” template and label it “DiffusionDemo”



When you have located the file and named the template, click upload. If the upload is successful, you will get a message telling you that you can save the template to the MDCS.



The saved template will then appear in the “Template Manager”

This screenshot shows the 'Materials Data Curation System' interface. At the top, a dark header bar displays the system name and a welcome message: 'Welcome, admin. Thanks for logging in.' On the right side of the header are links for 'Logout', 'My Profile', and 'Help'. Below the header is a navigation bar with tabs: 'Home', 'User Management', 'Templates & Types' (which is currently selected), 'Repositories', and 'Website'. Underneath the navigation bar is a secondary menu with links: 'Manage Templates', 'Manage Types', and 'Manage XSLT'. The main content area is titled 'Template Manager'. At the top of this section is a button labeled 'Upload Template' with an upward arrow icon. Below it is a table listing three templates:

Template name	Filename	Status	Actions
Image-demo	Image-diffusioncouple.xsd	Registered	<a href="#">Versions</a> <a href="#">Edit</a> <a href="#">Delete</a> <a href="#">Modules</a> <a href="#">Exporters</a> <a href="#">Results</a>
image4test	image-test.xsd	Registered	<a href="#">Versions</a> <a href="#">Edit</a> <a href="#">Delete</a> <a href="#">Modules</a> <a href="#">Exporters</a> <a href="#">Results</a>
DemoDiffusion	mod.demo.diffusion.xsd	Registered	<a href="#">Versions</a> <a href="#">Edit</a> <a href="#">Delete</a> <a href="#">Modules</a> <a href="#">Exporters</a> <a href="#">Results</a>

## Template Manager

This screenshot shows the same 'Template Manager' page as the previous one, but with a red oval highlighting the 'Exporters' link in the actions column for the 'DemoDiffusion' template. This indicates that the user has clicked on this link to explore export options for that specific template.

Now that the template has been loaded, we check the available “Exporter” options. To do this click on the “Exporters” in the “DemoDiffusion” row.

This screenshot shows the 'Template Manager' page again, but without the red oval. It displays the same three templates and their details as in the previous screenshots.

## Template Manager

This screenshot shows the 'Template Manager' page with a red oval highlighting the 'Exporters' link in the actions column for the 'DemoDiffusion' template, indicating that the user has clicked on it.

Next a menu with a choice of available options will appear

The screenshot shows a web browser window titled "Materials Data Curation System". The URL is 127.0.0.1:8000/admin/exporters?id=56ccb1bfff8b1ef54c18cebc. The page has a dark header with the system name and a "Logout" link. Below the header is a navigation bar with links: Home, User Management, Templates & Types, Repositories, Website, Manage Templates, Manage Types, and Manage XSLT. The main content area is titled "Exporter Manager" and contains the sub-instruction "Select exporters you want to associate with the template." A table lists five exporter types: XML, XSLT, JSON, CSV, and POP. Each row has a "Exporter name" column and a toggle switch column. The XML, JSON, and CSV rows have their toggle switches set to the "on" position, indicated by a green checkmark inside the button. The XSLT and POP rows have their toggle switches set to the "off" position, indicated by a grey circle. At the bottom right of the table is a "Save Template" button.

Chose to toggle on the CSV exporter.

This screenshot is identical to the one above it, showing the "Exporter Manager" page. The only difference is that the CSV exporter's toggle switch is now set to the "on" position, indicated by a green checkmark inside the button. All other exporters (XML, XSLT, JSON) still have their toggle switches set to the "off" position (grey circles).

You will then be asked to save the template.

Welcome, admin. Thanks for logging in.

Logout | My Profile | Help

Home User Management Templates & Types Repositories Website

Manage Templates Manage Types Manage XSLT

Exporter Manager

Select exporters you want to associate with the template.

Exporter name	
XML	<input type="checkbox"/>
XSLT	<input type="checkbox"/>
JSON	<input checked="" type="checkbox"/>
CSV	<input checked="" type="checkbox"/>
POP	<input type="checkbox"/>

Save Template

Home Data Curation Data Exploration Composer Contact Top ^

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Website template by Arcsin

After adding the “Exporters,” return the Template Manager

Welcome, admin. Thanks for logging in.

Logout | My Profile | Help

Home User Management Templates & Types Repositories Website

Manage Templates Manage Types Manage XSLT

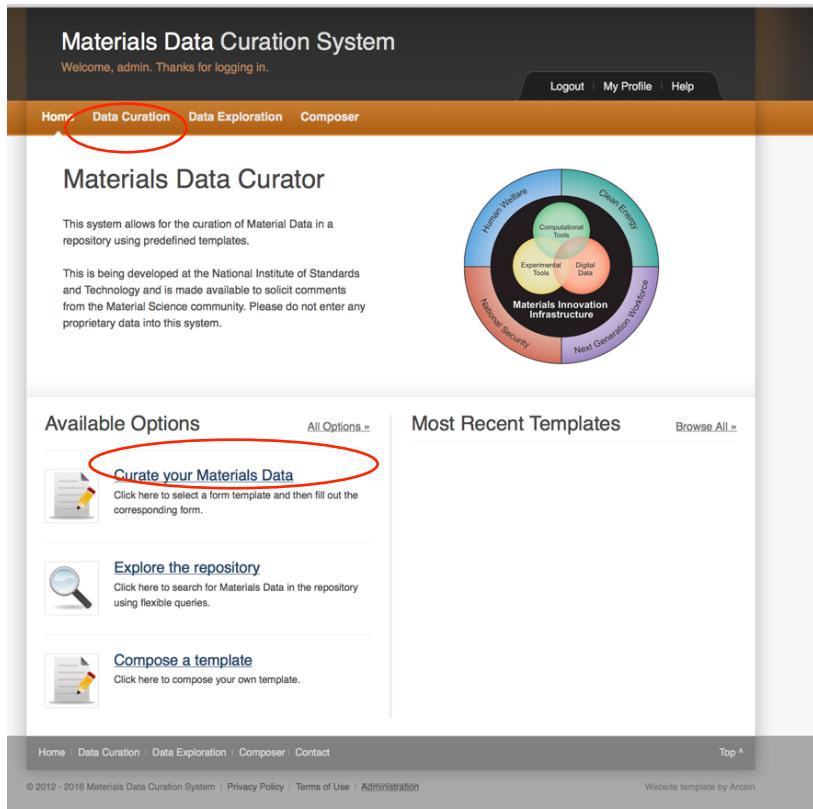
Template Manager

Template name	Filename	Status	Actions
Image-demo	Image-diffusioncouple.xsd	Registered	Versions  Edit  Delete  Modules  Exporters  Results
image4test	image-test.xsd	Registered	Versions  Edit  Delete  Modules  Exporters  Results
DemoDiffusion	mod.demo.diffusion.xsd	Registered	Versions  Edit  Delete  Modules  Exporters  Results

Upload Template

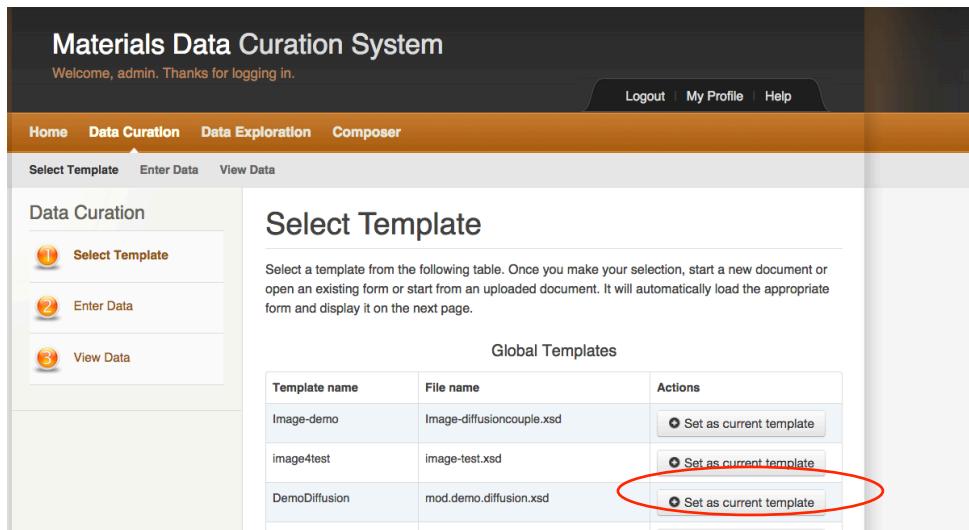
So return to “Home” screen.

From the “Home” screen, select “Data Curation” on the navigation ribbon or from the “Available Options”



The screenshot shows the Materials Data Curation System interface. At the top, there's a dark header bar with the title "Materials Data Curation System" and a welcome message "Welcome, admin. Thanks for logging in.". Below the header is a navigation bar with four items: "Home", "Data Curation" (which is highlighted with a red circle), "Data Exploration", and "Composer". To the right of the navigation bar are links for "Logout", "My Profile", and "Help". The main content area has a title "Materials Data Curator". It contains two sections: "Available Options" and "Most Recent Templates". The "Available Options" section includes three items: "Curate your Materials Data" (with a pencil icon), "Explore the repository" (with a magnifying glass icon), and "Compose a template" (with a document icon). The "Most Recent Templates" section has a link "Browse All". At the bottom of the page, there's a footer with links for "Home", "Data Curation", "Data Exploration", "Composer", and "Contact". The footer also includes copyright information: "© 2012 - 2016 Materials Data Curation System | Privacy Policy | Terms of Use | Administration" and "Website template by Arcsin".

Select “DemoDiffusion” template in the Data Curation Menu



This screenshot shows the "Data Curation" menu. On the left, there are three numbered options: "Select Template" (with a yellow info icon), "Enter Data" (with a blue file icon), and "View Data" (with a green document icon). The "Select Template" option is selected. The main content area is titled "Select Template" and contains a table with the following data:

Global Templates		
Template name	File name	Actions
Image-demo	Image-diffusioncouple.xsd	<input checked="" type="radio"/> Set as current template
image4test	image-test.xsd	<input checked="" type="radio"/> Set as current template
DemoDiffusion	mod.demo.diffusion.xsd	<input checked="" type="radio"/> Set as current template

4. Create a new document “new”

5. The next step is to select the type of diffusion experiment. In this case it is “chemical diffusivity”

6. Review of schema information (enter material, sample preparation, measurement conditions, composition profile, micrograph)
7. Now return “Select Template” menu and select “DemoDiffusion” template and this time we will upload a partially completed entry

127.0.0.1:8000/curate/

## Materials Data Curation System

Welcome, admin. Thanks for logging in.

Logout | My Profile | Help

**Home Data Curation Data Exploration Composer**

Select Template Enter Data View Data

**Data Curation**

- 1 Select Template**
- 2 Enter Data**
- 3 View Data**

### Select Template

Select a template from the following table. Once you make your selection, start a new document or open an existing form or start from an uploaded document. It will automatically load the appropriate form and display it on the next page.

Template	Actions
Image-TEM.xsd	<input type="button" value="Set as current template"/>
DSC-therm.xsd	<input type="button" value="Set as current template"/>
image-TEM.xsd	<input type="button" value="Set as current template"/>
DemoDiffusion.xsd	<input type="button" value="Set as current template"/>
Thermal-Image.xsd	<input type="button" value="Set as current template"/>
DSC-therm-Image.xsd	<input type="button" value="Set as current template"/>
test-Image.xsd	<input type="button" value="Set as current template"/>

**Template Loaded**

Please choose one of the following options to start curating data:

Create a new document:

Open an existing form:

Open an existing XML document:  No file chosen

TEM-Image      Image-TEM4.xsd

Open the file Test-DiffusionCouple-IN100IN718.xml

**Template Loaded**

Please choose one of the following options to start curating data:

Create a new document:

Open an existing form:

Open an existing XML document:  Test-Diffusio...N100IN718.xml

Upon opening the “Test-DiffusionCouple IN100IN17.xml” file, you will see that much of the information has been already entered. We enter the composition of IN100, the excel file containing the measured composition profiles, and the micrograph of the diffusion couple.

**Materials Data Curation System**

Welcome, admin. Thanks for logging in.

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Home Data Curation Data Exploration Composer

Select Template Enter Data View Data

**Data Curation**

- 1 Select Template
- 2 Enter Data
- 3 View Data

## Data Entry

Here you can fill in the Materials Data form. Once it is completed, you can go to 'View Data' to review what you have entered. You won't be able to reach the review page before the document is valid according to the selected template. From the review page, you will be able to curate the data. The 'Save Form' button allows you to save partial data that you may want to edit later. This will only save a temporary document and won't actually curate data. All grayed elements are optional. Thus, all elements written in black are required. The document may still be valid with empty elements. There are no validation on empty fields if no such constraint is defined in the template. Thus, an empty string of characters may not raise a validation error, but an empty number will.

Clear Fields Save Form Download

- experiment
  - experimentType
    - Choose chemicalDiffusivity
    - chemicalDiffusivity
    - material
      - materialName IN100
      - phase
        - name FCC
        - crystalStructure
          - spaceGroup
          - wyckoffSequence
      - Composition
        - quantityUnit mass percent
    - material
      - materialName IN718
      - phase
        - name FCC
        - crystalStructure
          - spaceGroup
          - wyckoffSequence
      - Composition

*Need enter phase and composition*

**Materials Data Curation System**

Welcome, admin. Thanks for logging in.

Logout | My Profile | Help

Home Data Curation Data Exploration Composer

Select Template Enter Data View Data

## Data Curation

- 1 Select Template
- 2 Enter Data
- 3 View Data

## Data Entry

Here you can fill in the Materials Data form. Once it is completed, you can go to 'View Data' to review what you have entered. You won't be able to reach the review page before the document is valid according to the selected template. From the review page, you will be able to curate the data. The 'Save Form' button allows you to save partial data that you may want to edit later. This will only save a temporary document and won't actually curate data. All grayed elements are optional. Thus, all elements written in black are required. The document may still be valid with empty elements. There are no validation on empty fields if no such constraint is defined in the template. Thus, an empty string of characters may not raise a validation error, but an empty number will.

Clear Fields Save Form Download

- experiment
- experimentType
- Choose chemicalDiffusivity
  - chemicalDiffusivity
  - material
    - materialName IN100
  - phase
    - name FCC
  - crystalStructure
    - spaceGroup
    - wyckoffSequence
  - Composition
  - material
    - materialName IN718
  - phase
    - name FCC

Now enter the composition of IN100: Ni-15Co-10Cr-5.5Al-3Mo-4.7Ti (wt.%). Select the "quantity Unit" as "mass percent." Click on "Select Elements" to enter the composition.

- Composition
  - quantityUnit mass percent
- constituents
  - Select Elements

No element selected.

After selecting “Select Element” a periodic table will appear.

**Periodic Table** X

		Select one element by clicking on the element.																																	
		IA		IIA		IIIB		IVB		VB		VIB		VIIIB		IB		IIB		IIIA		IVA		VA		VIA		VIIA		0					
1	H	2	Li	3	Na	4	K	5	Rb	6	Cs	7	Fr	He	B	C	N	O	F	Ne	Al	Si	P	S	Cl	Ar	Ge	As	Se	Br	Kr				
Unq	Unp	Unh	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	In	Sn	Sb	Te	I	Xe	Tc	Ru	Rh	Pd	Ag	Cd	Tl	Pb	Bi	Po	At	Rn				
La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg																										
Ba	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	Lu	Yb	Tm	Ho	Er	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
Lanthanides		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu																				
Actinides		Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr																				

**Actions**

Element	Quantity	Purity	Error	Actions	
Ni	<input type="text"/>	<input type="text"/>	<input type="text"/>	<button>Remove</button>	
				<button>Save</button>	<button>Cancel</button>

Enter the composition and purity for each element. (Entries for purity and error are required)

**Periodic Table**

Select one element by clicking on the element.																		0
1	H	IIA	IA	IIIB	IVB	VB	VIB	VIIB	VIIIB	IB	IIB	Al	III A	IV A	V A	VIA	VII A	He
2	Li	Be										B	C	N	O	F	Ne	
3	Na	Mg										Si	P	S	Cl	Ar		
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac	Unq	Unp	Unh												
Lanthanides			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
Actinides			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

Element	Quantity	Purity	Error	Actions
Ni	61.8	0.999	0.001	<button>Remove</button>
Cr	10	0.999	0.001	<button>Remove</button>
Co	15	0.999	0.001	<button>Remove</button>
Al	5.5	0.999	0.001	<button>Remove</button>
Mo	3	0.999	0.001	<button>Remove</button>
Ti	4.7	0.999	0.001	<button>Remove</button>

After entering the composition, click on “Save” and the composition table will now appear

- experiment
- experimentType
  - Choose
  - chemicalDiffusivity
- material 
  - materialName
- phase
  - name
- crystalStructure
  - spaceGroup
  - wyckoffSequence
- Composition
  - quantityUnit
  - constituents
    - Select Elements

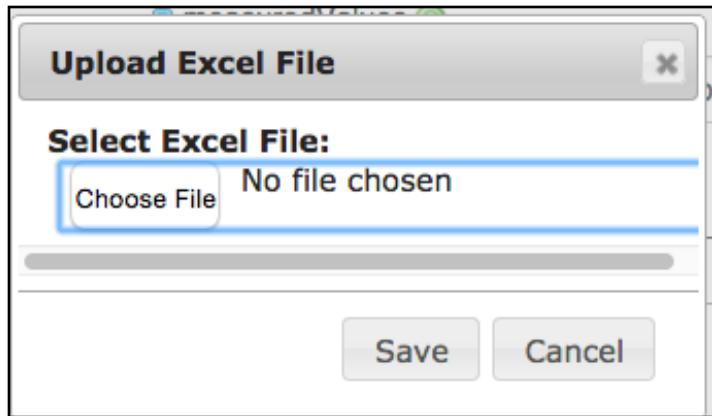
Element	Quantity	Purity	Error
Ni	61.8	0.999	0.001
Cr	10	0.999	0.001
Co	15	0.999	0.001
Al	5.5	0.999	0.001
Mo	3	0.999	0.001
Ti	4.7	0.999	0.001
- materialForm 
  - Choose
  - singleCrystalline
- material 
  - materialName
- phase
  - name
- crystalStructure
  - spaceGroup
  - wyckoffSequence

Now enter information on the “materialForm.” In this case the materials is polycrystalline with an average size of 100 µm.

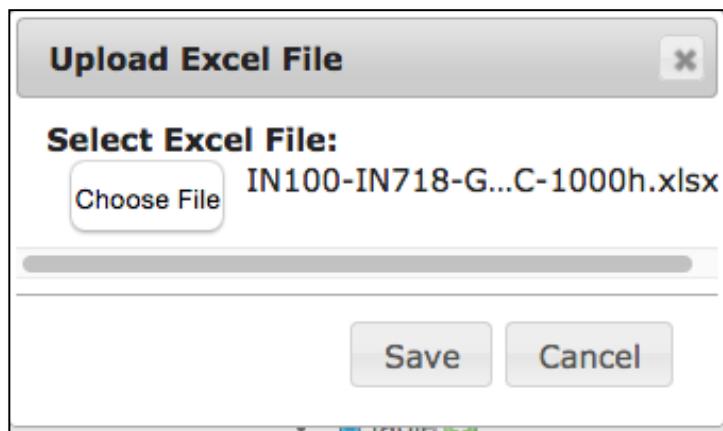
- materialForm 
- Choose  
- polycrystalline
- averageGrainSize
- length  

Now scroll down to “Measured Values” and enter the “measuredValues” as “Composition Profiles,” enter “Profile” as the value type, and “click” on “Upload Load Excel”

- experimentalMethod
  - Choose  
  - direct
    - Choose  
    - EPMA
      - Choose  
      - EPMAInstrumentBrand
- dataCollectionMethod
- measuredValues 
  - measurementDescription  
  - value  
    - Choose  
    - profile
      - table 
        - Upload Excel File
        - No file selected
  - table 
    - Upload Excel File
    - No file selected
- dataAnalysis
  - dataAnalysisMethod 
  - micrographOfStructure 



In the pop-up window, choose IN100-IN718 GE-1150C-1000h.xlsx file and "Save"



After uploading the Excel file, the table will appear in the form.

Now add the micrograph to the data record.

- dataAnalysis
  - dataAnalysisMethod
  - micrographOfStructure
- fileExtension
- reference
  - 
  - No files selected

Enter the file type and upload the micrograph (IN100-IN718-crop.TIFF)

- measuredValues 
- measurementDescription
- value  
- Choose  
- profile
- table 
- 

Distance	Co	Fe	C
0.1845	0.1845	0.1845	0.1845
0.1831	0.1831	0.1831	0.1831
0.181	0.181	0.181	0.181
0.1828	0.1828	0.1828	0.1828
100.0	0.0009	0.1824	0.1824

- dataAnalysis
- dataAnalysisMethod 
- micrographOfStructure  
- fileExtension
- reference
- No files selected
- id
- citation
- Choose  
- DOI
- DOI

- measuredValues
- measurementDescription
- value
- Choose
- profile
- table 

Upload Excel File

Distance	Co	Fe	Cr
um	wt. fraction	wt. fraction	wt. fraction
0.0	0.0013	0.1845	0.18
25.0	0.0014	0.1831	0.18
50.0	0.0014	0.181	0.18
75.0	0.0012	0.1828	0.18
100.0	0.0009	0.1824	0.18
- dataAnalysis
- dataAnalysisMethod
- micrographOfStructure
- fileExtension
- reference
- Uploaded File: IN100-IN718-crop.tif
- Handle: <http://127.0.0.1:8000/rest/blob?id=571e4cd1f8b1ef25dc53ac3e>
- id
- citation
- Choose
- DOI

You can now view the entered data in the XML format and save the data to the repository.

The screenshot shows a web-based application for data curation. The URL in the address bar is 127.0.0.1:8000/curate/view-data. The top navigation bar includes 'Select Template', 'Enter Data', and 'View Data'. The left sidebar, titled 'Data Curation', has three items: 'Select Template', 'Enter Data', and 'View Data', with 'View Data' circled in red. The main content area is titled 'View Data' and contains a message about previewing curated data in XML format. It features a red circle around the 'Download XML' and 'Save to repository' buttons. Below this is a hierarchical XML tree structure representing experimental data:

```
experiment
  experimentType
    chemicalDiffusivity
      material
        materialName : IN100
        phase
          name : FCC
          crystalStructure :
        Composition
          quantityUnit : mass fraction
          constituents
            constituent
              element : Ni
              quantity : 61.8
              purity : 0.999
              error : 0.001
            constituent
              element : Cr
              quantity : 10
              purity : 0.999
              error : 0.001
            constituent
              element : Co
              quantity : 15
              purity : 0.999
              error : 0.001
            constituent
              element : Al
              quantity : 5.5
              purity : 0.999
              error : 0.001
            constituent
```

**Materials Data Curation System**

Welcome, admin. Thanks for logging in.

Logout | My Profile | Help

Home Data Curation Data Exploration Composer

Select Template Enter Data View Data

**Data Curation**

- 1 Select Template
- 2 Enter Data
- 3 View Data

**View Data**

This is a preview of the curated data in XML format. As part of this demo, please save your data to the repository so that we can better evaluate our system. You can also click the download button for a copy on your local machine.

[Download XML](#) [★ Save to repository](#)

```

<?xml version="1.0" encoding="UTF-8"?>
<experiment>
    <experimentType></experimentType>
    <chemicalDiffusivity>
        <material>
            <materialName>Rene-88</materialName>
            <phase>
                <name>FCC</name>
                <crystalStructure></crystalStructure>
            </phase>
            <Composition>
                <quantityUnit>mass percent</quantityUnit>
                <constituents>
                    <constituent>
                        <element>Ni</element>
                        <quantity>58.1</quantity>
                        <purity>0.999</purity>
                        <error>0.001</error>
                    </constituent>
                    <constituent>
                        <element>Cr</element>
                        <quantity>10</quantity>
                    </constituent>
                </constituents>
            </Composition>
        </material>
    </chemicalDiffusivity>
</experiment>

```

**Materials Data Curation System**

Welcome, admin. Thanks for logging in.

Logout | My Profile | Help

Home Data Curation Data Exploration Composer

Select Template Enter Data View Data

**Data Curation**

- 1 Select Template
- 2 Enter Data
- 3 View Data

**View Data**

This is a preview of the curated data in XML format. As part of this demo, please save your data to the repository so that we can better evaluate our system. You can also click the download button for a copy on your local machine.

[Save to Repository](#) [Download XML](#) [★ Save to repository](#)

**Save to Repository**

Save data to the repository. You can also click the download button for a copy on your local machine.

**Save As:** GE-DiffusionCouple-R88IN100.

**Save**

```

<?xml version="1.0" encoding="UTF-8"?>
<experiment>
    <experimentType></experimentType>
    <chemicalDiffusivity>
        <material>
            <materialName>Rene-88</materialName>
            <phase>
                <name>FCC</name>
                <crystalStructure></crystalStructure>
            </phase>
            <Composition>
                <quantityUnit>mass percent</quantityUnit>
                <constituents>
                    <constituent>
                        <element>Ni</element>
                    </constituent>
                </constituents>
            </Composition>
        </material>
    </chemicalDiffusivity>
</experiment>

```

You can also download a copy of the XML entry.

**Materials Data Curation System**

Welcome, admin. Thanks for logging in.

Logout | My Profile | Help

Home Data Curation Data Exploration Composer

Select Template Enter Data View Data

**Data Curation**

1 Select Template  
2 Enter Data  
3 View Data

**View Data**

This is a preview of the curated data in XML format. As part of this demo, please save your data to the repository so that we can better evaluate our system. You can also click the download button for a copy on your local machine.

Download XML Save to repository

experiment

- experimentType
- chemicalDiffusivity
  - material
    - materialName : Rene-88
    - phase
      - name : FCC
      - crystalStructure :
    - Composition
      - quantityUnit : mass percent
      - constituents
        - constituent
          - element : Ni
          - quantity : 58.1
          - purity : 0.999
          - error : 0.001
        - constituent
          - element : Cr
          - quantity : 10

In the “Data Exploration” tutorial we will then view this data and export the spreadsheet.