

Data Curation: Simple TEM Tutorial

Adding a Template

1: Select “Administration”

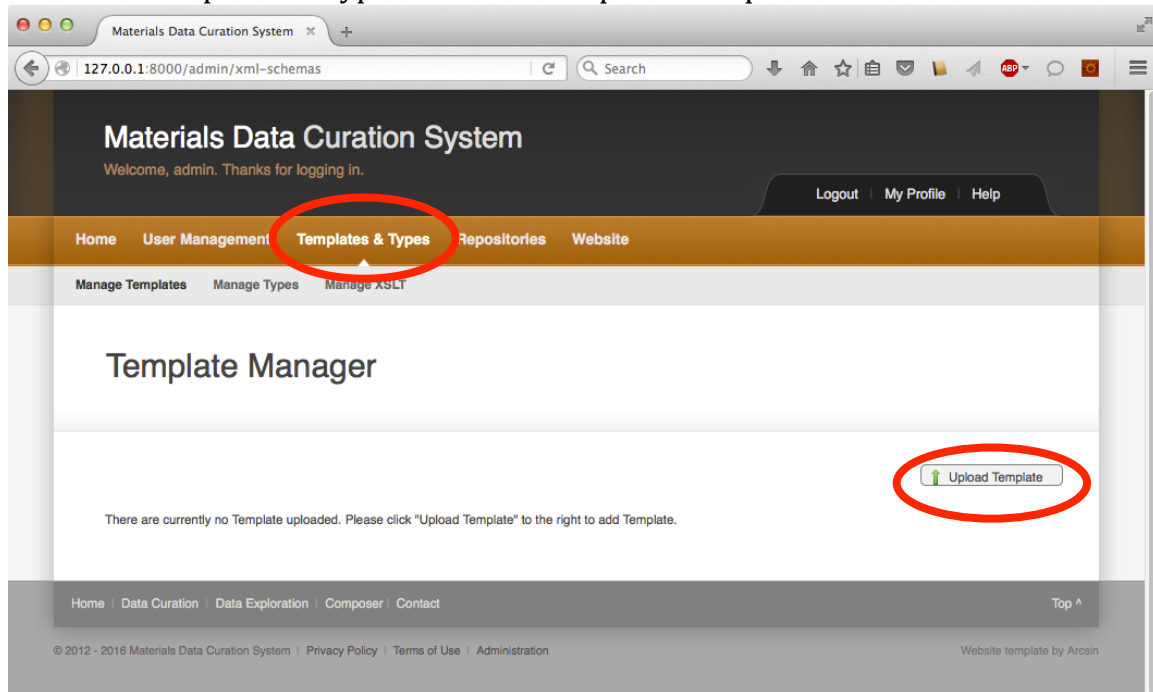
The screenshot shows a web browser window displaying the Materials Data Curation System. The browser's address bar shows the URL 127.0.0.1:8000. The page has a dark header with the title "Materials Data Curation System" and a welcome message "Welcome, admin. Thanks for logging in." Navigation links include "Logout", "My Profile", and "Help". Below the header is a brown navigation bar with links: "Home", "Data Curation", "Data Exploration", and "Composer".

The main content area is titled "Materials Data Curator". It contains two paragraphs: "This system allows for the curation of Material Data in a repository using predefined templates." and "This is being developed at the National Institute of Standards and Technology and is made available to solicit comments from the Material Science community. Please do not enter any proprietary data into this system." To the right of the text is a circular diagram with four segments: "Human Welfare", "Clean Energy", "Next Generation Workforce", and "National Security". In the center of the diagram are three overlapping circles labeled "Computational Tools", "Experimental Tools", and "Digital Data", with the text "Materials Innovation Infrastructure" at the bottom.

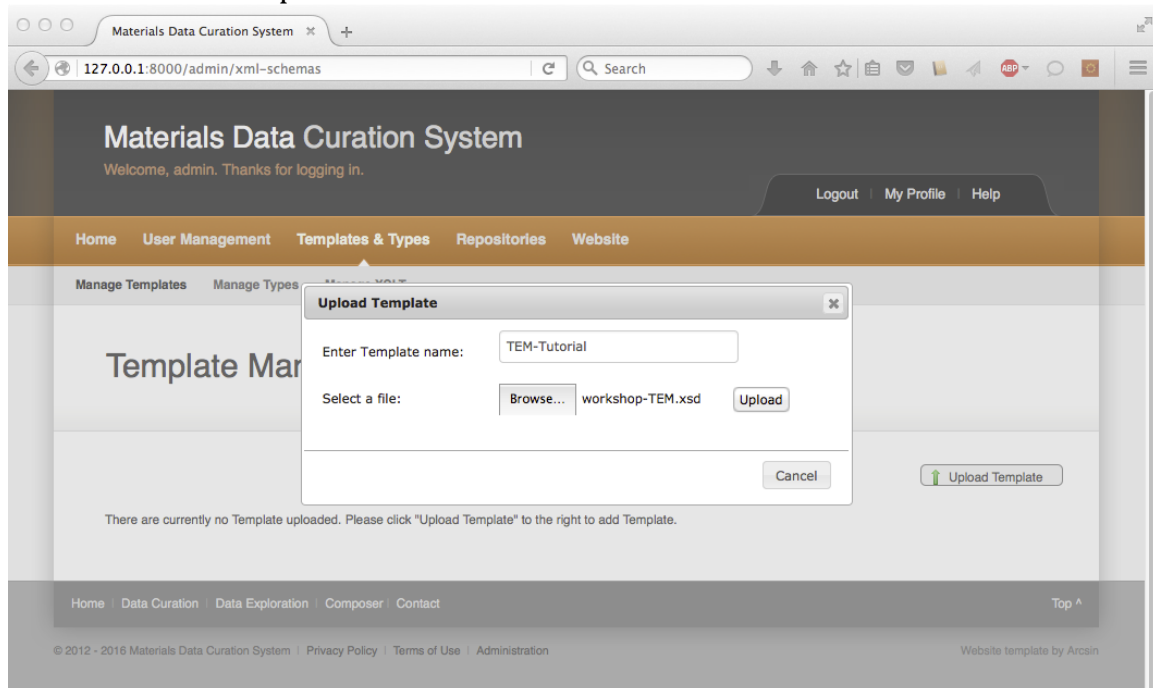
Below the main content area are two columns. The left column is titled "Available Options" and contains three links with icons: "Curate your Materials Data" (with a document icon), "Explore the repository" (with a magnifying glass icon), and "Compose a template" (with a document icon). The right column is titled "Most Recent Templates" and contains a link "Browse All".

The footer of the page is a dark gray bar. It contains navigation links: "Home", "Data Curation", "Data Exploration", "Composer", and "Contact". On the right side of the footer is a "Top ^" link. At the bottom of the footer, there is a copyright notice "© 2012 - 2016 Materials Data Curation System | Privacy Policy | Terms of Use" and a link "Administration" which is circled in red. On the far right of the footer is the text "Website template by Arcsin".

2: Select “Templates & Types” and select “Upload Template”



3: Navigate to the TEM Tutorial folder and select “workshop-TEM.xsd”. Enter “TEM-Tutorial” as the template name.



4: Click on “Home”

The screenshot shows a web browser window with the URL `127.0.0.1:8000/admin/xml-schemas/manage-schemas`. The page header includes the title "Materials Data Curation System" and a welcome message: "Welcome, admin. Thanks for logging in." The navigation bar has links for "Home", "User Management", "Templates & Types", "Repositories", and "Website". The "Home" link is circled in red. Below the navigation bar, there are sub-links: "Manage Templates", "Manage Types", and "Manage XSLT". The main content area is titled "Template Manager" and features an "Upload Template" button. A table lists the templates:

Template name	Filename	Status	Actions
TEM-Tutorial	workshop-TEM.xsd	Registered	Versions Edit Delete Modules Exporters Results

The footer contains copyright information: "© 2012 - 2016 Materials Data Curation System" and links for "Privacy Policy", "Terms of Use", and "Administration". It also includes a "Top" link and the text "Website template by Arcsin".

Curate TEM Micrograph

1: Click on “Data Curation” and set “TEM-Tutorial” as the current template.

The screenshot shows a web browser window with the address bar displaying '127.0.0.1:8000/curate/'. The page title is 'Materials Data Curation System'. Below the title, there is a welcome message: 'Welcome, admin. Thanks for logging in.' and links for 'Logout', 'My Profile', and 'Help'. The main navigation bar includes 'Home', 'Data Curation', 'Data Exploration', and 'Composer'. The 'Data Curation' section is active, showing a sidebar with three options: 'Select Template' (highlighted with a red circle and the number 1), 'Enter Data' (with a red circle and the number 2), and 'View Data' (with a red circle and the number 3). The main content area is titled 'Select Template' and contains instructions: '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.' Below this, there are two sections: 'Global Templates' and 'User Defined Templates'. The 'Global Templates' section contains a table with one row: 'TEM-Tutorial' with file name 'workshop-TEM.xsd' and an action button 'Set as current template'. The 'User Defined Templates' section contains a message: 'Create your own templates using the [Composer](#) and you will be able to use them from this section.'

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.

Global Templates

Template name	File name	Actions
TEM-Tutorial	workshop-TEM.xsd	Set as current template

User Defined Templates

Create your own templates using the [Composer](#) and you will be able to use them from this section.

Home | Data Curation | Data Exploration | Composer | Contact

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2: Select “Create a new document”. Type in “Co-L06-1000h-900C” and click “Start”

The screenshot shows a web browser window with the address bar displaying "127.0.0.1:8000/curate/". The page title is "Materials Data Curation System" and the subtitle is "Welcome, admin. Thanks for logging in." The navigation bar includes links for "Home", "Data Curation", "Data Exploration", and "Composer". The "Data Curation" section is active, showing a sidebar with three steps: "1 Select Template", "2 Enter Data", and "3 View Data". The main content area is titled "Select Template" and contains a table of "Global Templates". A modal dialog box titled "Template Loaded" is open, prompting the user to choose an option to start curating data. The options are: "Create a new document:" (selected), "Open an existing form:", and "Open an existing XML document:". The "Create a new document:" option has a text input field containing "Co-L06-1000h-900C". The "Open an existing XML document:" option has a "Browse..." button and the text "No file selected.". A "Start" button is at the bottom right of the dialog box.

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.

Global Templates

Template name	File name	Actions
TEM-1		Set as current template

Template Loaded

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

☒ Create a new document:

Co-L06-1000h-900C

☐ Open an existing form:

.....

☐ Open an existing XML document:

Browse... No file selected.

Start

3: The following information will be entered via the web interface in the next few steps:

<?xml		version="1.0" encoding="utf-8"						
measurement	core	title		TEM Measurement of Co-11W-9.4Al				
		contactPoint	fn	John Smith				
			hasEmail	data@nist.gov				
		keyword		TEM				
		material	quantity-unit		mole percent			
	composition		constituent	ele...	qua...	purity	error	
				(3 r...	1 Co	81.75	1	0
				2 W	10	1	0	
				3 Al	8.25	1	0	
	phases		FCC, FCC_L12					
	anneal		time	value	1000			
				unit	h			
			temperature	value	900			
				unit	C			
	trans...	instrument-ID		FEI Titan 80-300				
imaging-mode		Bright Field Image						
accelerat...		value	300					
		unit	kV					
supporting-files								

4: Enter “core” metadata:

The screenshot shows a web browser window with the address bar displaying '127.0.0.1:8000/curate/enter-data'. The page has a top navigation bar with 'Home', 'Data Curation', 'Data Exploration', and 'Composer'. Below this is a sub-navigation bar with 'Select Template', 'Enter Data', and 'View Data'. The main content area is titled 'Data Entry' and contains a paragraph explaining the process: '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.'

Below the text are three buttons: 'Clear Fields', 'Save Form', and 'Download'. The form itself is a tree structure starting with 'measurement', which has a sub-section 'core'. The 'core' section contains several fields: 'title' (filled with 'TEM measurement of Co-11W-9.'), 'description' (grayed out), 'contactPoint' (with a sub-field 'fn' filled with 'John Smith'), 'hasEmail' (filled with 'data@nist.gov'), and 'keyword' (filled with 'TEM'). Below these are several more grayed-out fields: 'modified', 'publisher', 'accessLevel', 'identifier', 'bureauCode', and 'programCode'. The 'core' section also has a sub-section 'material' which contains the field 'transmission-electron-microscopy'.

The footer of the page contains a navigation bar with 'Home', 'Data Curation', 'Data Exploration', 'Composer', and 'Contact', a 'Top ^' link, and a copyright notice: '© 2012 - 2016 Materials Data Curation System | Privacy Policy | Terms of Use | Administration'. The website template is credited to 'Arcsin'.

5: Enter composition by clicking “Select Elements” and enter the composition via the periodic table

The screenshot shows the Materials Data Curation System web application. The browser address bar displays "127.0.0.1:8000/curate/enter-data". The page has a dark header with the title "Materials Data Curation System" and a welcome message "Welcome, admin. Thanks for logging in." Navigation links include "Logout", "My Profile", and "Help". A secondary navigation bar contains "Home", "Data Curation", "Data Exploration", and "Composer". Below this, a sub-navigation bar shows "Select Template", "Enter Data", and "View Data".

The "Enter Data" section is active, displaying a "Data Curation" sidebar with three steps: "1 Select Template", "2 Enter Data", and "3 View Data". The main content area features a "Periodic Table" modal window. The modal has a title bar with a close button. Inside, it displays a periodic table with elements color-coded by groups. A text prompt says "Select one element by clicking on the element." Below the periodic table, there are sections for "Lanthanides" and "Actinides".

Below the periodic table, there is a table for entering composition data:

Element	Quantity	Purity	Error	Actions
Co	<input type="text" value="81.75"/>	<input type="text" value="1"/>	<input type="text" value="0"/>	<button>Remove</button>
W	<input type="text" value="10"/>	<input type="text" value="1"/>	<input type="text" value="0"/>	<button>Remove</button>
Al	<input type="text" value="8.25"/>	<input type="text" value="1"/>	<input type="text" value="0"/>	<button>Remove</button>

At the bottom of the modal, there are "Save" and "Cancel" buttons. To the right of the modal, there is a "Download" button and some text: "View what you... to the selected... s you to save... tually curate data... may still be valid... template. Thus,".

The footer of the page includes "© 2012 - 2016 Materials Data Curation System" and "Website template by Arcsin".

6: Select “mole percent” quantity unit and enter phase and annealing metadata:

Materials Data Curation System

127.0.0.1:8000/curate/enter-data

View Data

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

- measurement
 - core
 - material
 - quantity-unit: mole percent
 - composition
 - Select Elements

Element	Quantity	Purity	Error
Co	81.75	1	0
W	10	1	0
Al	8.25	1	0
- phases: FCC, FCC_L12
- anneal
 - time
 - value: 1000
 - unit: h
 - uncertainty
 - temperature
 - value: 900
 - unit: C
 - uncertainty
- transmission-electron-microscopy

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7: Enter the TEM image metadata:

Materials Data Curation System

127.0.0.1:8000/curate/enter-data

3 View Data

partial data that you may want to curate. You can only save a temporary document and must always 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

- measurement
 - core
 - material
 - transmission-electron-microscopy
 - instrument-ID FEI Titan 80-300
 - sample-ID
 - user-ID
 - acquisition-date-time
 - metadata
 - imaging-mode Bright Field Image
 - tilt-zone-axis
 - accelerating-voltage
 - value 300
 - unit kV
 - uncertainty
 - supporting-files
 - file
 - name
 - type
 - downloadURL
 - accessURL
 - local

Upload File

No files selected

Home | Data Curation | Data Exploration | Composer | Contact

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8: Expand “supporting-files”, “file”, and “downloadURL”. Click on “Upload File” and select Co-L06-1000h-900C.jpg. Click “Save”.

The screenshot shows the Materials Data Curation System interface. The browser address bar displays "127.0.0.1:8000/curate/enter-data". The page title is "Materials Data Curation System". A sidebar on the left contains a "View Data" button. The main content area displays a form with a tree structure of fields. The "measurement" section is expanded, showing "core", "material", and "transmission-electron-microscopy". The "transmission-electron-microscopy" section is further expanded, showing "instrument-ID" (FEI Titan 80-300), "sample-ID", "user-ID", "acquisition-date-time", and "metadata". An "Upload File" dialog box is open, showing a "Browse..." button and the file "Co-L06-1000h-900C.jpg". The dialog box has "Save" and "Cancel" buttons. Below the dialog box, the "supporting-files" section is expanded, showing "file" (with a red minus icon), "name", "type", "downloadURL" (with a red minus icon), and "accessURL". The "file" section is further expanded, showing "name", "type", "downloadURL", and "accessURL". The "downloadURL" field has an "Upload File" button. Below the "downloadURL" field, it says "No files selected". The footer contains navigation links: "Home", "Data Curation", "Data Exploration", "Composer", and "Contact". It also includes copyright information: "© 2012 - 2016 Materials Data Curation System" and "Privacy Policy", "Terms of Use", and "Administration". The website template is by Arcsin.

Materials Data Curation System

127.0.0.1:8000/curate/enter-data

Search

View 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

- measurement
 - core
 - material
 - transmission-electron-microscopy
 - instrument-ID FEI Titan 80-300
 - sample-ID
 - user-ID
 - acquisition-date-time
 - metadata

Upload File

Browse... Co-L06-1000h-900C.jpg

Save Cancel

- uncertainty
- supporting-files
 - file
 - name
 - type
 - downloadURL
 - accessURL
 - local

Upload File

No files selected

Home Data Curation Data Exploration Composer Contact

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Website template by Arcsin

9: A URL should be present. Click on “View Data”.

The screenshot shows a web browser window with the address bar displaying "127.0.0.1:8000/curate/enter-data". The page title is "Materials Data Curation System". On the left sidebar, there is a button labeled "View Data" with a circular icon containing the number 3, which is circled in red. The main content area displays a form for entering data. At the top of the form, there are three buttons: "Clear Fields", "Save Form", and "Download". The form is organized into a hierarchical structure with expandable sections:

- measurement**
 - core**
 - material**
 - transmission-electron-microscopy**
 - instrument-ID**: FEI Titan 80-300
 - sample-ID**
 - user-ID**
 - acquisition-date-time**
 - metadata**
 - imaging-mode**: Bright Field Image
 - tilt-zone-axis**
 - accelerating-voltage**
 - value**: 300
 - unit**: kV
 - uncertainty**
 - supporting-files**
 - file**
 - name**
 - type**
 - downloadURL**

Below the form, there is an "Upload File" button. Underneath it, the text "Uploaded File: Co-1.06-1000h-900C.jpg" is displayed. At the bottom of the form, the text "Handle: <http://127.0.0.1:8000/rest/blob?id=56d45fa51813cd10fb6eadb>" is shown, with the URL circled in red. The footer of the page contains links: "Home | Data Curation | Data Exploration | Composer | Contact" and a "Top ^" link.

10: The metadata should be rendered as shown below. Click on “Save to repository”.

The screenshot displays the 'Materials Data Curation System' interface. The browser address bar shows '127.0.0.1:8000/curate/view-data'. The page header includes a welcome message for 'admin' and navigation links for 'Logout', 'My Profile', and 'Help'. The main navigation bar has tabs for 'Home', 'Data Curation', 'Data Exploration', and 'Composer'. Below this, a sub-navigation bar shows 'Select Template', 'Enter Data', and 'View Data'. The left sidebar, under 'Data Curation', lists three steps: '1 Select Template', '2 Enter Data', and '3 View Data'. The main content area is titled 'View Data' and contains a message: '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.' Below the message are two buttons: 'Download XML' and 'Save to repository'. The 'Save to repository' button is circled in red. The data is presented as a tree structure:

- measurement
 - core
 - title : TEM measurement of Co-11W-9.4Al
 - contactPoint
 - fn : John Smith
 - hasEmail : data@nist.gov
 - keyword : TEM
 - material
 - quantity-unit : mole percent
 - composition
 - constituent
 - element : Co
 - quantity : 81.75
 - purity : 1
 - error : 0
 - constituent
 - element : W
 - quantity : 10
 - purity : 1
 - error : 0
 - constituent
 - element : Al
 - quantity : 8.25

11: The document name should be populated. Click “Save”.

The screenshot shows a web browser window with the address bar displaying "127.0.0.1:8000/curate/view-data". The page title is "Materials Data Curation System" with a welcome message: "Welcome, admin. Thanks for logging in." The navigation bar includes links for "Home", "Data Curation", "Data Exploration", and "Composer". The "Data Curation" section is active, showing a sidebar with three steps: "1 Select Template", "2 Enter Data", and "3 View Data". The main content area is titled "View Data" and contains a message: "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." Below this message are two buttons: "Download XML" and "Save to repository". A "Save to Repository" dialog box is open, prompting the user to "Save data to the repository" and asking for a "Save As:" name. The input field contains "Co-L06-1000h-900C.xml" and a "Save" button is visible. The background data is structured as follows:

```
measurement
├── quantity-unit : mole percent
├── composition
│   ├── constituent
│   │   ├── element : Co
│   │   ├── quantity : 81.75
│   │   ├── purity : 1
│   │   └── error : 0
│   ├── constituent
│   │   ├── element : W
│   │   ├── quantity : 10
│   │   ├── purity : 1
│   │   └── error : 0
│   └── constituent
│       ├── element : Al
│       └── quantity : 8.25
```