

Data Curation: Simple TEM Tutorial

Adding a Template

1: Select “Administration”

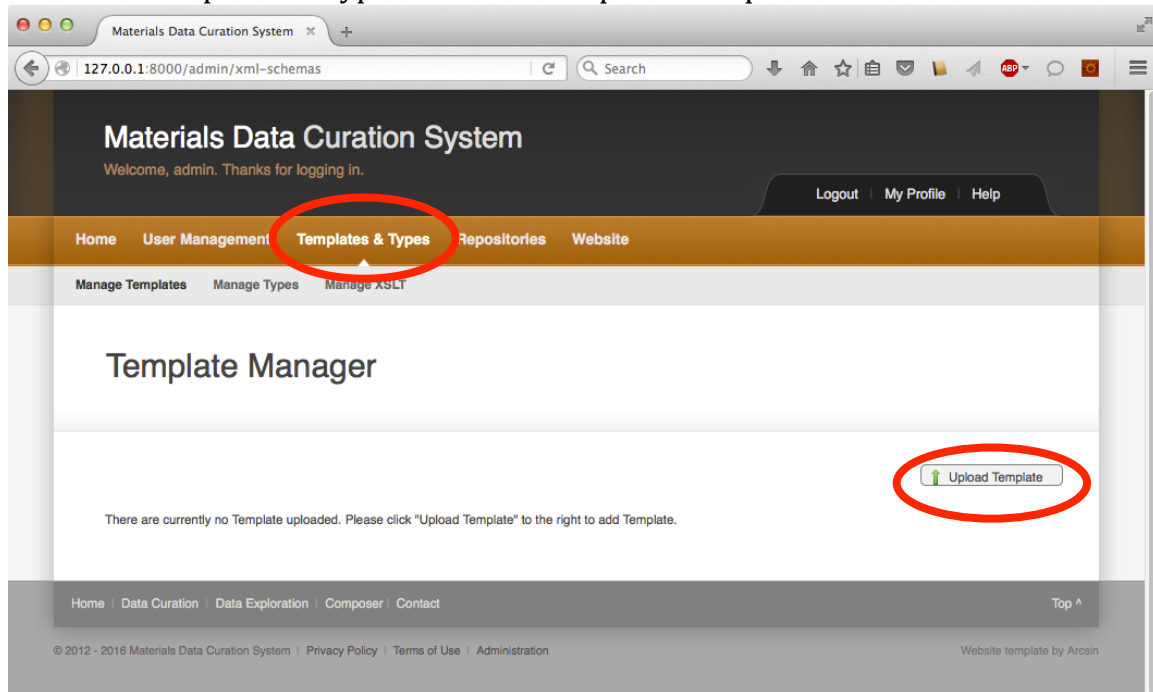
The screenshot shows a web browser window displaying the Materials Data Curation System. The browser's address bar shows the URL 127.0.0.1:8000. The page has a dark header with the title "Materials Data Curation System" and a welcome message "Welcome, admin. Thanks for logging in." Navigation links include "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.

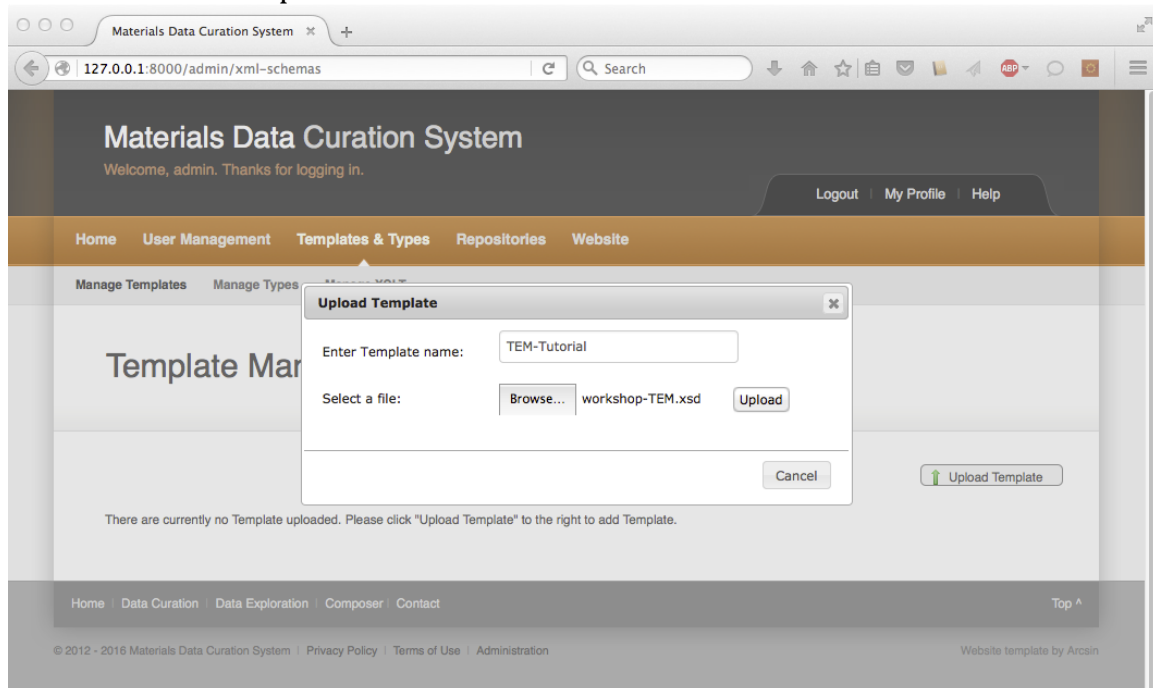
Below the main content area are two columns. The left column is titled "Available Options" and contains three links with icons: "Curate your Materials Data" (with a document icon), "Explore the repository" (with a magnifying glass icon), and "Compose a template" (with a document icon). The right column 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 address bar displaying `127.0.0.1:8000/admin/xml-schemas/manage-schemas`. 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 menu is highlighted in orange and includes the following items: "Home", "User Management", "Templates & Types", "Repositories", and "Website". The "Home" link is circled in red. Below this menu, there are sub-links: "Manage Templates", "Manage Types", and "Manage XSLT".

The main content area is titled "Template Manager". It features an "Upload Template" button with an upward arrow icon. Below this is a table with the following data:

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

The footer of the page contains the following text: "© 2012 - 2016 Materials Data Curation System | Privacy Policy | Terms of Use | Administration" and "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 navigation links: '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 the following text: '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 text, there is a table titled 'Global Templates' with the following content:

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

Below the table, there is a section titled 'User Defined Templates' with the text: 'Create your own templates using the [Composer](#) and you will be able to use them from this section.'

The footer of the page includes a navigation bar with links: 'Home', 'Data Curation', 'Data Exploration', 'Composer', and 'Contact'. The copyright notice is '© 2012 - 2016 Materials Data Curation System' and the website template is by 'Arcsin'.

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

The screenshot shows the Materials Data Curation System web application. The browser address bar displays "127.0.0.1:8000/curate/". The page header includes the title "Materials Data Curation System" and a welcome message "Welcome, admin. Thanks for logging in." with links for "Logout", "My Profile", and "Help". The main navigation bar contains "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

Create y

templates

to use them from this section.

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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:

Materials Data Curation System

127.0.0.1:8000/curate/enter-data

Home Data Curation Data Exploration Composer

Select Template Enter Data View Data

Data Curation

- Select Template
- Enter Data
- 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

- measurement
 - core
 - title TEM measurement of Co-11W-9.
 - description
 - contactPoint
 - fn John Smith
 - hasEmail data@nist.gov
 - keyword TEM
 - modified
 - publisher
 - accessLevel
 - identifier
 - bureauCode
 - programCode
 - material
 - transmission-electron-microscopy

Home | Data Curation | Data Exploration | Composer | Contact

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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

Select Template

Enter Data

View Data

1 Select Template

2 Enter Data

3 View Data

Periodic Table

IA

0

1 H IIA

Select one element by clicking on the element.

IIIA IVA VA VIA VIIA He

2 Li Be

B C N O F Ne

3 Na Mg IIIB IVB VB VIB VIIB VIIIB IB IIB

Al 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
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>

Save

Cancel

Download

How what you

to the selected

s you to save

actually curate data.

may still be valid

template. Thus,

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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

Home | Data Curation | Data Exploration | Composer | Contact

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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. The form only saves a temporary document and does not 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

- 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 has a sidebar with a 'View Data' button. The main content area contains a form with a tree structure of fields. A dialog box titled 'Upload File' is open, showing a 'Browse...' button and the filename 'Co-L06-1000h-900C.jpg'. Below the dialog, the 'supporting-files' section is expanded, showing a 'file' section with 'name' and 'type' fields, and a 'downloadURL' field with an 'Upload File' button. The footer contains navigation links: Home, Data Curation, Data Exploration, Composer, Contact, and a 'Top' link. Copyright information for 2012-2016 and the website template by Arcsin are also present.

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 Upload File
 - accessURL
 - local

Home Data Curation Data Exploration Composer Contact Top

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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 contains a form with the following fields and options:

- 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 and a message "Uploaded File: Co-1.06-1000h-900C.jpg". A red circle highlights the "Handle" field, which contains the URL: <http://127.0.0.1:8000/rest/blob?id=56d45fa51813cd10fb6eadb>. At the bottom of the page, there is a footer with 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'. The 'Data Curation' tab is active, showing a sidebar with three steps: '1 Select Template', '2 Enter Data', and '3 View Data'. The 'View Data' step is selected, leading to the 'View Data' page. This page contains a message about saving data to the repository and two buttons: 'Download XML' and 'Save to repository'. The 'Save to repository' button is circled in red. Below the buttons is a tree view of the metadata:

```
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 : 0.05
```

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 subtitle "Welcome, admin. Thanks for logging in." and navigation links "Logout", "My Profile", and "Help". The main navigation bar includes "Home", "Data Curation", "Data Exploration", and "Composer". The "Data Curation" section has sub-links "Select Template", "Enter Data", and "View Data".

The "View Data" page displays a preview of curated data in XML format. A "Save to Repository" dialog box is open, prompting the user to "Save data to the repository." and "Save As:". The "Save As:" field contains the text "Co-L06-1000h-900C.xml". A "Save" button is visible in the dialog.

The XML data structure is shown as follows:

```
measurement
├── 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
```