

# Data Curation: Simple TEM Tutorial

## Adding a Template

### 1: Select “Administration”

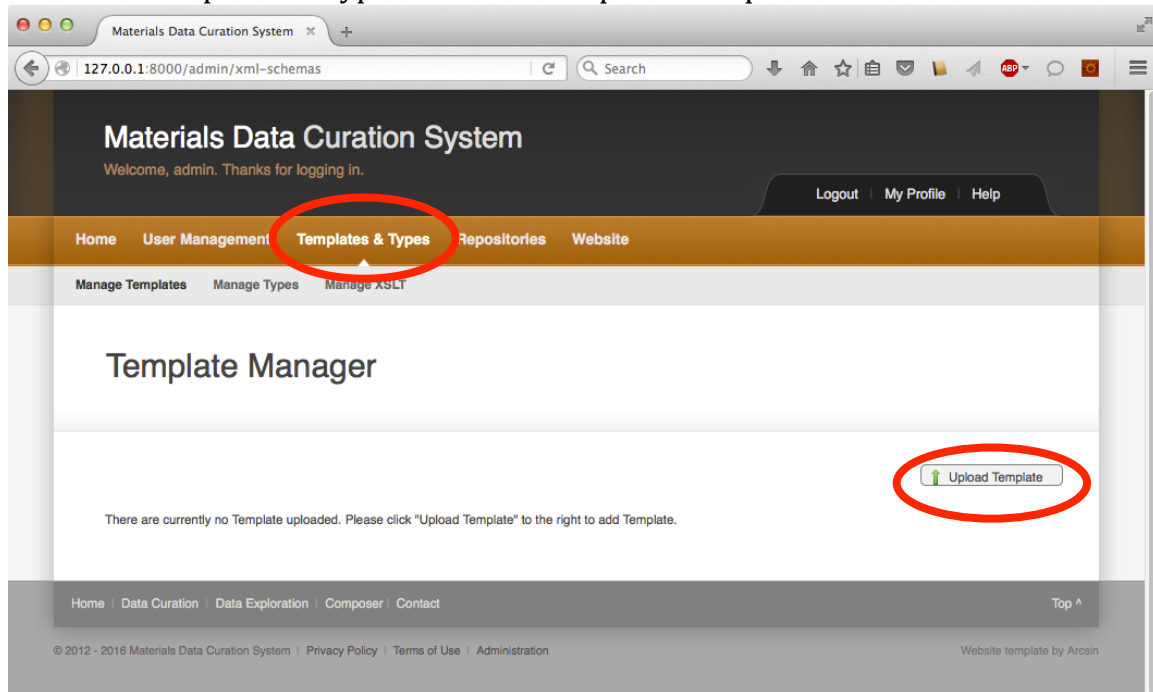
The screenshot shows a web browser window displaying the Materials Data Curation System. The browser's address bar shows the URL `127.0.0.1:8000`. The page has a dark header with the title "Materials Data Curation System" and a welcome message "Welcome, admin. Thanks for logging in." Navigation links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

The main content area is titled "Materials Data Curator" and includes a description of the system's purpose and its development at the National Institute of Standards and Technology. To the right is a circular diagram representing the "Materials Innovation Infrastructure", with segments for Human Welfare, Clean Energy, Next Generation Workforce, and National Security, and internal components for Computational Tools, Experimental Tools, and Digital Data.

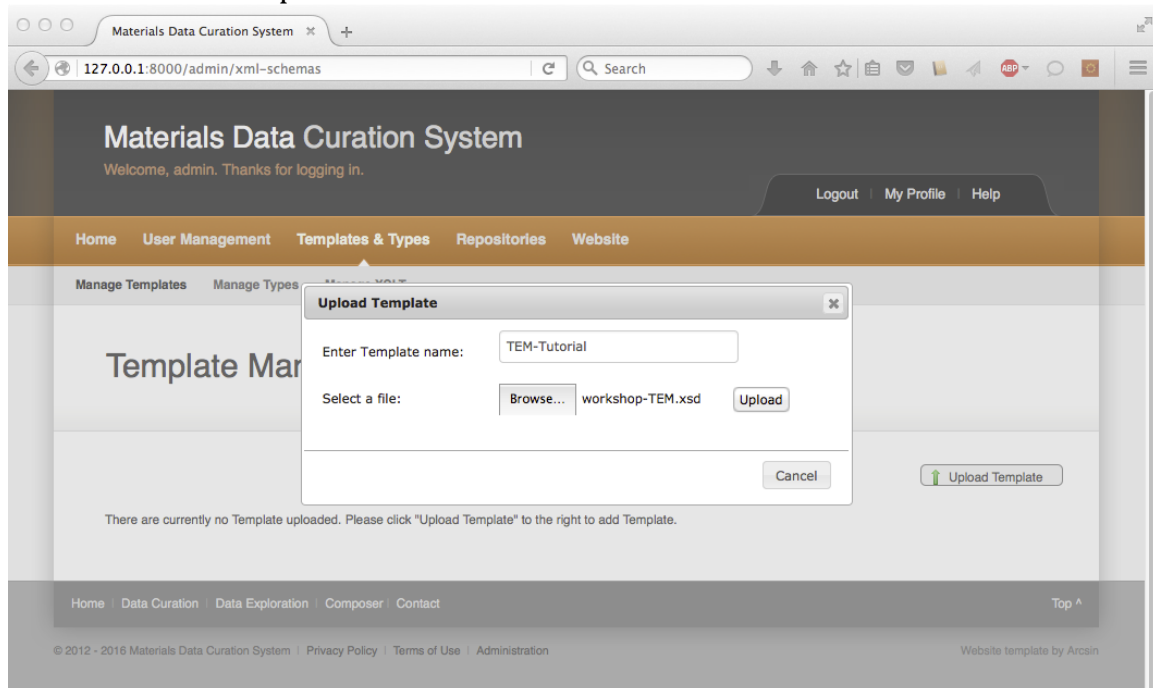
Below this, there are two columns: "Available Options" and "Most Recent Templates". The "Available Options" column lists three actions: "Curate your Materials Data", "Explore the repository", and "Compose a template", each with an icon and a brief description. The "Most Recent Templates" column is currently empty.

The footer contains a navigation bar with "Home", "Data Curation", "Data Exploration", "Composer", and "Contact". Below this, a copyright notice "© 2012 - 2016 Materials Data Curation System" is followed by links for "Privacy Policy", "Terms of Use", and "Administration" (which is circled in red). The footer also includes 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.



# Adding Modules to the TEM-Tutorial Template

## 1: Select “Modules”

The screenshot shows the Materials Data Curation System admin interface. The browser address bar displays `127.0.0.1:8000/admin/xml-schemas`. The page title is "Materials Data Curation System" with a welcome message for the admin user. The navigation menu includes "Home", "User Management", "Templates & Types", "Repositories", and "Website". The "Templates & Types" section is active, showing sub-links for "Manage Templates", "Manage Types", and "Manage XSLT". The "Template Manager" page displays a table with the following data:

Template name	Filename	Status	Actions
TEM-Tutorial	workshop-TEM.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>

The "Modules" link is circled in red. An "Upload Template" button is located above the table. The footer contains copyright information for 2012-2016 and a link to the website template by Arcsin.

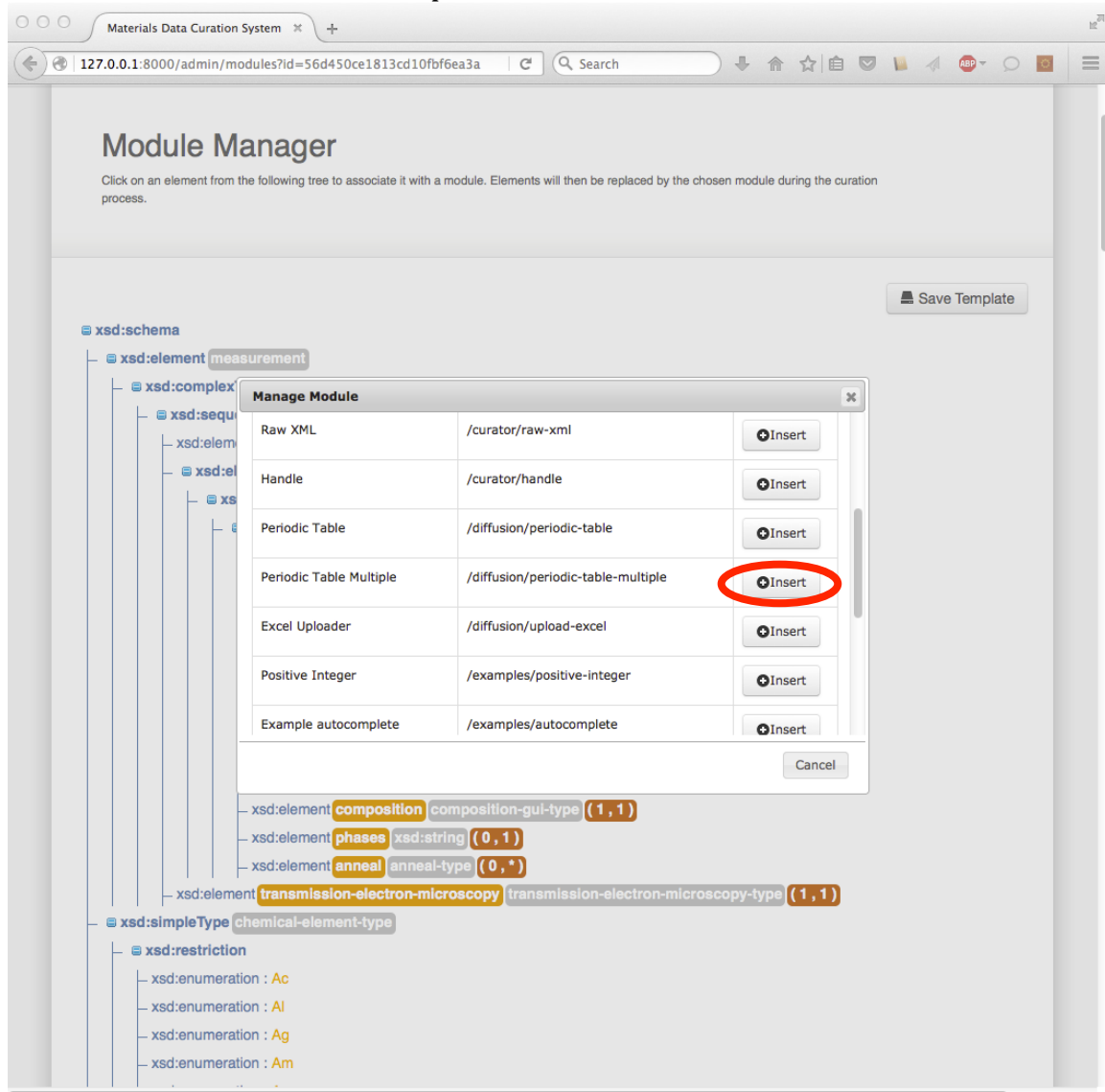
2: Scroll to “composition”. Click on “xsd:element” to the left of composition.

The screenshot shows the Materials Data Curation System Module Manager interface. The browser address bar indicates the URL: 127.0.0.1:8000/admin/modules?id=56d450ce1813cd10fbf6ea3a. The page title is "Module Manager". Below the title, a message states: "Click on an element from the following tree to associate it with a module. Elements will then be replaced by the chosen module during the curation process."

The main content area displays an XSD schema tree. The root node is `xsd:schema`. It contains a child node `xsd:element` with the attribute `measurement`. This node is expanded, showing a child node `xsd:complexType`. This node is also expanded, showing a child node `xsd:sequence`. This node is expanded, showing a child node `xsd:element` with the attribute `core` and the attribute `core-type` with the value `(1,1)`. This node is expanded, showing a child node `xsd:complexType`. This node is expanded, showing a child node `xsd:sequence`. This node is expanded, showing a child node `xsd:element` with the attribute `quantity-unit`. This node is expanded, showing a child node `xsd:simpleType`. This node is expanded, showing a child node `xsd:restriction`. This node is expanded, showing a list of enumerations: `mass fraction`, `mass percent`, `mole fraction`, `mole percent`, `volume fraction`, and `volume percent`. The `composition` element is highlighted with a red circle. It has the attribute `composition-gui-type` with the value `(1,1)`. Below it, there is a child node `xsd:string` with the attribute `(0,1)`. Below that, there is a child node `anneal` with the attribute `anneal-type` with the value `(0,*)`. Below that, there is a child node `transmission-electron-microscopy` with the attribute `transmission-electron-microscopy-type` with the value `(1,1)`. At the bottom of the tree, there is a child node `xsd:simpleType` with the attribute `chemical-element-type`. This node is expanded, showing a list of enumerations: `Ac`, `Al`, `Ag`, and `Am`.

A "Save Template" button is located in the top right corner of the main content area.

3: Scroll to “Periodic Table Multiple” and click on insert.



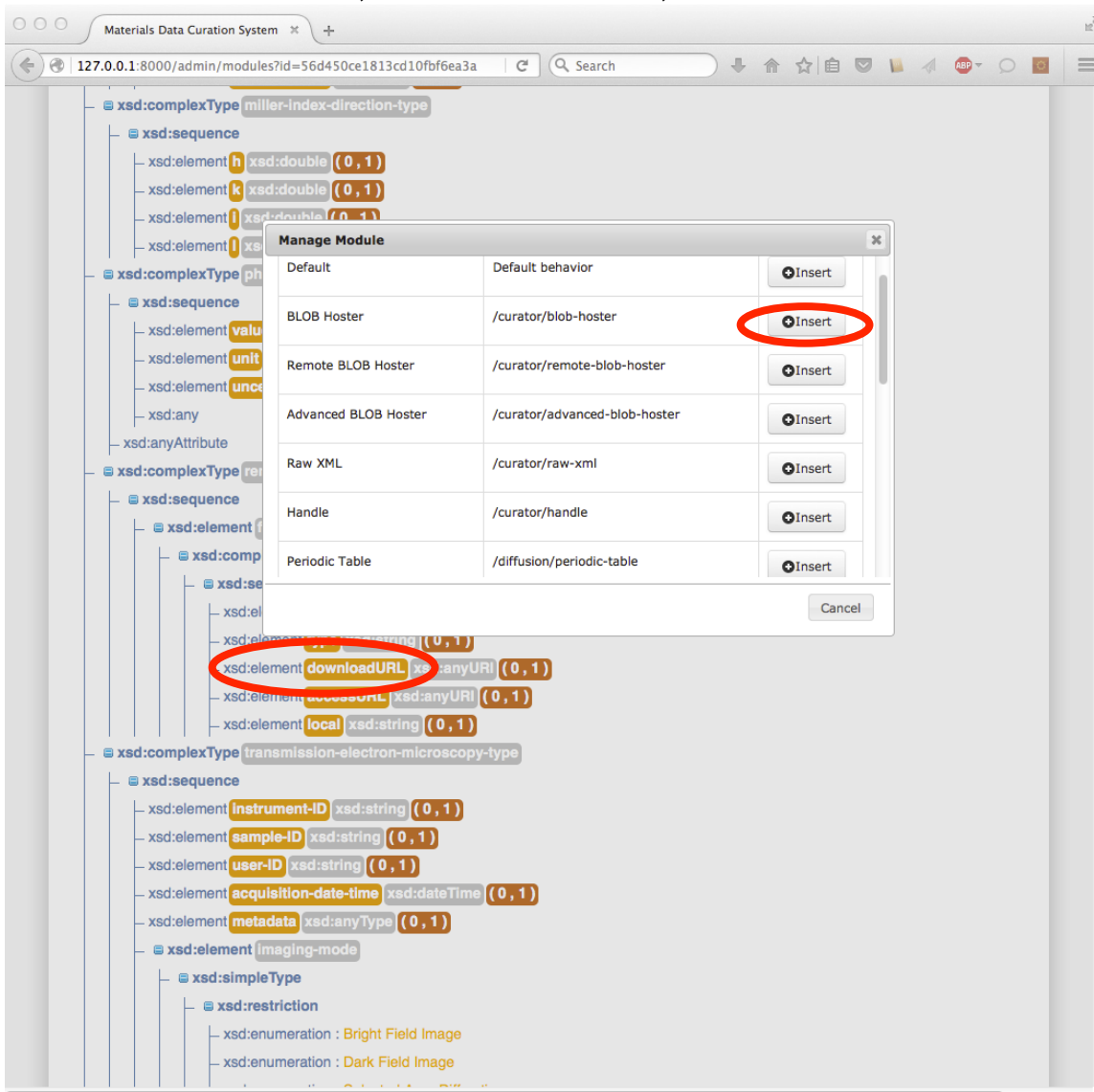
#### 4: Notice the addition of “/diffusion/periodic-table-multiple”

The screenshot shows the Materials Data Curation System Module Manager interface. The browser address bar indicates the URL: 127.0.0.1:8000/admin/modules?id=56d450ce1813cd10fbf6ea3a. The page title is "Module Manager". Below the title, a note states: "Click on an element from the following tree to associate it with a module. Elements will then be replaced by the chosen module during the curation process."

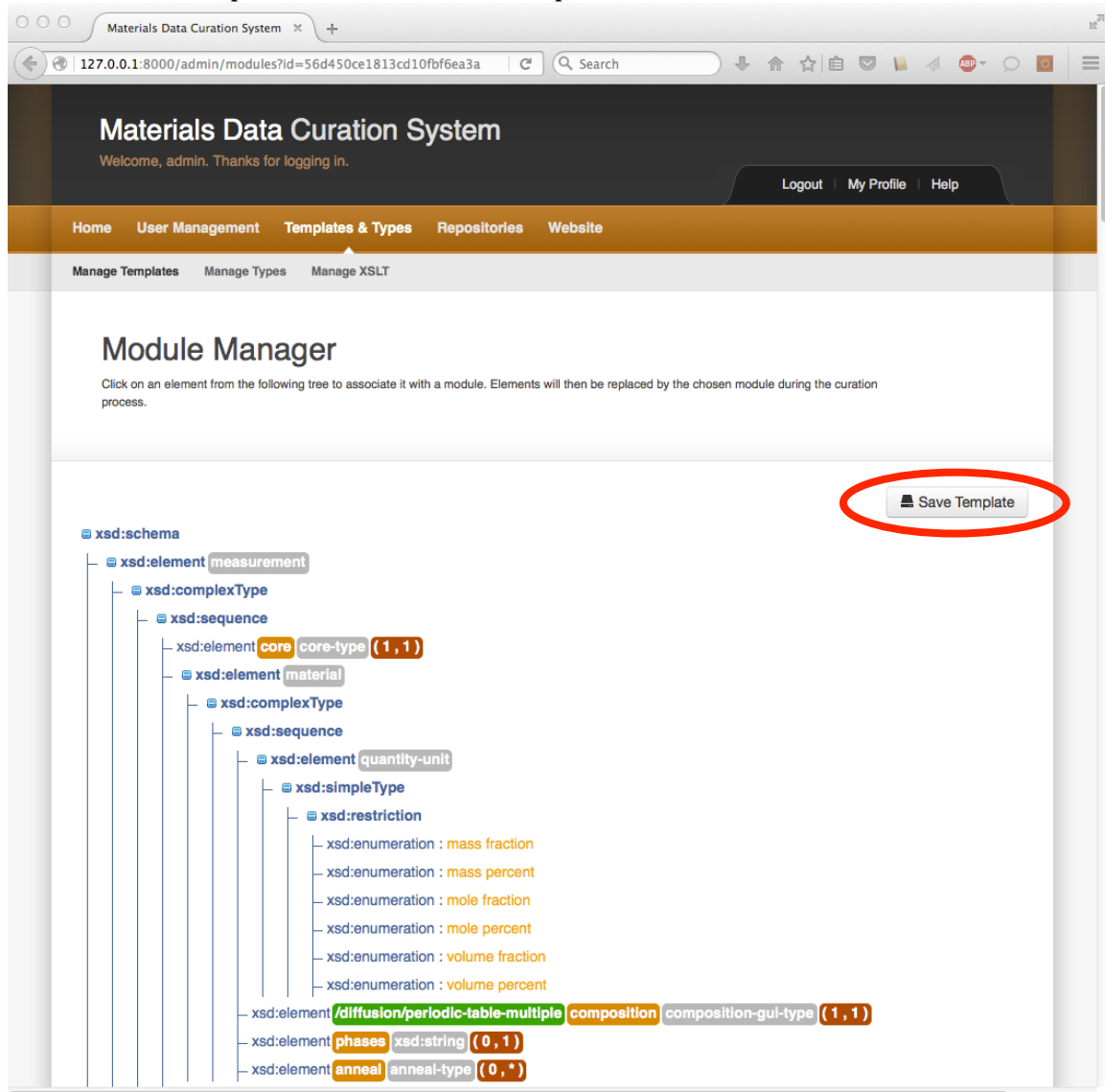
A "Save Template" button is located in the top right corner. The main content area displays an XSD schema tree structure:

- xsd:schema**
  - xsd:element measurement**
    - xsd:complexType**
      - xsd:sequence**
        - xsd:element core** core-type (1,1)
        - xsd:element material**
          - xsd:complexType**
            - xsd:sequence**
              - xsd:element quantity-unit**
                - xsd:simpleType**
                  - xsd:restriction**
                    - xsd:enumeration : mass fraction
                    - xsd:enumeration : mass percent
                    - xsd:enumeration : mole fraction
                    - xsd:enumeration : mole percent
                    - xsd:enumeration : volume fraction
                    - xsd:enumeration : volume percent
                - xsd:element /diffusion/periodic-table-multiple** composition composition-gui-type (1,1) (highlighted with a red circle)
                - xsd:element phase** phase-type (0,1)
                - xsd:element anneal** anneal-type (0,\*)
                - xsd:element transmission-electron-microscopy** transmission-electron-microscopy-type (1,1)
  - xsd:simpleType chemical-element-type**
    - xsd:restriction**
      - xsd:enumeration : Ac
      - xsd:enumeration : Al
      - xsd:enumeration : Ag
      - xsd:enumeration : Am

5: Scroll to “downloadURL”, click on “xsd:element”, and insert “BLOB Hoster”:



## 6: Scroll to the top and click on “Save Template”





## 7: Click on “Home”

The screenshot shows the Materials Data Curation System admin interface. The browser address bar displays `127.0.0.1:8000/admin/xml-schemas/manage-schemas`. The page header includes the system name and a welcome message for the admin user. The top navigation bar contains 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 for 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, with one entry 'TEM-Tutorial' having a status of 'Registered' and various action links. The footer contains copyright information and a link to the website template by Arcsin.

Materials Data Curation System

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

Upload Template

| Template name | Filename         | Status     | Actions  |
|---------------|------------------|------------|--|
| TEM-Tutorial  | workshop-TEM.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> |

Home | Data Curation | Data Exploration | Composer | Contact

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## 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 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 | <a href="#">Set as current template</a> |

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 for 'Home', 'Data Curation', 'Data Exploration', 'Composer', and 'Contact', along with a 'Top ^' link. The footer also contains copyright information: '© 2012 - 2016 Materials Data Curation System' and links for 'Privacy Policy', 'Terms of Use', and 'Administration'. The footer also mentions 'Website template 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         |           | <a href="#">Set as current template</a> |

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

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

The screenshot displays the Materials Data Curation System web application. The browser address bar shows the URL `127.0.0.1:8000/curate/enter-data`. The application header includes the title "Materials Data Curation System" and a welcome message for the admin user. Navigation tabs at the top include "Home", "Data Curation", "Data Exploration", and "Composer". The "Data Curation" tab is active, showing sub-tabs for "Select Template", "Enter Data", and "View Data".

A "Periodic Table" modal window is open, displaying a color-coded periodic table. Below the table, there are sections for "Lanthanides" and "Actinides". To the right of the periodic table, a text box provides instructions: "Select one element by clicking on the element." Below this, a table lists the elements currently in the composition:

| Element | Quantity | Purity | Error | Actions |
|---------|----------|--------|-------|---------|
| Co      | 81.75    | 1      | 0     | Remove  |
| W       | 10       | 1      | 0     | Remove  |
| Al      | 8.25     | 1      | 0     | Remove  |

At the bottom of the modal, there are "Save" and "Cancel" buttons. The main page also features a "Download" button and a "Top" link.

## 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. 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 title is "Materials Data Curation System". A sidebar on the left contains a "View Data" button. The main content area features a form with a "Clear Fields" button, a "Save Form" button, and a "Download" button. The form is organized into sections: "measurement", "core", "material", and "transmission-electron-microscopy". The "transmission-electron-microscopy" section includes fields for "instrument-ID" (FEI Titan 80-300), "sample-ID", "user-ID", "acquisition-date-time", and "metadata". A modal dialog 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, a "downloadURL" field with an "Upload File" button, and a "local" section. The footer contains navigation links: "Home", "Data Curation", "Data Exploration", "Composer", and "Contact". The copyright notice is "© 2012 - 2016 Materials Data Curation System | Privacy Policy | Terms of Use | Administration". The website template is by Arcsin.

Materials Data Curation System

127.0.0.1:8000/curate/enter-data

View Data

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
  - local

Home | Data Curation | Data Exploration | Composer | Contact

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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:

- Buttons: Clear Fields, Save Form, Download
- Form 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". Below this, the "Handle" is displayed as: <http://127.0.0.1:8000/rest/blob?id=56d45fa51813cd10fb6eadb>, which is circled in red. The footer 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 the URL `127.0.0.1:8000/curate/view-data`. The page header includes the system name and a welcome message for the admin user. The navigation bar contains 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 about saving data to the repository. Below the message are two buttons: 'Download XML' and 'Save to repository', with the latter being circled in red. The metadata is displayed in 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 : 9.4
```

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 message states: "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." Buttons for "Download XML" and "Save to repository" are visible.

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 present.

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
```