

Composer: Simple DiffusionDemo

Change an “instance”

In this example we want to change the schema to allow one to enter multiple phase for a given material.

1: At the Home screen navigate to “Composer”

The screenshot shows the Materials Data Curation System interface. At the top, there's a navigation bar with tabs: Home, Data Curation, Data Exploration, and Composer (which is circled in red). Below the navigation bar is a banner with the text "Materials Data Curation System" and "Welcome, admin. Thanks for logging in." On the right side of the banner 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 pencil and paper icon, which is also circled in red). 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 (which is underlined), Contact, and Administration. The footer also includes copyright information: "© 2012 - 2016 Materials Data Curation System | Privacy Policy | Terms of Use | Administration" and "Website template by Arcsin".

2: Select “DiffusionDemo” Template as the current template

The screenshot shows the 'Materials Data Curation System' interface. The left sidebar has 'Composer' selected. The main area is titled 'Start Template'. It displays a table of global templates:

Template name	File name	Actions
New Base Template	new_base_template.xsd	<input type="radio"/> Select as start template
Image-demo	Image-diffusioncouple.xsd	<input checked="" type="radio"/> Set as current template
image-test	image-test.xsd	<input type="radio"/> Set as current template
DemoDiffusion	mod.demo.diffusion.xsd	Current template

3: Select “Compose Template” on the left-side menu

The screenshot shows the 'Materials Data Curation System' interface. The left sidebar has 'Composer' selected. The main area is titled 'Start Template'. It displays a table of global templates:

Template name	File name	Actions
New Base Template	new_base_template.xsd	<input type="radio"/> Select as start template
Image-demo	Image-diffusioncouple.xsd	<input checked="" type="radio"/> Set as current template
image-test	image-test.xsd	<input type="radio"/> Set as current template
DemoDiffusion	mod.demo.diffusion.xsd	Current template
ThermoMLdraft	ThermoML-draft.xsd	<input type="radio"/> Set as current template
test-image	image-test.xsd	<input type="radio"/> Set as current template
TEM-Image	Image-TEM4.xsd	<input type="radio"/> Set as current template

The 'Compose Template' link in the left sidebar is circled in red.

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compose/build-template

Materials Data Curation System

Welcome, admin. Thanks for logging in.

Logout | My Profile | Help

Home **Data Curation** **Data Exploration** **Composer**

Start Template **Compose Template**

Composer

- Select Template**
- Compose Template**

Legend

- Name**
- Type**
- (minOccurs, maxOccurs)**

Compose Template

Please click on an element of the tree to start composing the template. A menu will appear and you will be able to interact with that element.

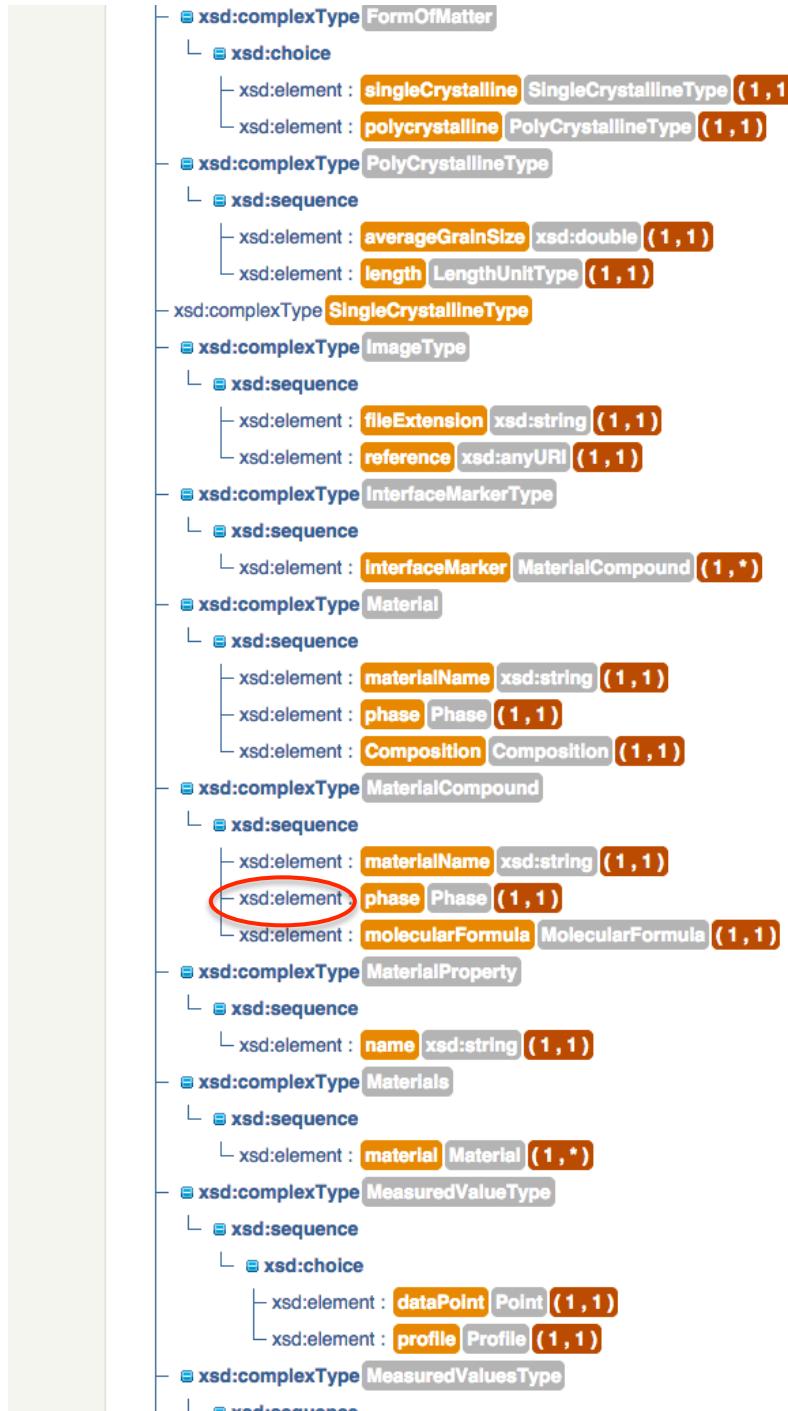
[Download](#) [Save as Template](#) [Save as Type](#)

```

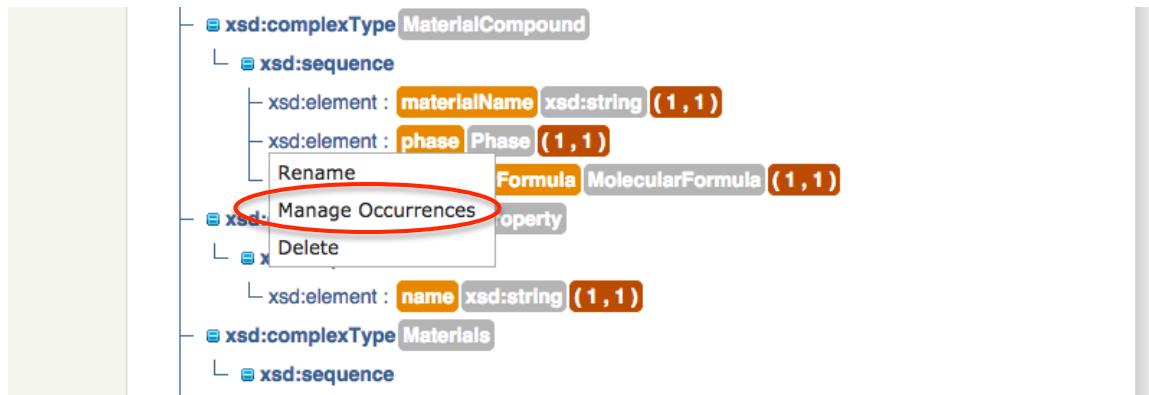
xsd:schema
└ xsd:element : experiment Experiment (1,1)
  └ xsd:complexType CatalogNumber
    └ xsd:sequence
      └ xsd:element : id xsd:string (1,1)
      └ xsd:element : catalogTitle CatalogTitle (1,1)
  └ xsd:complexType CatalogTitle
    └ xsd:sequence
      └ xsd:element : name xsd:string (1,1)
  └ xsd:simpleType ChemicalElement
    └ xsd:restriction
      └ xsd:enumeration : Ac
      └ xsd:enumeration : Al
      └ xsd:enumeration : Ag
      └ xsd:enumeration : Am
      └ xsd:enumeration : Ar
      └ xsd:enumeration : As
      └ xsd:enumeration : At
      └ xsd:enumeration : Au
      └ xsd:enumeration : B
      └ xsd:enumeration : Ba
      └ xsd:enumeration : Bh
      └ xsd:enumeration : Bi
      └ xsd:enumeration : Be
      └ xsd:enumeration : Bk
      └ xsd:enumeration : Br
      └ xsd:enumeration : C
      └ xsd:enumeration : Ca
      └ xsd:enumeration : Cd

```

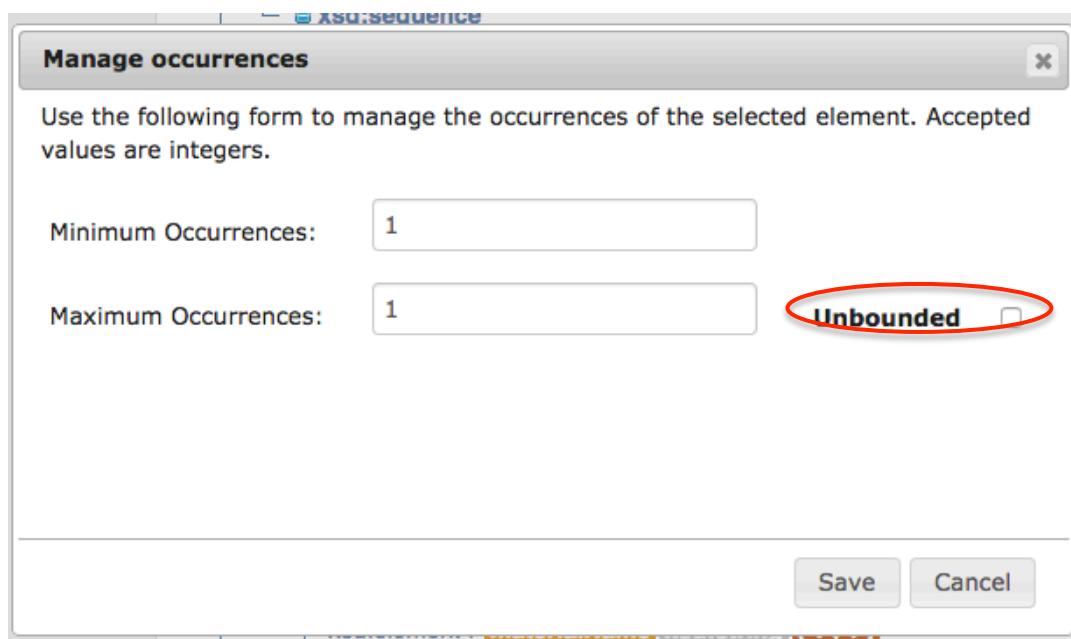
4. Scroll a little more than half way down the schema and find the “element” labelled “phase” and click on the element.



After clicking on “element” a box will appear with 3 choices: Rename, Manage Occurrences, and Delete. Select “Manage Occurrences”



A new pop-up window will appear where you can change the number of occurrences that “phase” is allowed. Change it to “Unbounded” and click “Save”.



Manage occurrences

Use the following form to manage the occurrences of the selected element. Accepted values are integers.

Minimum Occurrences:

Maximum Occurrences: **Unbounded**

Save **Cancel**

Now the number of occurrences for phase should be (1,*)



Now scroll to the top of the page and save the template as “DiffusionDemo-2”.

The screenshot shows the 'Materials Data Curation System' interface with the 'Composer' tab selected. On the left, there's a sidebar with 'Composer' buttons (Select Template, Compose Template) and a legend for 'Name', 'Type', and '(minOccurs, maxOccurs)'. The main area is titled 'Compose Template' with instructions: 'Please click on an element of the tree to start composing the template. A menu will appear and you will be able to interact with that element.' Below this are three buttons: 'Download', 'Save as Template' (which is highlighted with a red circle), and 'Save as Type'. A hierarchical tree view shows an 'xsd:schema' node with an 'experiment' element (1,1), which has a 'CatalogNumber' complex type. This type contains a sequence with an 'id' element (1,1) and a 'catalogTitle' element (1,1). There are also 'CatalogTitle' and 'ChemicalElement' complex types, and a 'ChemicalElement' simple type with enumerations: 'Ac', 'Al', 'Ag', 'Am', and 'Ar'.

This screenshot shows the same interface after a template has been saved. A 'Save Template' dialog box is open in the foreground, prompting for a name. The 'Name:' field contains 'DiffusionDemo-2'. Below the dialog, the tree view shows the same schema structure as the previous screenshot, with the 'Save as Template' button still highlighted by a red circle.

Now return to the “Data Curation” menu. You should now see under the “User Defined Templates” the DiffusionDemo-2 template.

User Defined Templates	
Template name	Actions
image3a	<input type="button"/> Set as current template
image4a	<input type="button"/> Set as current template
test2	<input type="button"/> Set as current template
DemoDiffusion-cec	<input type="button"/> Set as current template
Diffusion-cec-phase	<input type="button"/> Set as current template
DiffusionDemo-2	<input type="button"/> Set as current template

Select the template and read in the existing GE-DiffusionCouple-R88-IN100.xml document.

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
Image-demo	Image-diffusioncouple.xsd	+ Set as current template
image4test	image-test.xsd	+ Set as current template
DemoDiffusion	mod.demo.diffusion.xsd	+ Set as current template
ThermoMLdraft	ThermoML-draft.xsd	+ Set as current template
test-in	Template Loaded	+ Set as current template
Interco	<input type="radio"/> Create a new document: <input type="text"/>	+ Set as current template
image	<input type="radio"/> Open an existing form: <input type="text"/>	+ Set as current template
Interco	<input checked="" type="radio"/> Open an existing XML document: <input type="file" value="DiffusionGE-Rene88IN100.xml"/>	+ Set as current template
TEM		+ Set as current template

Start

Local Templates		
Template name	Actions	
image3a	+ Set as current template	
image4a	+ Set as current template	
test2	+ Set as current template	
DemoDiffusion-cec	+ Set as current template	
Diffusion-cec-phase	+ Set as current template	
DiffusionDemo-2	+ Set as current template	

After reading the “GE-DiffusionCouple-R88-IN100” document, the Data Entry screen will appear. Notice there is now a “green” plus button next to phase. Click on it to add additional phase to the Rene-88 material.

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 Rene-88
 - phase
 - name FCC
- Composition
 - quantityUnit mass percent
 - constituents

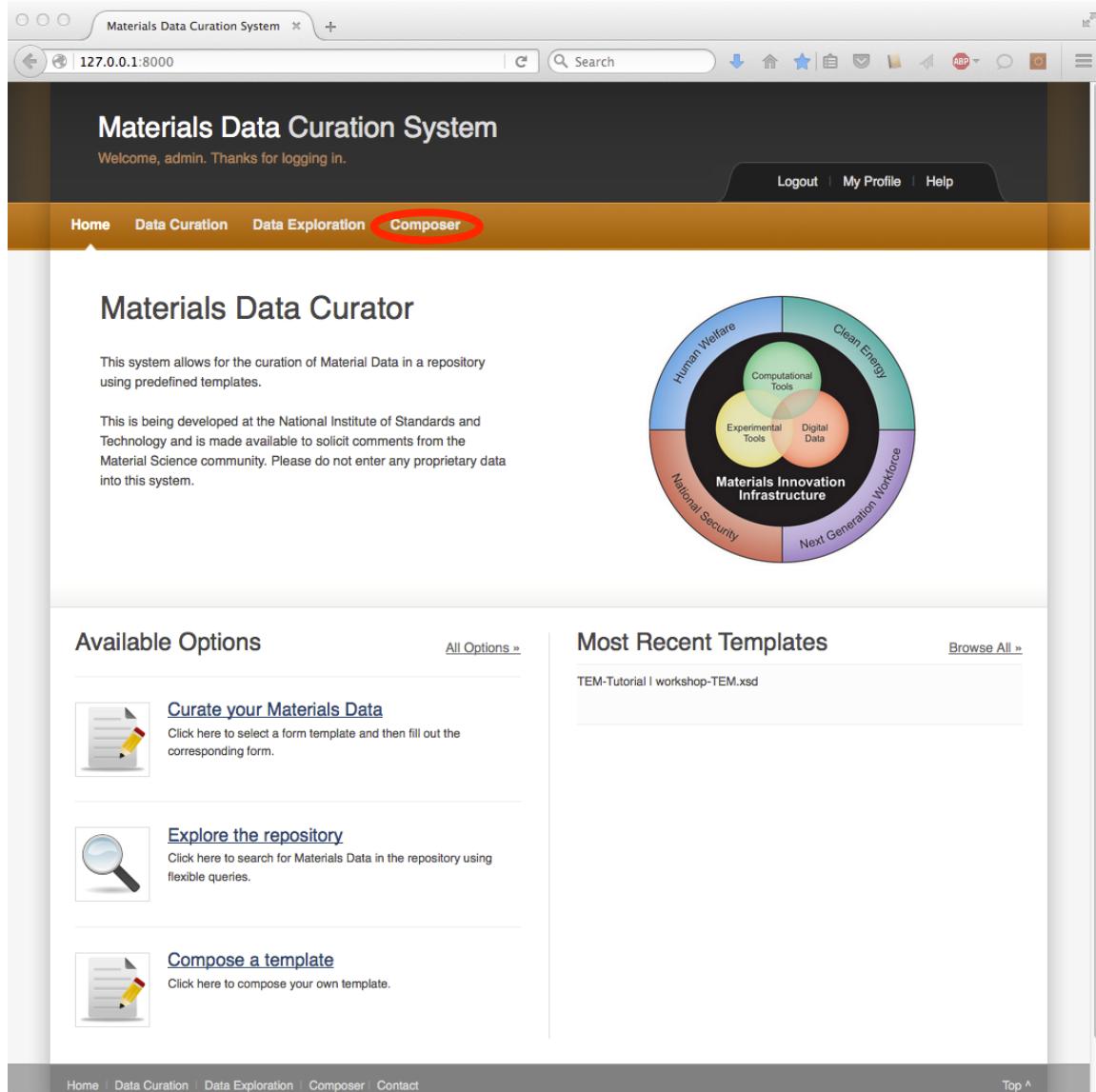
Element	Quantity	Purity	Error
Ni	58.1	0.999	0.001

Enter the “MC carbide” as a second phase.

- Choose chemicalDiffusivity
- chemicalDiffusivity
- material
 - materialName Rene-88
- phase
 - name FCC
- crystalStructure
 - spaceGroup
 - wyckoffSequence
- phase
 - name MC carbide
- crystalStructure
 - spaceGroup

Modifying an existing Template

1: Click on "Composer"



The screenshot shows a web browser window for the "Materials Data Curation System" at address 127.0.0.1:8000. The page title is "Materials Data Curation System". A banner at the top says "Welcome, admin. Thanks for logging in." with links for "Logout", "My Profile", and "Help". The navigation bar includes "Home", "Data Curation", "Data Exploration", and "Composer", with "Composer" circled in red. Below the navigation is a circular diagram titled "Materials Innovation Infrastructure" with segments for "Human Welfare", "Clean Energy", "Computational Tools", "Experimental Tools", "Digital Data", "National Security", and "Next Generation Workforce". The main content area has two sections: "Available Options" with links to "Curate your Materials Data", "Explore the repository", and "Compose a template"; and "Most Recent Templates" with a link to "TEM-Tutorial I workshop-TEM.xsd". The bottom navigation bar includes "Home", "Data Curation", "Data Exploration", "Composer", "Contact", and a "Top ^" link.

2: Select “TEM-Tutorial” as current template. Proceed to second step: “Compose Tempalte”

The screenshot shows the Materials Data Curation System Composer interface. The top navigation bar includes links for Home, Data Curation, Data Exploration, and Composer. The main content area is titled "Start Template". A message at the top states: "Select a new or existing start template from the following table to start composing. Once you make your selection, click on "Compose Template" to proceed. It will automatically load the appropriate template and display it on the next page." Below this is a yellow warning box: "⚠ No template selected. Select one in the table below." The "Global Templates" section contains a table:

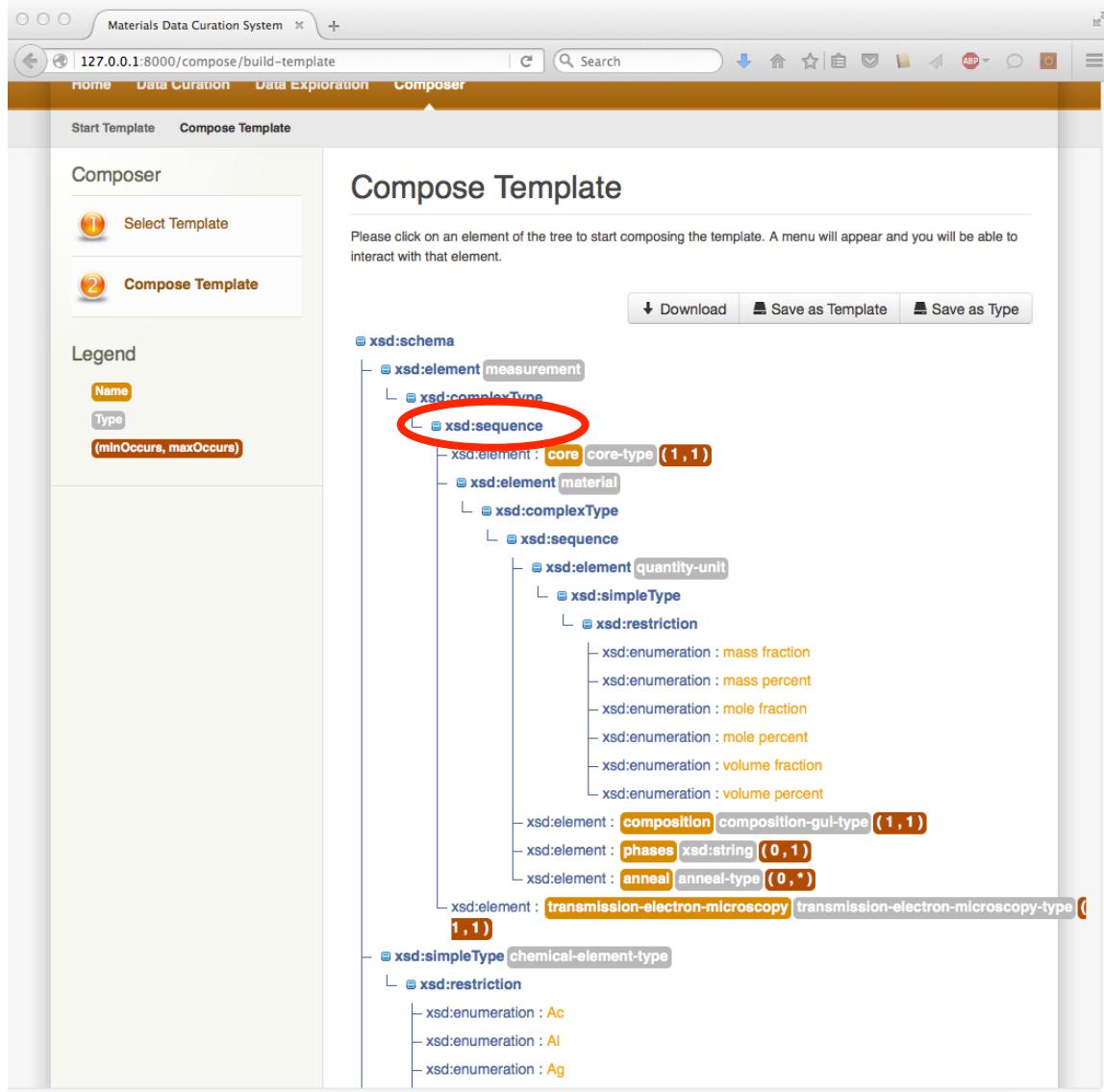
Template name	File name	Actions
New Base Template	new_base_template.xsd	<input checked="" type="radio"/> Select as start template
TEM-Tutorial	workshop-TEM.xsd	<input type="radio"/> Set as current template

The "TEM-Tutorial" row is circled in red. The "Set as current template" button is also highlighted with a red circle.

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

The bottom navigation bar includes links for Home, Data Curation, Data Exploration, Composer, Contact, and links for Copyright (© 2012 - 2016), Privacy Policy, Terms of Use, and Administration. It also indicates the website template is by Arcsin.

3: Click on the top-level xsd:sequence and select “Add Element”



4: Drop-down “No Buckets” menu and insert “note”

The screenshot shows the Materials Data Curation System Composer interface. The main window title is "Compose Template". A legend on the left indicates that orange circles represent "Name" and grey circles represent "Type". The "Composer" section has two items: "Select Template" and "Compose Template", with "Compose Template" being the active item.

A legend on the left also includes "(minOccurs, maxOccurs)" information. The main workspace shows a tree structure under "xsd:schema" with "xsd:element measurement". An "Insert an Element" dialog is open, showing a "No Buckets" category with a single item "note". The "note" item has a sub-item "note.xsd" and an "Insert" button. Below this is a "My Types" section.

The tree view below the dialog shows several schema elements:

- xsd:element : composition composition-gui-type (1,1)
- xsd:element : phases xsd:string (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

5: Notice new element

The screenshot shows a web-based XML schema editor for the 'Materials Data Curation System'. The URL is 127.0.0.1:8000/compose/build-template. On the left, there's a legend with three items: 'Name' (blue), 'Type' (orange), and '(minOccurs, maxOccurs)' (red). The main area displays an XML schema structure:

```
<xsd:schema>
  <xsd:element name="measurement">
    <xsd:complexType>
      <xsd:sequence>
        <xsd:element name="core">
          <xsd:complexType>
            <xsd:sequence>
              <xsd:element name="material">
                <xsd:complexType>
                  <xsd:sequence>
                    <xsd:element name="quantity-unit">
                      <xsd:simpleType>
                        <xsd:restriction>
                          <xsd:enumeration value="mass fraction"/>
                          <xsd:enumeration value="mass percent"/>
                          <xsd:enumeration value="mole fraction"/>
                          <xsd:enumeration value="mole percent"/>
                          <xsd:enumeration value="volume fraction"/>
                          <xsd:enumeration value="volume percent"/>
                    </xsd:sequence>
                    <xsd:element name="composition">
                      <xsd:complexType>
                        <xsd:sequence>
                          <xsd:element name="phases"/>
                          <xsd:element name="anneal"/>
                        </xsd:sequence>
                      </xsd:complexType>
                    </xsd:element>
                    <xsd:element name="transmission-electron-microscopy">
                      <xsd:complexType>
                        <xsd:sequence>
                          <xsd:element name="note"/>
                        </xsd:sequence>
                      </xsd:complexType>
                    </xsd:element>
                  </xsd:sequence>
                </xsd:complexType>
              </xsd:element>
            </xsd:sequence>
          </xsd:complexType>
        </xsd:element>
      </xsd:sequence>
    </xsd:complexType>
  </xsd:element>
<xsd:simpleType name="chemical-element">
  <xsd:restriction>
    <xsd:enumeration value="Ac"/>
    <xsd:enumeration value="Al"/>
    <xsd:enumeration value="Ag"/>
    <xsd:enumeration value="Am"/>
    <xsd:enumeration value="Ar"/>
    <xsd:enumeration value="As"/>
    <xsd:enumeration value="At"/>
    <xsd:enumeration value="Au"/>
    <xsd:enumeration value="B"/>
    <xsd:enumeration value="Ba"/>
  </xsd:restriction>
</xsd:simpleType>
```

A red oval highlights the 'note' element under the 'transmission-electron-microscopy' element, indicating it is a new or recently added element.

6: Scroll to the top and click “Save as Template”. Enter “TEM note” and click “save”.

The screenshot shows the 'Materials Data Curation System' interface. The title bar says 'Materials Data Curation System' and 'Welcome, admin. Thanks for logging in.' The navigation bar includes 'Home', 'Data Curation', 'Data Exploration', 'Composer', 'Logout', 'My Profile', and 'Help'. The main area is titled 'Compose Template' with the sub-instruction: 'Please click on an element of the tree to start composing the template. A menu will appear and you will be able to interact with that element.' On the left, there's a 'Composer' sidebar with 'Select Template' (highlighted with a red circle) and 'Compose Template' (highlighted with a red circle). Below it is a 'Legend' section with 'Name' (orange button), 'Type' (grey button), and '(minOccurs, maxOccurs)' (grey text). The central part shows an XML schema tree under 'xsd:schema'. Key elements include 'measurement' (xsd:element), 'core-type' (xsd:element), 'material' (xsd:element), 'composition-gui-type' (xsd:element), 'phase' (xsd:element), 'anneal-type' (xsd:element), and 'transmission-electron-microscopy-type' (xsd:element). The 'Save as Template' button in the top right toolbar is circled in red. The URL in the browser is '127.0.0.1:8000/compose/build-template'.

7: After selecting “Ok” click “home”

The screenshot shows the Materials Data Curation System interface. The top navigation bar includes links for Home, Data Curation, Data Exploration, and Composer. The Home link is circled in red. The main content area is titled "Compose Template". It displays an XML schema tree under the heading "xsd:schema". The tree structure includes "xsd:element measurement", "xsd:complexType", "xsd:sequence", "xsd:element core", "xsd:element material", and several "xsd:enumeration" and "xsd:element" nodes for "composition", "phases", "anneal", "transmission-electron-microscopy", and "note". A legend on the left defines symbols for "Name" (orange square), "Type" (grey square), and "(minOccurs, maxOccurs)" (orange text). A "Composer" sidebar on the left lists "Select Template" and "Compose Template". A "Legend" section on the left explains the symbols. A "Compose Template" section on the right contains instructions and download/save buttons. A "XML Data Saved" modal dialog is centered, stating "Saved to repository successfully." with an "Ok" button, which is also circled in red.

8: Click on “Data Curation” and set “TEM note” as the current template

The screenshot shows a web browser window for the "Materials Data Curation System" at the URL 127.0.0.1:8000/curate/. The page has a dark header with the system name and a "Logout | My Profile | Help" link. Below the header is a navigation bar with "Home", "Data Curation" (which is circled in red), "Data Exploration", and "Composer". A sub-navigation bar below the main menu includes "Select Template", "Enter Data", and "View Data". On the left, there's a sidebar titled "Data Curation" with three items: "Select Template" (circled in orange), "Enter Data", and "View Data". The main content area is titled "Select Template" and contains instructions about selecting a template from a table. It shows two sections: "Global Templates" and "User Defined Templates". In the "Global Templates" section, there's one entry: "Template name: TEM-Tutorial", "File name: workshop-TEM.xsd", and an "Actions" button labeled "Set as current template". In the "User Defined Templates" section, there's one entry: "Template name: TEM note", and an "Actions" button labeled "Set as current template" which is also circled in red. At the bottom of the page, there's a footer with links to "Home", "Data Curation", "Data Exploration", "Composer", "Contact", "Top ^", and copyright information: "© 2012 - 2016 Materials Data Curation System | Privacy Policy | Terms of Use | Administration".

9: Select “Create a new document”. Enter “test-interface” and click “Start”. Verify “note” element was added to the template.

The screenshot shows a web browser window for the "Materials Data Curation System" at the URL 127.0.0.1:8000/curate/enter-data. The page has a dark header with the system name and a "Logout | My Profile | Help" link. Below the header is a navigation bar with "Home", "Data Curation", "Data Exploration", and "Composer". Under "Data Curation", there are three options: "Select Template", "Enter Data" (which is highlighted in orange), and "View Data". The main content area is titled "Data Entry". It contains a list of required fields: "measurement", "core", "material", "technique", and "note". The "note" field is circled in red. Below the list are two input fields: "title" with the value "Surface Preparation" and "text" with the value "Grind with 600 grit sandpaper, rot". At the bottom right of the form are buttons for "Clear Fields", "Save Form", and "Download". The footer includes links for "Home", "Data Curation", "Data Exploration", "Composer", "Contact", "Top ^", and copyright information: "© 2012 - 2016 Materials Data Curation System | Privacy Policy | Terms of Use | Administration". It also mentions "Website template by Arcsin".