

Composer: Simple DiffusionDemo

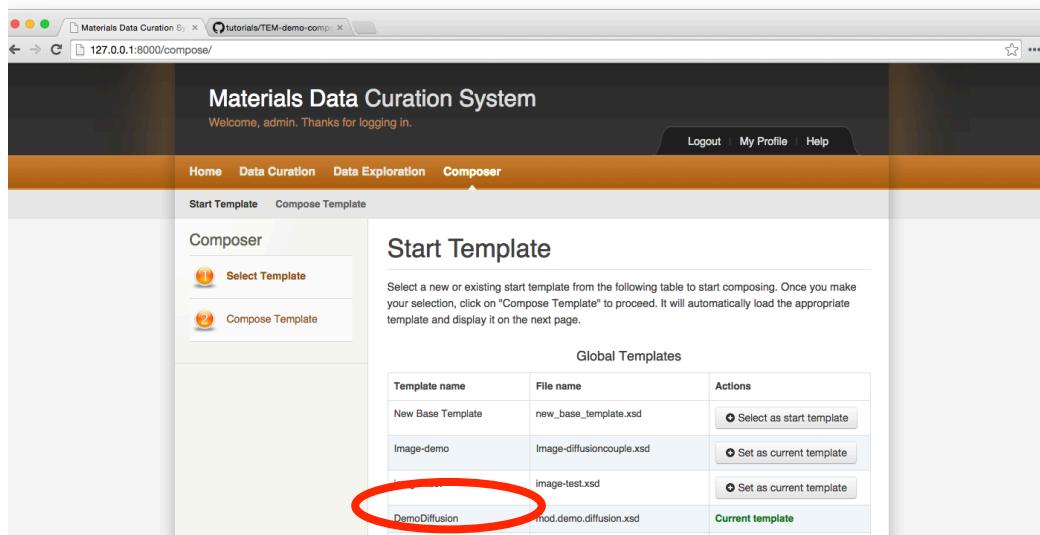
Change an “instance”

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 ». Below the main content is a footer with links for Home, Data Curation, Data Exploration, Composer (highlighted in blue), 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".

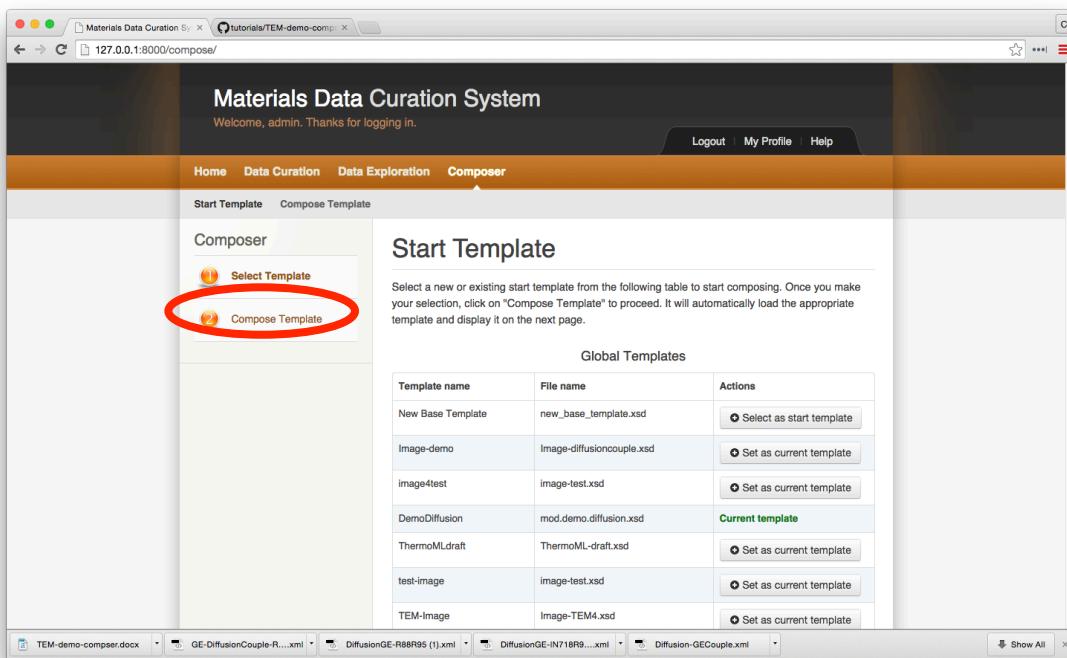
2: Select “DiffusionDemo” Template as the current template



The screenshot shows the 'Materials Data Curation System' interface. The top navigation bar includes 'Home', 'Data Curation', 'Data Exploration', and 'Composer'. Below this, a secondary menu has 'Start Template' and 'Compose Template' options. The main content area is titled 'Start Template' and contains a table of 'Global Templates'. One row, 'DemoDiffusion', is highlighted with a green background and labeled 'Current template'. A red circle surrounds the 'Compose Template' link in the sidebar.

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



This screenshot is identical to the one above, showing the 'Materials Data Curation System' interface with the 'Composer' tab selected. The left sidebar has 'Select Template' and 'Compose Template' links, with 'Compose Template' circled in red. The main content area displays the 'Start Template' page and the 'Global Templates' table, where 'DemoDiffusion' is marked as 'Current template'.

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

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

1 Select Template

2 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.

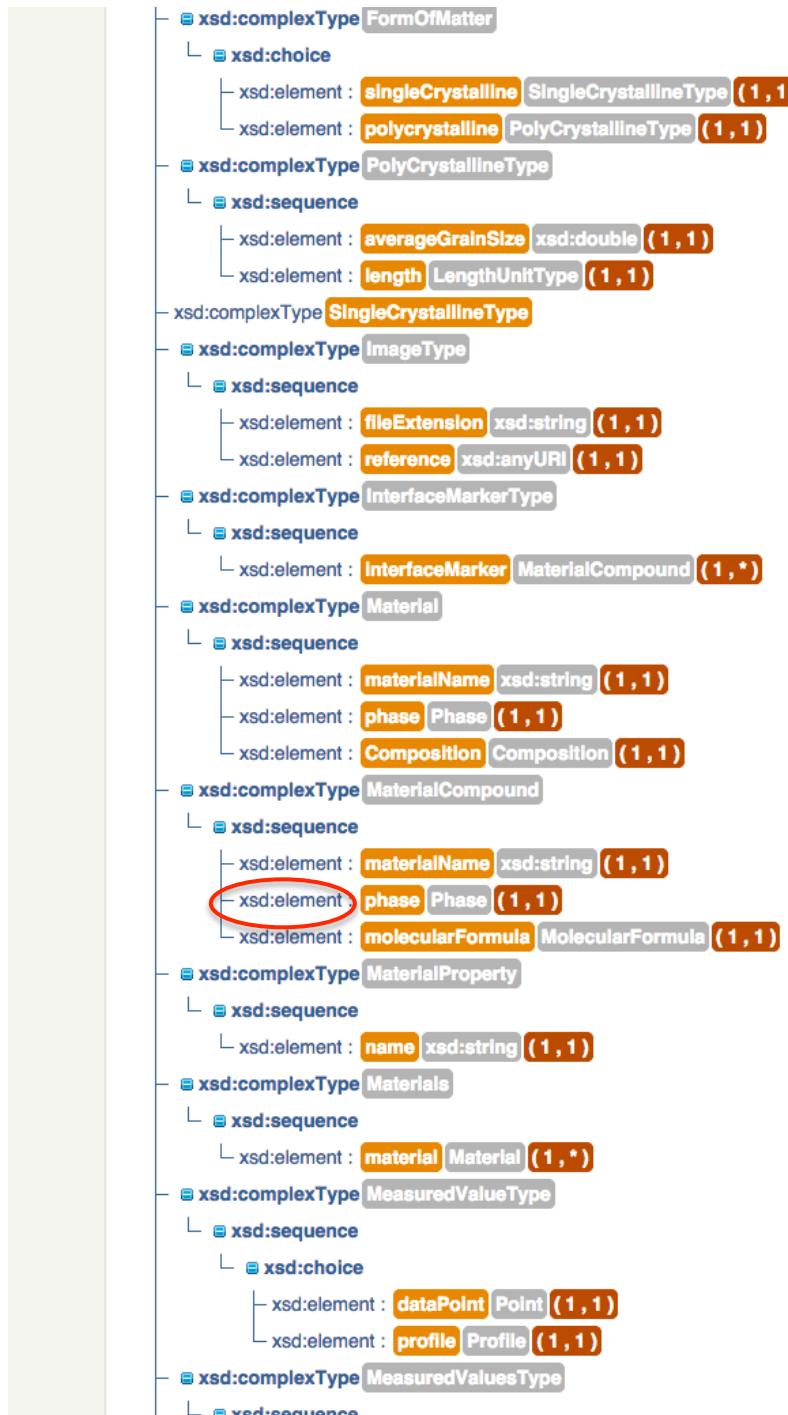
Download **Save as Template** **Save as Type**

```

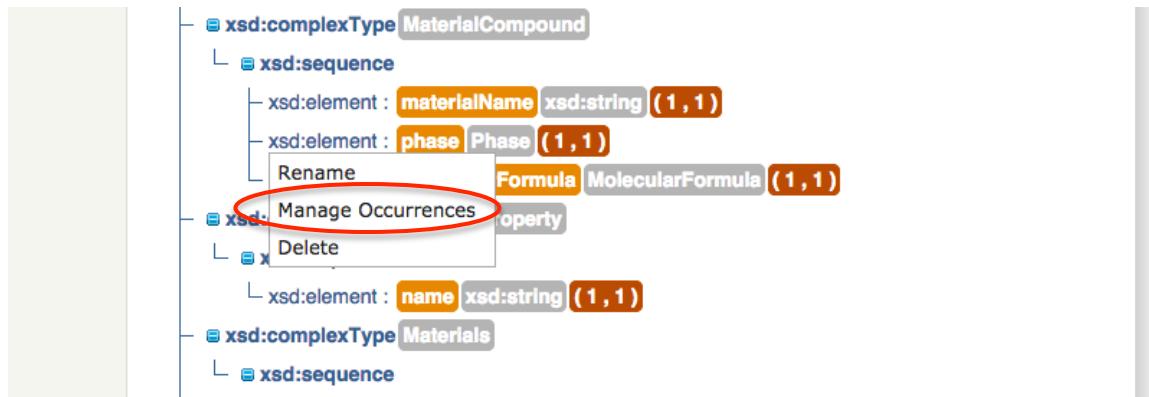
xsd:schema
└ xsd:element : experiment Experiment (1,1)
  └ xsd:complexType CatalogNumber
    └ xsd:sequence
      └ xsd:element : id xsd:string (1,1)
      └ xsd:element : catalogTitle CatalogTitle (1,1)
  └ xsd:complexType CatalogTitle
    └ xsd:sequence
      └ xsd:element : name xsd:string (1,1)
  └ 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

```

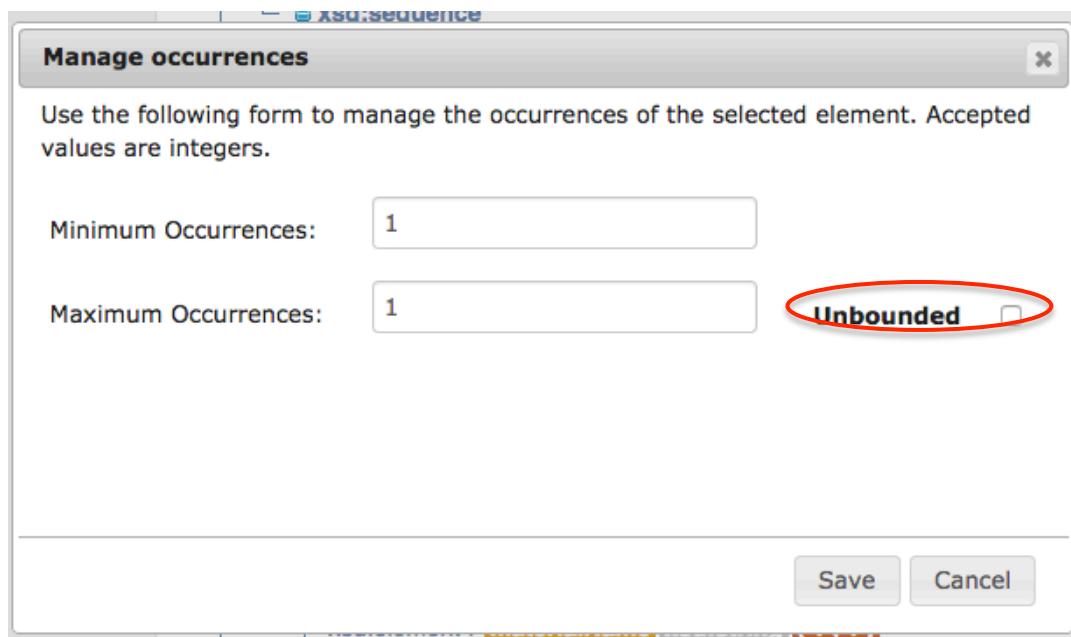
4. Scroll a little more than half way down the schema and find the “element” labelled “phase” and click on the element.

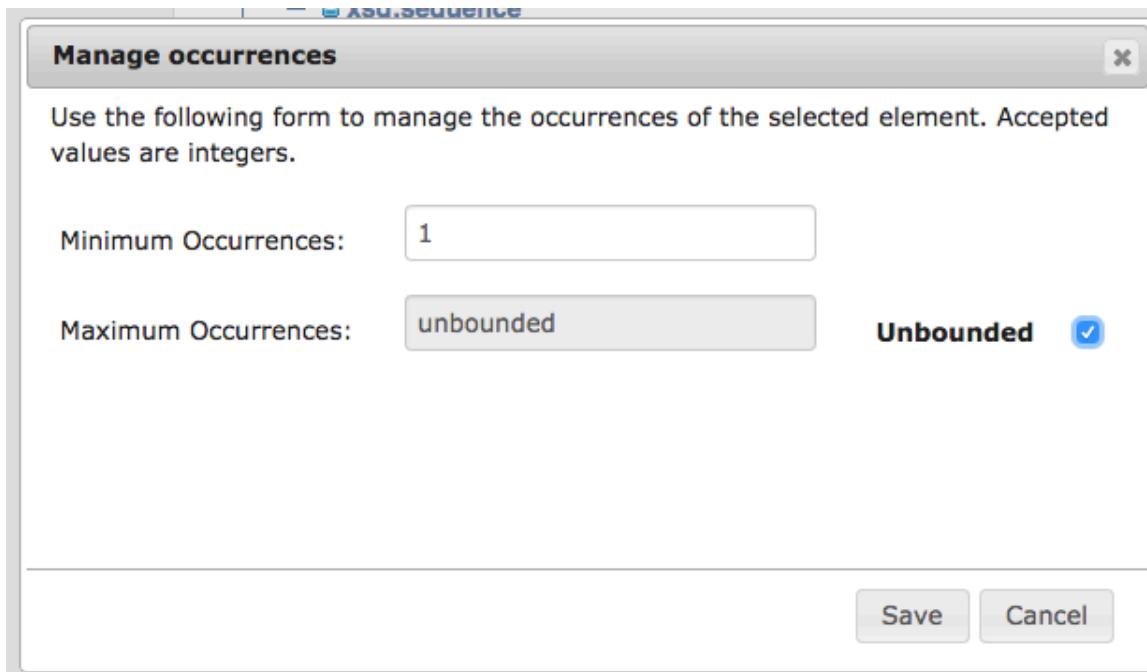


After clicking on “element” a box will appear with 3 choices: Rename, Manage Occurrences, and Delete. Select “Manage Occurrences”

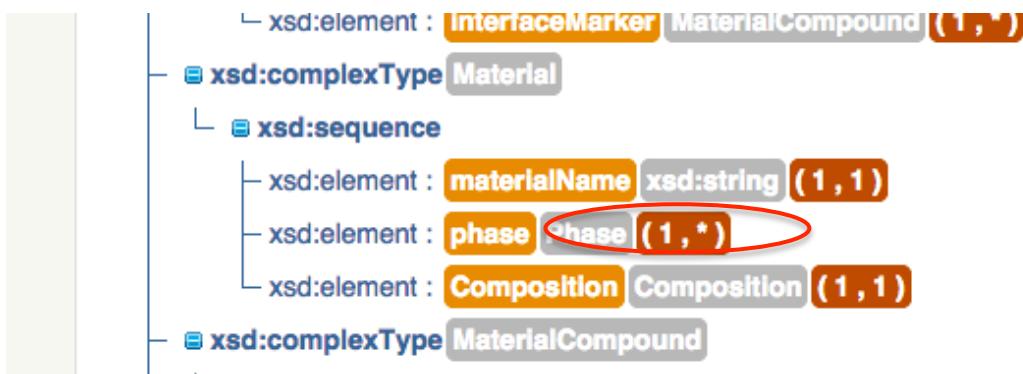


A new pop-up window will appear where you can change the number of occurrences that “phase” is allowed. Change it to “Unbounded” and click “Save”.





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'. To the right is a hierarchical tree view of an XML schema:

```
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
```

This screenshot shows the same interface after a template has been composed. 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 'ChemicalElement' node expanded, listing its enumerations: 'Ag', 'Al', 'Am', and 'Ar'. The 'Save' and 'Cancel' buttons are at the bottom of the dialog.

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" value="Set as current template"/>
image4a	<input type="button" value="Set as current template"/>
test2	<input type="button" value="Set as current template"/>
DemoDiffusion-cec	<input type="button" value="Set as current template"/>
Diffusion-cec-phase	<input type="button" value="Set as current template"/>
DiffusionDemo-2	<input type="button" value="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

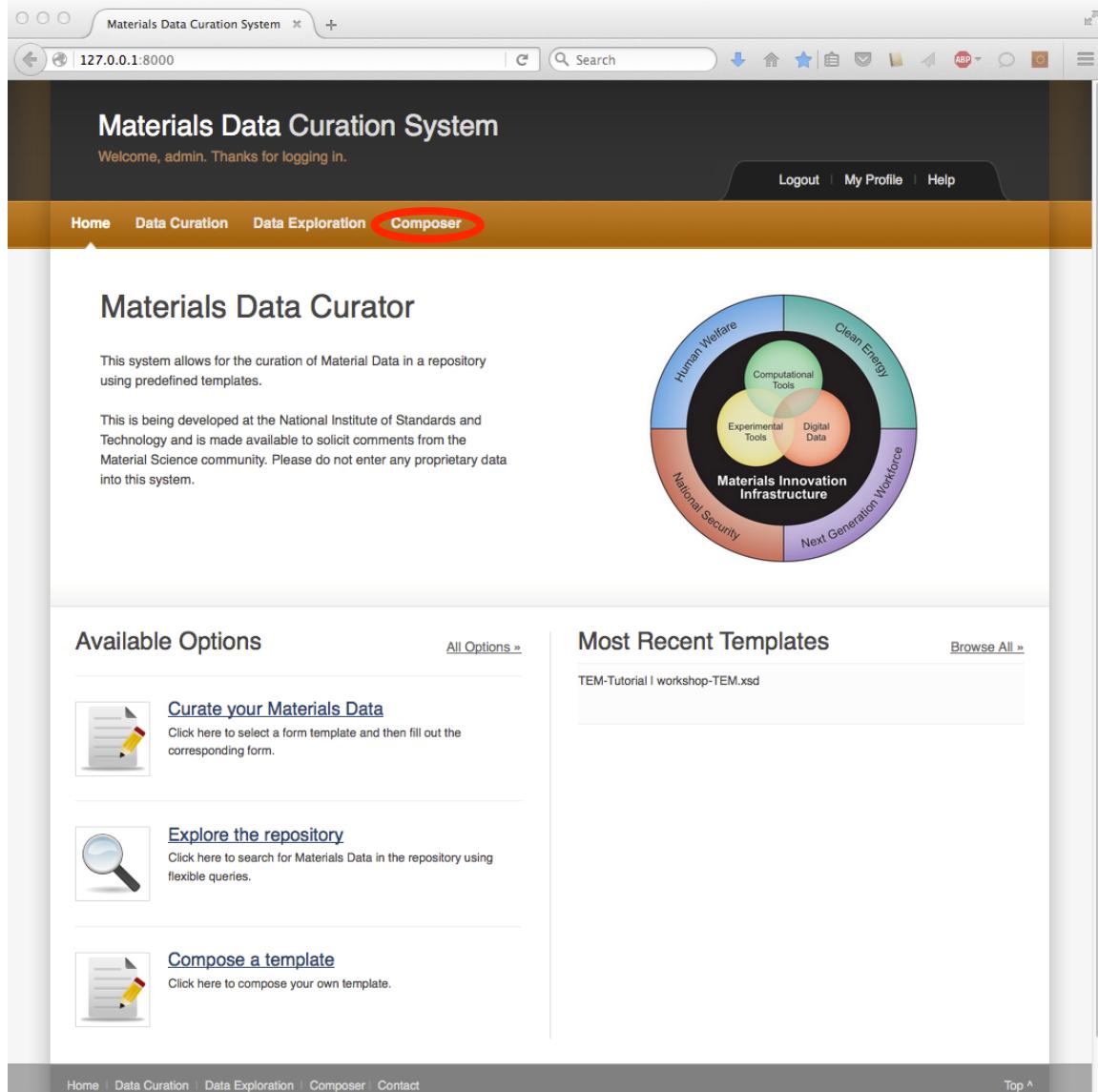
Element	Quantity	Purity	Error
Ni	58.1	0.999	0.001

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 welcome message "Welcome, admin. Thanks for logging in." is displayed. The top navigation bar includes links for "Logout", "My Profile", and "Help". Below the navigation, a secondary menu bar has tabs: "Home", "Data Curation", "Data Exploration", and "Composer", with "Composer" circled in red. The main content area is titled "Materials Data Curator". It contains a brief description of the system's purpose, a note about its development at NIST, and a circular diagram illustrating the "Materials Innovation Infrastructure". The diagram is divided into four quadrants: "Human Welfare" (top-left), "Clean Energy" (top-right), "National Security" (bottom-left), and "Next Generation Workforce" (bottom-right). The center of the circle is labeled "Computational Tools", "Experimental Tools", and "Digital Data". The entire circle is labeled "Materials Innovation Infrastructure". Below the diagram, there are 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 shows a single item: "TEM-Tutorial I workshop-TEM.xsd" with a link to "Browse All". At the bottom of the page, there is a footer with links for "Home", "Data Curation", "Data Exploration", "Composer", and "Contact".

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:

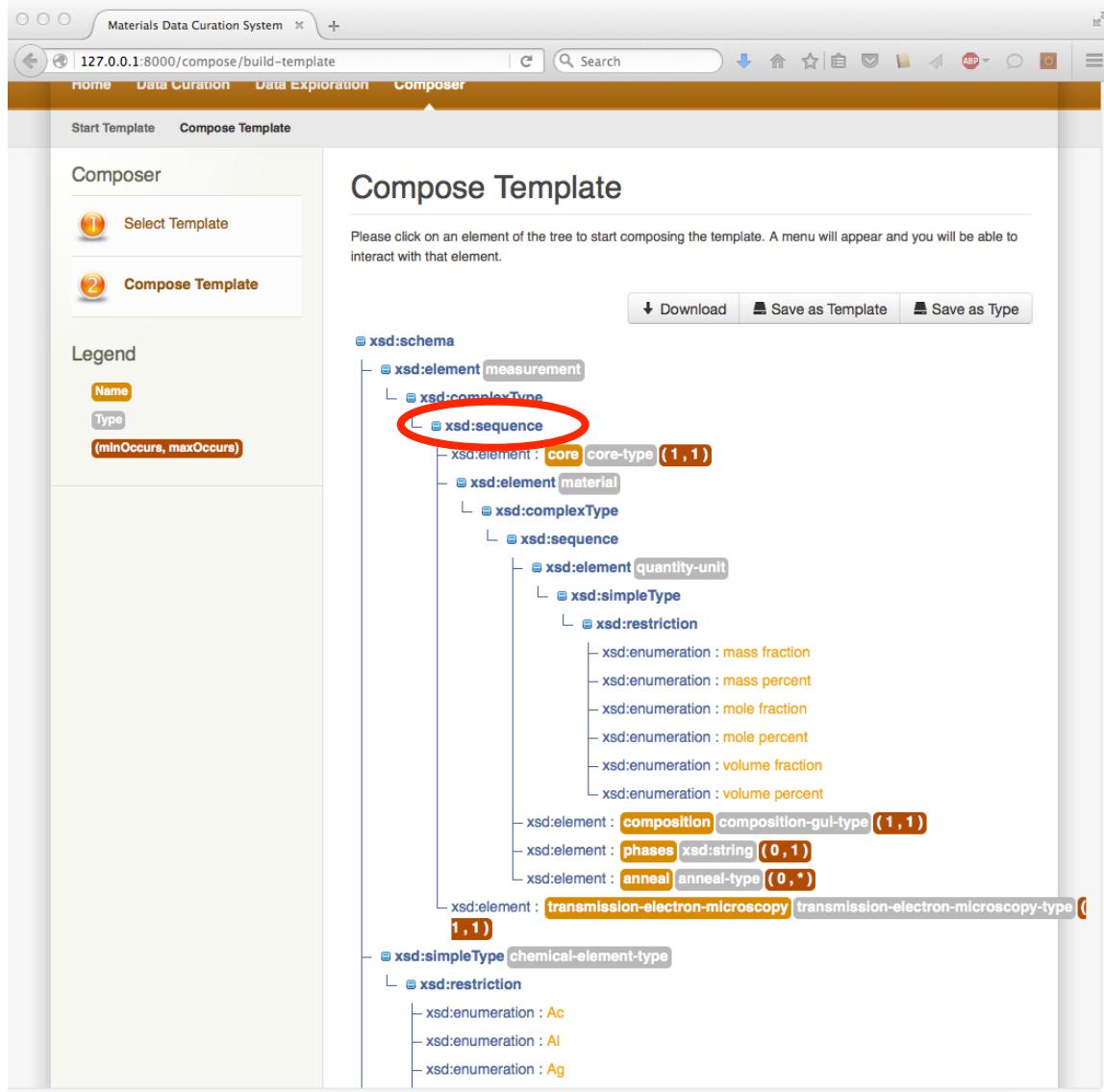
Template name	File name	Actions
New Base Template	new_base_template.xsd	<input checked="" type="radio"/> Select as start template
TEM-Tutorial	workshop-TEM.xsd	<input type="radio"/> Set as current template

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 footer includes links for Home, Data Curation, Data Exploration, Composer, Contact, Privacy Policy, Terms of Use, Administration, and a note: "Website template 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 also shows "(minOccurs, maxOccurs)".

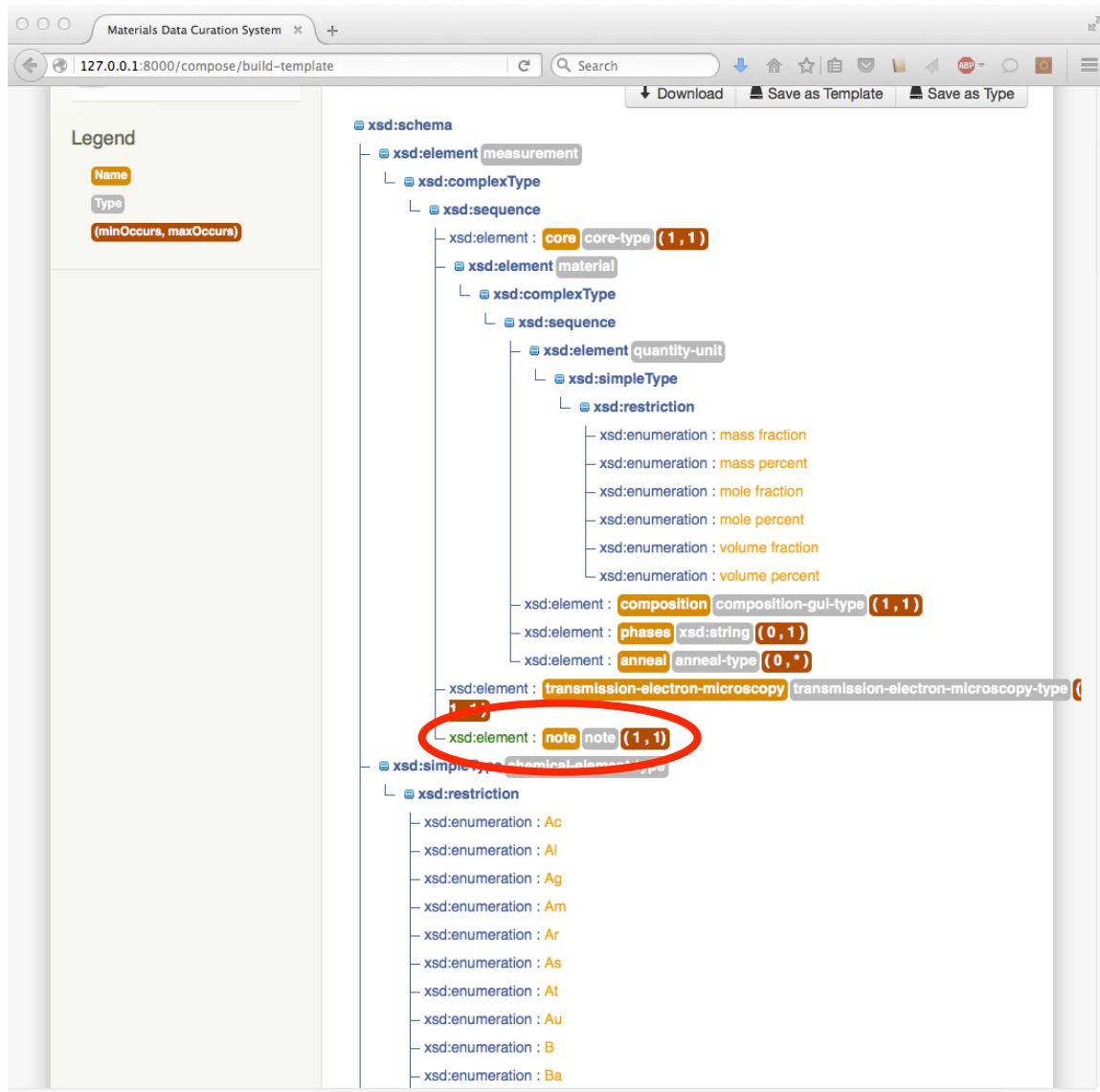
A modal dialog titled "Insert an Element" is open, prompting the user to select the type of element to insert. It lists "xsd:schema" and "xsd:element measurement". Under "xsd:element measurement", there is a section titled "No Buckets" containing a table with one row:

note	note.xsd	<input type="button" value="Insert"/>
------	----------	---------------------------------------

Below the table is a link "My Types". At the bottom right of the modal is a "Cancel" button.

In the background, the tree view shows various XSD elements and their types, such as "composition", "composition-gui-type", "phases", "volume percent", "anneal", "transmission-electron-microscopy", "chemical-element-type", "Ac", "Al", and "Ag".

5: Notice new 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 '127.0.0.1:8000/compose/build-template'. The top navigation bar includes 'Logout', 'My Profile', and 'Help'. Below the navigation is a toolbar with 'Home', 'Data Curation', 'Data Exploration', and 'Composer'. The main area is titled 'Compose Template' with a 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' and 'Compose Template' buttons, and a 'Legend' section showing icons for 'Name', 'Type', and '(minOccurs, maxOccurs)'. The central content area displays an XML schema tree under the 'xsd:schema' node. The tree structure is as follows:

```
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 composition composition-gui-type (1,1)
              - xsd:element phase xsd:string (0,*) 
              - xsd:element anneal anneal-type (0,*) 
        - xsd:element transmission-electron-microscopy transmission-electron-microscopy-type (1,1)
```

At the top right of the main area, there are three buttons: 'Download', 'Save as Template' (which is highlighted with a red oval), and 'Save as Type'. The 'Save as Template' button is located at approximately [340, 540, 360, 780].

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 highlighted with a red circle. Below the navigation is a toolbar with 'Start Template' and 'Compose Template'. The main area is titled 'Compose Template' and contains a legend for 'Name' and 'Type' with '(minOccurs, maxOccurs)' information. A tree view shows an 'xsd:schema' structure with nodes like 'measurement', 'core', 'material', 'composition', 'phases', 'anneal', 'transmission-electron-microscopy', and 'note'. A modal dialog box titled 'XML Data Saved' is displayed, stating 'Saved to repository successfully.' and has 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 the Materials Data Curation System interface. At the top, there is a navigation bar with links for Home, Data Curation, Data Exploration, and Composer. The 'Data Curation' link is highlighted with a red circle. Below the navigation bar, there is a sub-navigation menu for 'Data Curation' with three items: 'Select Template' (highlighted with a red circle), 'Enter Data', and 'View Data'. The main content area is titled 'Select Template'. It contains two sections: 'Global Templates' and 'User Defined Templates'. In the 'Global Templates' section, there is 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 is 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 is a footer with links for Home, Data Curation, Data Exploration, Composer, Contact, and a 'Top ^' link. The footer also includes copyright information: '© 2012 - 2016 Materials Data Curation System | Privacy Policy | Terms of Use | Administration' and 'Website template by Arcsin'.

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

The screenshot shows the Materials Data Curation System interface. The top navigation bar includes links for Home, Data Curation, Data Exploration, Composer, Logout, My Profile, and Help. Below the navigation is a sub-menu with Select Template, Enter Data, and View Data. The main content area is titled "Data Entry". It contains a list of required fields: measurement, core, material, technique (electron-microscopy), and note. The "note" field is highlighted with a red oval. The "title" field contains "Surface Preparation" and the "text" field contains "Grind with 600 grit sandpaper, rot". At the bottom right of the entry form are buttons for Clear Fields, Save Form, and Download. The footer includes links for Home, Data Curation, Data Exploration, Composer, Contact, Top, and Administration, along with copyright information (© 2012 - 2016) and a note about the website template (Website template by Arcsin).