

Data Exploration: Simple Diffusion Tutorial

Upload past student data

To synthesize student usage in the past, execute the IPython (Jupyter) Notebook “-Tutorial-Setup”:

The screenshot shows a Jupyter Notebook interface with the title "IP[y]: Notebook diffusion-Tutorial-Setup". The notebook contains the following code:

```
Populate local MDCS instance with student data and metadata

Import MDCS API tool module
In [1]: import mdcs

Host and user information
In [2]: user='admin'
        pswd='admin'
        host='http://127.0.0.1:8000'
        template_name='DemoDiffusion'

List of file prefixes for micrograph images and XML metadata
In [3]: name_list=[

        "GE-DiffusionCouple-IN100-IN718",
        "GE-DiffusionCouple-IN718-R95",
        "GE-DiffusionCouple-R95-R88"
    ]

For each name in the list:


- Upload micrograph
- Read XML metadata
- Replace generic URL with unique URL for micrograph
- Upload XML metadata record


In [4]: for name in name_list:
    xml_name=name+".xml"
    tif_name=name+".tif"

    print "Uploading:",tif_name
    url = mdcs.blob.upload(tif_name,host,user,pswd)

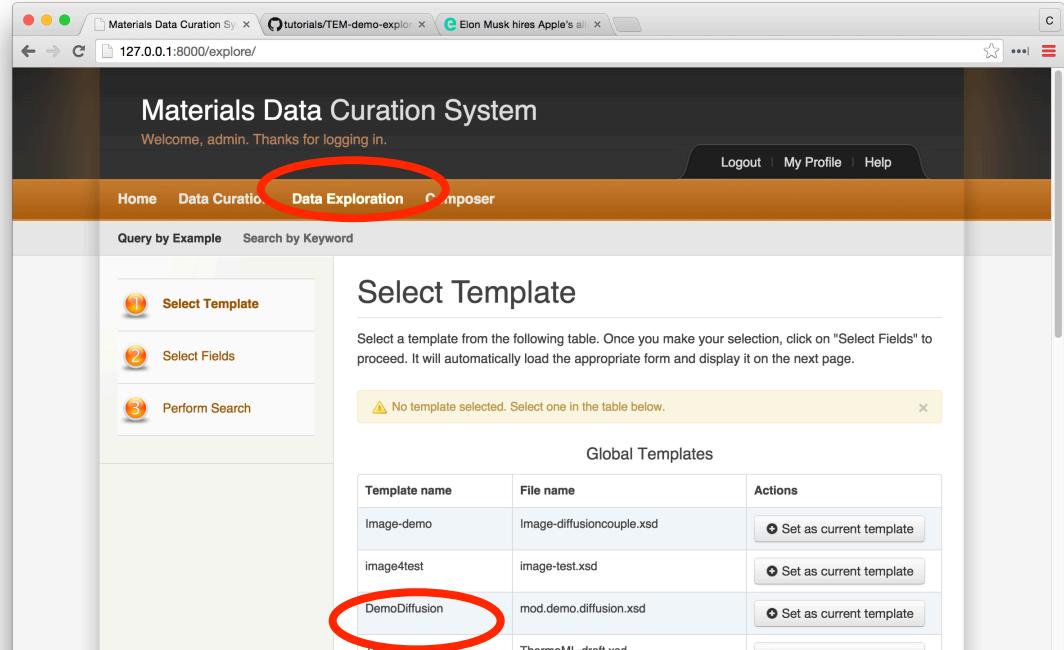
    print "Reading:",xml_name
    with open(xml_name, 'r') as f:
        content = f.read()
    content = content.replace("http://127.0.0.1:8000/rest/blob?id=REPLACE-ME-BLOB-ID",url)

    print "Uploading:",xml_name
    response = mdcs.curate_as(xml_name,name,host,user,pswd,template_title=template_name,content=content)
    print "Response:",response

Uploading: GE-DiffusionCouple-IN100-IN718.tif
Reading: GE-DiffusionCouple-IN100-IN718.xml
Uploading: GE-DiffusionCouple-IN100-IN718.xml
Response: 201
Uploading: GE-DiffusionCouple-IN718-R95.tif
Reading: GE-DiffusionCouple-IN718-R95.xml
Uploading: GE-DiffusionCouple-IN718-R95.xml
Response: 201
Uploading: GE-DiffusionCouple-R95-R88.tif
Reading: GE-DiffusionCouple-R95-R88.xml
Uploading: GE-DiffusionCouple-R95-R88.xml
Response: 201
```

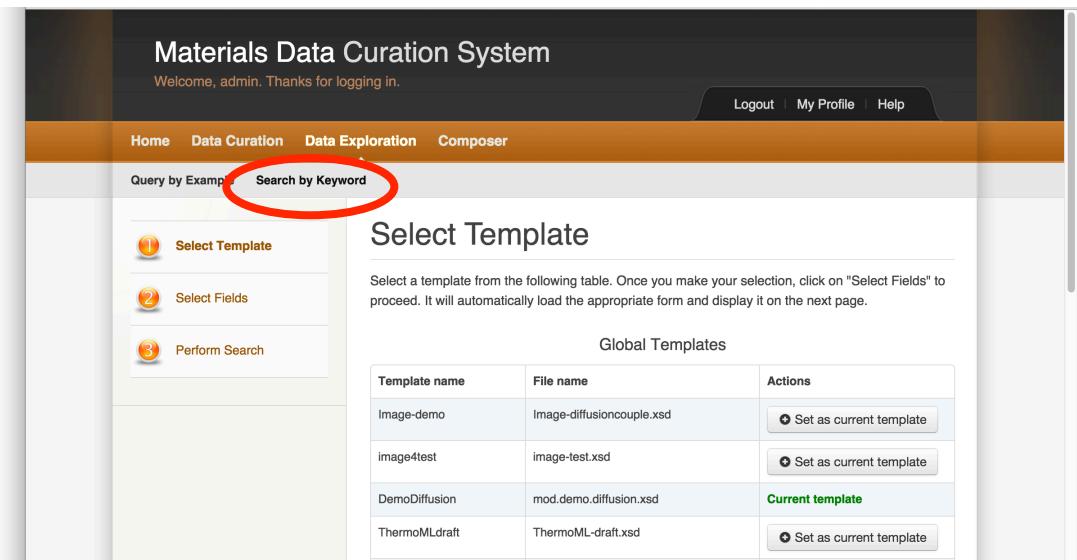
Explore Student Diffusion Data by Alloy Name

1: From the MDCS homepage, click on “Data Exploration” then click on “Search by Keyword”:



The screenshot shows the Materials Data Curation System homepage. At the top, there is a navigation bar with links for Home, Data Curation, Data Exploration (which is highlighted with a red circle), and Composer. Below the navigation bar, there are two search options: "Query by Example" and "Search by Keyword". The main content area is titled "Select Template". It contains a table titled "Global Templates" with columns for "Template name", "File name", and "Actions". The table lists several templates, including "Image-demo", "image4test", "DemoDiffusion" (which is circled in red), and "ThermoML-draft". A message at the top of the template selection area says: "Select a template from the following table. Once you make your selection, click on "Select Fields" to proceed. It will automatically load the appropriate form and display it on the next page." A yellow warning message below the table says: "No template selected. Select one in the table below."

Template name	File name	Actions
Image-demo	Image-diffusioncouple.xsd	<input type="radio"/> Set as current template
image4test	image-test.xsd	<input type="radio"/> Set as current template
DemoDiffusion	mod.demo.diffusion.xsd	<input type="radio"/> Set as current template
ThermoML-draft	ThermoML-draft.xsd	<input type="radio"/> Set as current template



This screenshot is identical to the previous one, showing the Materials Data Curation System homepage. However, the "Search by Keyword" link in the navigation bar is now circled in red. The rest of the interface, including the template selection table and messages, remains the same.

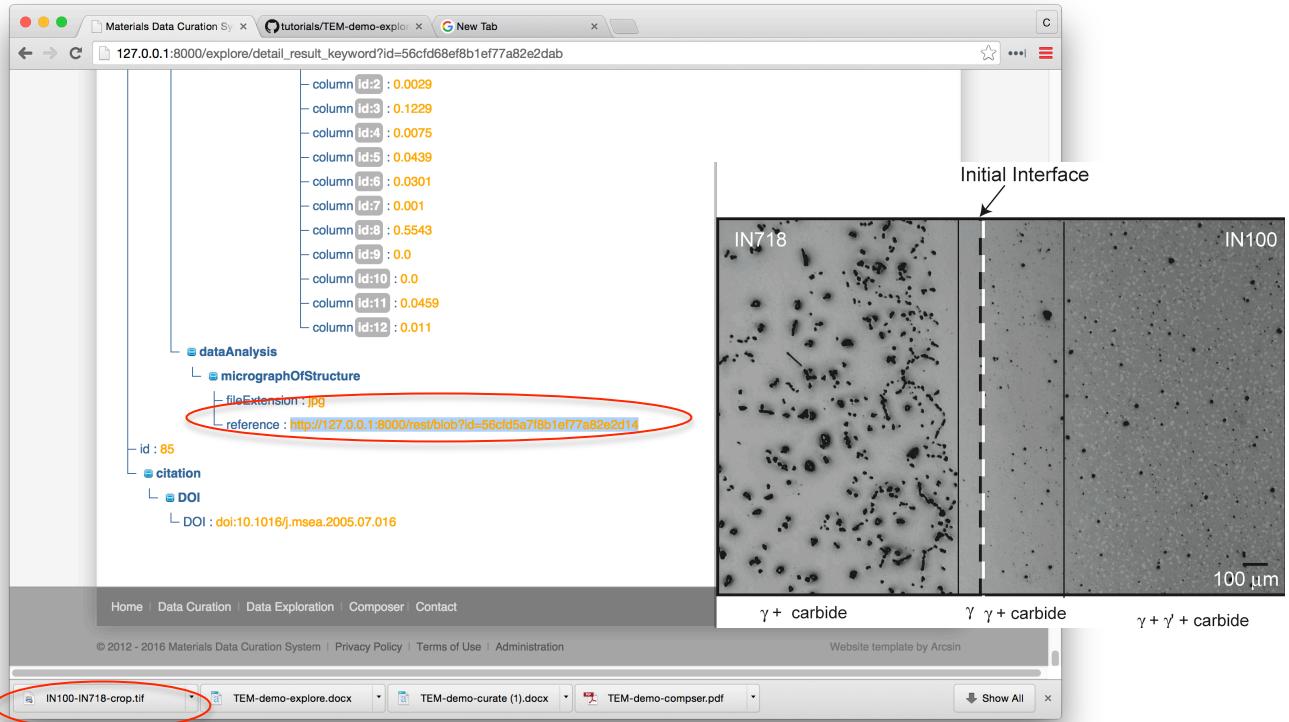
2: Search for all records containing the “IN100” alloy

The screenshot shows the Materials Data Curation System interface. The top navigation bar includes links for Home, Data Curation, Data Exploration, and Composer, along with Logout, My Profile, and Help. Below the navigation is a search bar with options for "Query by Example" and "Search by Keyword". The main content area is titled "Search by keyword" and contains a search input field with the text "IN100". An "Export" button is located to the right of the search field. Below the search field, it says "2 results" and lists two items: "DiffusionGE-IN718R95.xml" and "GE-DiffusionCouple-IN100IN718.xml".

Select “GE-DiffusionCouple-IN100IN718” to expand the view.

The screenshot shows the expanded view of the "GE-DiffusionCouple-IN100IN718.xml" record. The title "GE-DiffusionCouple-IN100IN718.xml" is at the top. On the right, there is a "Back to Results" button. The left side features a hierarchical tree view of the XML structure. The tree starts with "experiment", which has children "experimentType", "chemicalDiffusivity", and "material". The "material" node has a child "materialName" with the value "IN100". It also has a "phase" node, which has a "name" child with the value "FCC". The "phase" node also has a "crystalStructure" child, which in turn has a "Composition" child. The "Composition" child has a "quantityUnit" child with the value "mass percent".

Scroll down to the bottom of the screen to find the link to the attached micrograph. In a new browser tab, enter the link and the micrograph will download.



Now if one wants to export the composition profiles, return the “Results”. Scroll back to the top of the page.

The screenshot shows the 'Materials Data Curation System' homepage with the title 'GE-DiffusionCouple-IN100IN718.xml'. A red oval highlights the 'Back to Results' button in the top right corner of the main content area. The sidebar on the left shows a detailed hierarchical tree structure of experimental data, including 'experiment', 'experimentType', 'chemicalDiffusivity', 'material', 'phase', 'Composition', and 'quantityUnit'. The 'material' node is expanded to show 'materialName : IN100' and 'phase' node 'name : FCC'.

Select both data sets to export and click on “Export”

The screenshot shows the Materials Data Curation System interface. In the search bar, 'IN100' has been entered. Below the search bar, there are two results listed:

- [DiffusionGE-IN718R95.xml](#) DemoDiffusion
- [GE-DiffusionCouple-IN100IN718.xml](#) DemoDiffusion

A red circle highlights the 'Export' button located at the bottom right of the search results area.

Chose to export the files as a “CSV” files.

The screenshot shows the Materials Data Curation System interface with the 'Export' dialog box open. The dialog box asks to choose an export format, with 'CSV' selected. Below the dialog box, the search results for 'IN100' are shown again, and a red circle highlights the 'Export' button at the bottom right of the results area.

The files will then download and appear in folder labelled CSV.

The screenshot shows a Mac OS X Finder window titled 'CSV 3'. Inside the window, there are two files listed:

- DiffusionGE-IN718R95.csv
- GE-DiffusionCouple-IN100IN718.csv

Both files were modified today at 9:52 PM.

Below the Finder window, a portion of a Microsoft Excel spreadsheet is visible, showing data for the 'GE-DiffusionCouple-IN100IN718' file. The data includes columns for Distance, C, Fe, Cr, V, Ti, Mo, Ni, W, Ta, Al, and C fractions.