

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)

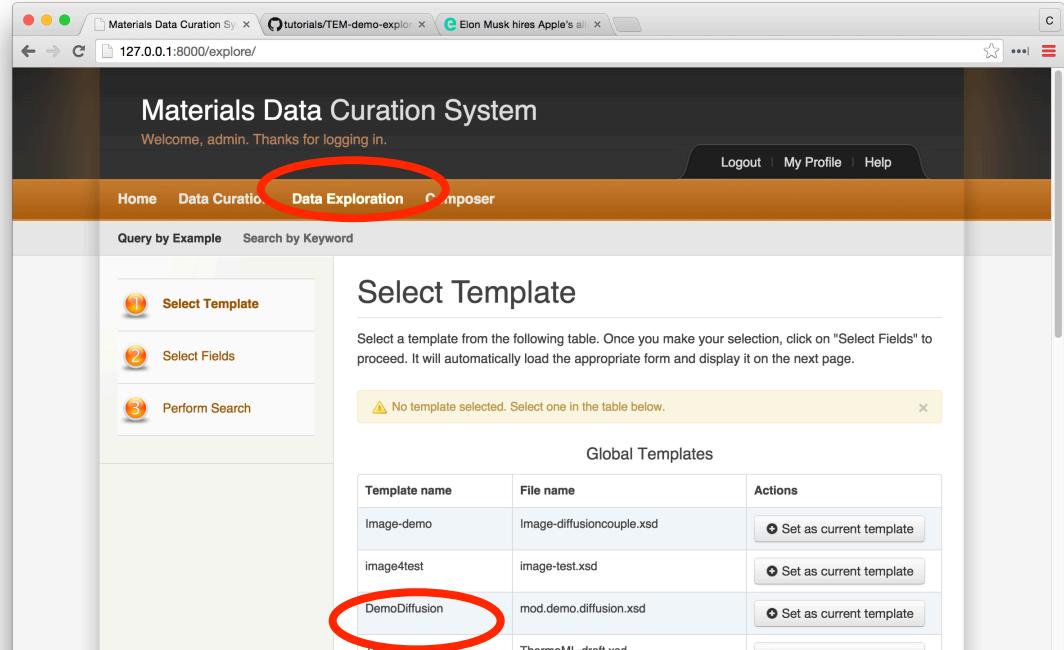
    print "Reading:",xml_name
    with open(xml_name, 'r') as f:
        content = f.read()
    content = content.replace("http://127.0.0.1:8000/rest/blob?id=REPLACE-ME-BLOB-ID",url)

    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
```

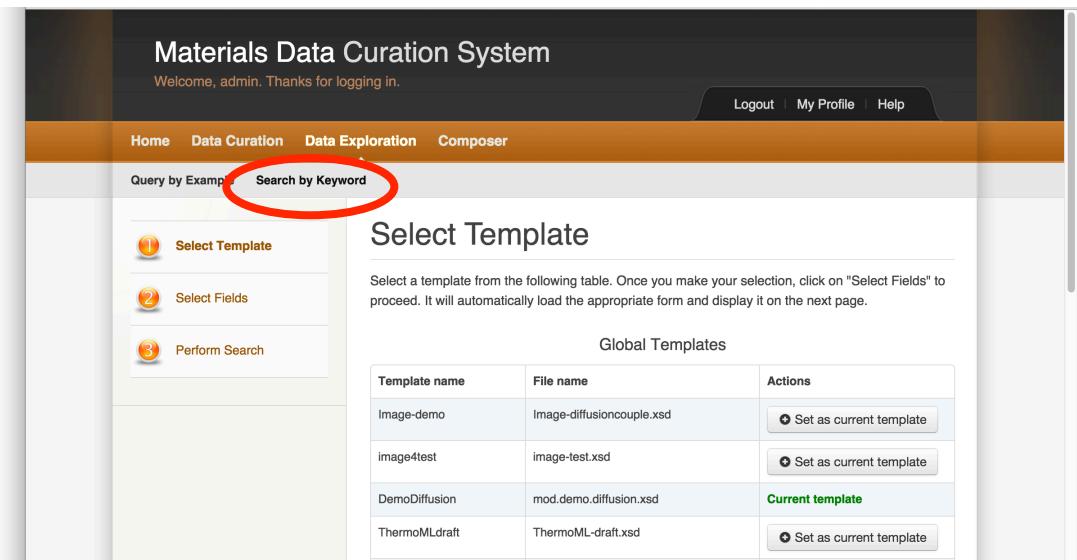
Explore Student Diffusion Data by Alloy Name

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



The screenshot shows the Materials Data Curation System homepage. The navigation bar at the top has 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 of "Global Templates" with columns for "Template name", "File name", and "Actions". A message at the top right says "No template selected. Select one in the table below." The table data is as follows:

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 similar 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 is identical to the first screenshot, including the "Select Template" page with its table of global templates.

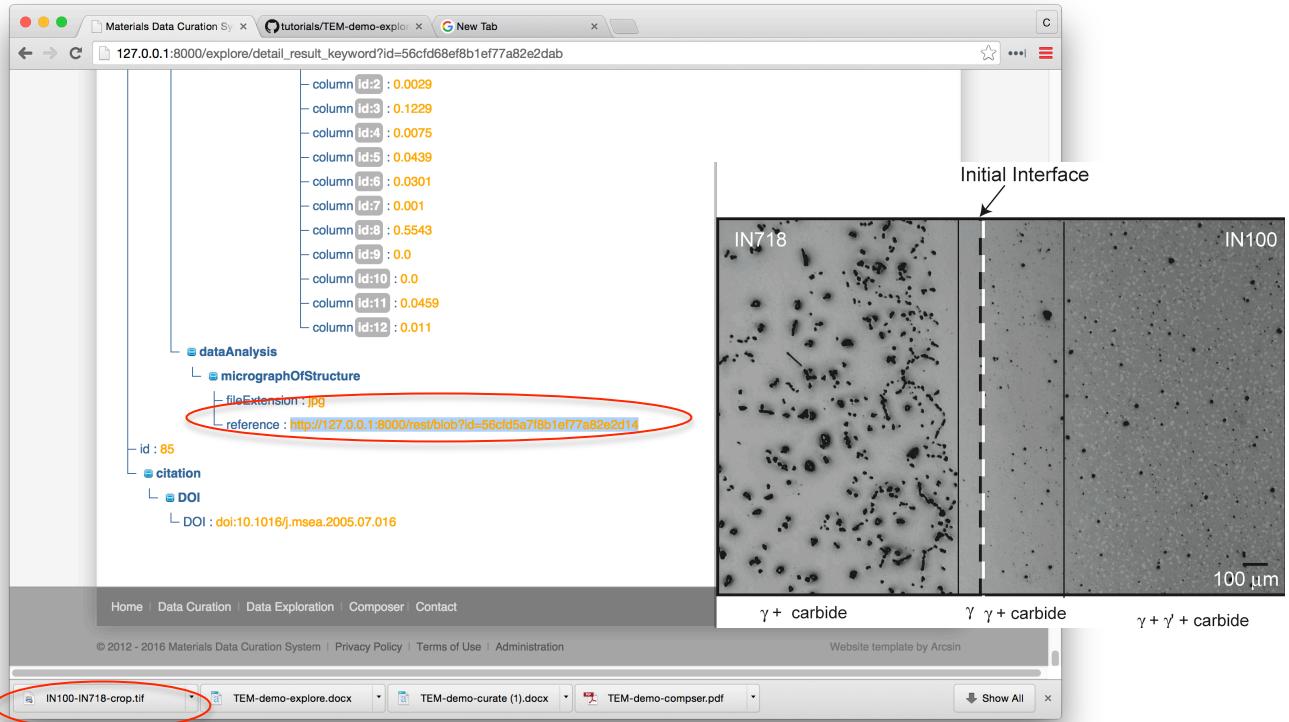
2: Search for all records containing the “IN100” alloy

The screenshot shows the Materials Data Curation System interface. The top navigation bar includes links for Home, Data Curation, Data Exploration, Composer, Logout, My Profile, and Help. Below the navigation is a search bar with the placeholder "Search by Keyword". A user has entered "IN100" into the search field. To the right of the search bar is an "Export" button. On the left, there is a sidebar titled "Refine by Template" which lists various global templates with checkboxes, some of which are checked (e.g., DemoDiffusion, TEM-Image-ZT). The main search results area displays "2 results" for "IN100". The first result is "DiffusionGE-IN718R95.xml" and the second is "GE-DiffusionCouple-IN100IN718.xml". Both results are associated with the "DemoDiffusion" template.

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

The screenshot shows the expanded view of the XML record "GE-DiffusionCouple-IN100IN718.xml". The page title is "GE-DiffusionCouple-IN100IN718.xml". At the top right is a "Back to Results" button. The main content area displays a hierarchical tree structure of the XML data. The root node is "experiment", which contains "experimentType", "chemicalDiffusivity", and "material". The "material" node has a child node "materialName" with the value "IN100". It also contains a "phase" node, which has a "name" node with the value "FCC" and a "crystalStructure" node. The "crystalStructure" node has a child node "Composition", which has a "quantityUnit" node 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.

Materials Data Curation System

Welcome, admin. Thanks for logging in.

Logout | My Profile | Help

Home Data Curation Data Exploration Composer

Query by Example Search by Keyword

GE-DiffusionCouple-IN100IN718.xml

experiment

- experimentType**
- chemicalDiffusivity**
- material**
- phase**
- Composition**

materialName : IN100
name : FCC
crystalStructure :
quantityUnit : mass percent

Back to Results

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

Materials Data Curation System

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Home Data Curation Data Exploration Composer

Query by Example Search by Keyword

Refine by Template

Global Templates

- DemoDiffusion
- TEM-Image
- Interdiffusion
- ThermoMLdraft
- Interdiffusion3-2
- Image-demo
- test-image
- image2-test
- image3
- image4-test
- TEM-Image-ZT

Search by keyword

IN100

Export

2 results

- DiffusionGE-IN718R95.xml DemoDiffusion
- GE-DiffusionCouple-IN100IN718.xml DemoDiffusion

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

Materials Data Curation System

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Home Data Curation Data Exploration Composer

Query by Example Search by Keyword

Refine by Template

Global Templates

- DemoDiffusion
- TEM-Image
- Interdiffusion
- ThermoMLdraft
- Interdiffusion3-2
- Image-demo
- test-image
- image2-test
- image3
- image4-test
- TEM-Image-ZT

Search by keyword

Export

Please Choose one of the following export format:

- CSV
- JSON
- XML

2 results

Export

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

CSV 3

CSV 3

Name	Date Modified
DiffusionGE-IN718R95.csv	Today, 9:52 PM
GE-DiffusionCouple-IN100IN718.csv	Today, 9:52 PM

CSV 3

Distance, Cr, Fe, Ni, V, Ti, Mo, G, H, I, W, Ta, Al, C, Fraction

1, 0, 0.0113, 0.3845, 0.1899, 0, 0.0094, 0.0006, 0.0406, 0.54, 0, 0, 0.0042, 0.0055
2, 25, 0.0114, 0.1811, 0.1834, 0, 0.0092, 0.0003, 0.0406, 0.541, 0, 0, 0.0044, 0.0043
3, 50, 0.0112, 0.1812, 0.1841, 0, 0.0093, 0.0005, 0.0406, 0.541, 0, 0, 0.0044, 0.0043
4, 75, 0.0112, 0.1812, 0.1841, 0, 0.0093, 0.0005, 0.0413, 0.5411, 0, 0, 0.0044, 0.0043
5, 100, 0.0096, 0.1824, 0.1828, 0.0002, 0.0093, 0.0006, 0.0396, 0.542, 0, 0, 0.0046, 0.0085
6, 125, 0.0097, 0.1824, 0.1828, 0.0001, 0.0093, 0.0006, 0.0396, 0.5421, 0, 0, 0.0046, 0.0085
7, 150, 0.0012, 0.1817, 0.1818, 0, 0.0092, 0.0003, 0.0396, 0.5419, 0, 0, 0.0045, 0.0099
8, 100, 0.0114, 0.1827, 0.1835, 0, 0.009, 0.0009, 0.0391, 0.5389, 0, 0, 0.0046, 0.0113
9, 200, 0.0097, 0.1824, 0.1828, 0.0002, 0.0093, 0.0006, 0.0396, 0.541, 0, 0, 0.0046, 0.0085
10, 225, 0.0011, 0.1795, 0.1745, 0, 0.0114, 0.0009, 0.0391, 0.541, 0, 0, 0.0041, 0
11, 250, 0.0011, 0.1821, 0.1847, 0.0005, 0.0092, 0.0007, 0.0396, 0.5409, 0, 0, 0.0041, 0.0078
12, 275, 0.0013, 0.1821, 0.1852, 0, 0.0092, 0.0007, 0.0394, 0.5397, 0, 0, 0.0049, 0.0097
13, 300, 0.0013, 0.1821, 0.1841, 0.0005, 0.0092, 0.0007, 0.0397, 0.5409, 0, 0, 0.0051, 0.0064
14, 325, 0.0013, 0.1821, 0.1841, 0.0005, 0.0092, 0.0007, 0.0397, 0.5409, 0, 0, 0.0051, 0.0064
15, 350, 0.0013, 0.1824, 0.1848, 0.0005, 0.0092, 0.0007, 0.0398, 0.5409, 0, 0, 0.0051, 0.0064
16, 375, 0.0013, 0.1824, 0.1858, 0.0005, 0.0092, 0.0006, 0.0396, 0.5398, 0, 0, 0.0052, 0.0055
17, 400, 0.0013, 0.1824, 0.1858, 0.0005, 0.0092, 0.0006, 0.0396, 0.5398, 0, 0, 0.0052, 0.0055
18, 425, 0.0014, 0.1821, 0.186, 0, 0.0091, 0.0012, 0.0372, 0.5404, 0, 0, 0.0055, 0.007
19, 450, 0.0014, 0.1821, 0.186, 0.0003, 0.0091, 0.0012, 0.0372, 0.5404, 0, 0, 0.0055, 0.007
20, 475, 0.0014, 0.1821, 0.1867, 0.0005, 0.0091, 0.0012, 0.0364, 0.5401, 0, 0, 0.0057, 0.008
21, 500, 0.0015, 0.1814, 0.1868, 0, 0.0095, 0.0007, 0.0364, 0.5391, 0, 0, 0.0059, 0.0061
22, 525, 0.0015, 0.1814, 0.1868, 0, 0.0095, 0.0007, 0.0364, 0.5391, 0, 0, 0.0061, 0.0061
23, 550, 0.0015, 0.1815, 0.1868, 0.0001, 0.0095, 0.0007, 0.0361, 0.5392, 0, 0, 0.0062, 0.0064
24, 575, 0.0016, 0.1826, 0.1868, 0, 0.0097, 0.0015, 0.0364, 0.5392, 0, 0, 0.0067, 0.0071
25, 600, 0.0016, 0.1826, 0.1868, 0, 0.0097, 0.0015, 0.0364, 0.5392, 0, 0, 0.0067, 0.0071
26, 625, 0.0016, 0.1826, 0.1868, 0, 0.0097, 0.0015, 0.0364, 0.5392, 0, 0, 0.0067, 0.0071
27, 650, 0.0016, 0.1826, 0.1868, 0, 0.0097, 0.0015, 0.0364, 0.5392, 0, 0, 0.0067, 0.0071
28, 675, 0.0016, 0.1826, 0.1868, 0, 0.0097, 0.0015, 0.0364, 0.5392, 0, 0, 0.0067, 0.0071
29, 700, 0.0016, 0.1826, 0.1868, 0, 0.0097, 0.0015, 0.0364, 0.5392, 0, 0, 0.0067, 0.0071
30, 725, 0.0017, 0.1826, 0.1868, 0, 0.0097, 0.0015, 0.0364, 0.5392, 0, 0, 0.0067, 0.0071
31, 750, 0.0018, 0.1849, 0.1863, 0.0003, 0.0111, 0.0006, 0.0322, 0.5416, 0, 0, 0.0098, 0.007
32, 775, 0.0017, 0.1826, 0.186, 0, 0.0113, 0.0011, 0.0313, 0.5408, 0, 0, 0.0104, 0.0091
33, 800, 0.0017, 0.1826, 0.186, 0, 0.0113, 0.0011, 0.0313, 0.5408, 0, 0, 0.0104, 0.0091
34, 825, 0.0012, 0.1875, 0.185, 0, 0.0097, 0.0012, 0.0322, 0.5461, 0, 0, 0.0118, 0.0037
35, 850, 0.0114, 0.1849, 0.1829, 0.0011, 0.0117, 0.0011, 0.0301, 0.5467, 0, 0, 0.0114, 0.0061