

NIST Isotherm Database “AND”- Search Tool

Jack Tabb
Scott Research Group
Clemson University
DOE RAPID
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- TTU -- the website only has “OR”-search functionality

Results (450)

Title	Authors	Journal	Year	Adsorbents	Adsorbates	
▼ The Effect of Methyl Func...	Hui Liu et al.	Adv Funct Mater	2011	Zn(BDC)(DMBPY) 0...	Carbon Dioxide, ...	SHOW
▼ Hydrogen Selective NH2-MI...	Feng Zhang et al.	Adv Funct Mater	2012	NH2-MIL-53(Al)	Carbon Dioxide, ...	SHOW
▼ Gas-Sorption Selectivity ...	Ji Woong Yoon et al.	Adv Mater	2007	Zeolite 4A, CMS-...	Carbon Dioxide, ...	SHOW

The Solution

- “AND”-search made in Python

```
[jbtabb@localhost adsorbates_AND_search]$ python3 and_search_multi_adsorbates.py
Welcome to 'AND' search for NIST-ISODB!
Using the naming scheme from the NIST-ISODB, list the adsorbate materials
you wish to find isotherm data for.
    Ex: 'N2' instead of 'Nitrogen' and 'H2' instead of 'Hydrogen'
Enter adsorbates separated by a space. Then press enter:
CH4 N2

Checking for adsorbate synonyms...
Fetching JSON file from database...
Finding relevant entries...
Fetching JSON file from database...
24 out of 3342 entries matched your search parameters
Formatting entries...
Results printed to /home/jbtabb/Documents/ScottResearch/NIST_Isotherm_Data
base/adsorbates_AND_search/results/20180605_092337.txt
```

My Results

- Out of 24 results, ctrl+f “zeolite” gave 5 results with zeolite adsorbent.

```
DOI: 10.1021/acs.iecr.5b01608
title: Adsorption Equilibrium and Dynamics of Fixed Bed Adsorption of CH4/N2 in Binderless Beads of 5A Zeolite
journal: Industrial & Engineering Chemistry Research
year: 2015
authors: José A. C. Silva, Alexandre F. P. Ferreira, Patrícia A. P. Mendes, Adelino F. Cunha, Kristin Gleichman
adsorbentMaterial: Binderless Beads of Zeolite 5A
adsorbates: Nitrogen, Methane,
isotherms: 10.1021acs.iecr.5b01608.Isotherm1, 10.1021acs.iecr.5b01608.Isotherm2, 10.1021acs.iecr.5b01608.Isotherm3,
DOI: 10.1021/Ic061052d
title: Functionalities of One-Dimensional Dynamic Ultramicropores in Nickel(II) Coordination Polymers
journal: Inorganic Chemistry
year: 2006
authors: Shin-ichiro Noro, Ryo Kitaura, Susumu Kitagawa, Tomoyuki Akutagawa, Takayoshi Nakamura
adsorbentMaterial: [Ni2(NCS)4(azpy)4]n
adsorbates: Nitrogen, Methane,
isotherms: 10.1021Ic061052d.Isotherm1, 10.1021Ic061052d.Isotherm2, 10.1021Ic061052d.Isotherm3,
DOI: 10.1021/Ie200652e
title: Adsorption Measurements of Nitrogen and Methane in Hydrogen-Rich Mixtures at High Pressures
journal: Industrial & Engineering Chemistry Research
year: 2011
authors: Moises Bastos-Neto, Andreas Moeller, Reiner Staudt, Jürgen Böhm, Roger Gläser
adsorbentMaterial: Zeolite 5A
adsorbates: Nitrogen, Methane,
isotherms: 10.1021Ie200652e.isotherm1, 10.1021Ie200652e.isotherm10, 10.1021Ie200652e.isotherm11, 10.1021Ie200652e.isotherm12, 10.1021Ie200652e.isotherm13, 10.1021Ie200652e.isotherm14, 10.1021Ie200652e.isotherm15, 10.1021Ie200652e.isotherm16, 10.1021Ie200652e.isotherm17, 10.1021Ie200652e.isotherm18, 10.1021Ie200652e.isotherm19, 10.1021Ie200652e.isotherm2, 10.1021Ie200652e.isotherm3, 10.1021Ie200652e.isotherm4, 10.1021Ie200652e.isotherm5, 10.1021Ie200652e.isotherm6, 10.1021Ie200652e.isotherm7, 10.1021Ie200652e.isotherm8, 10.1021Ie200652e.isotherm9
```

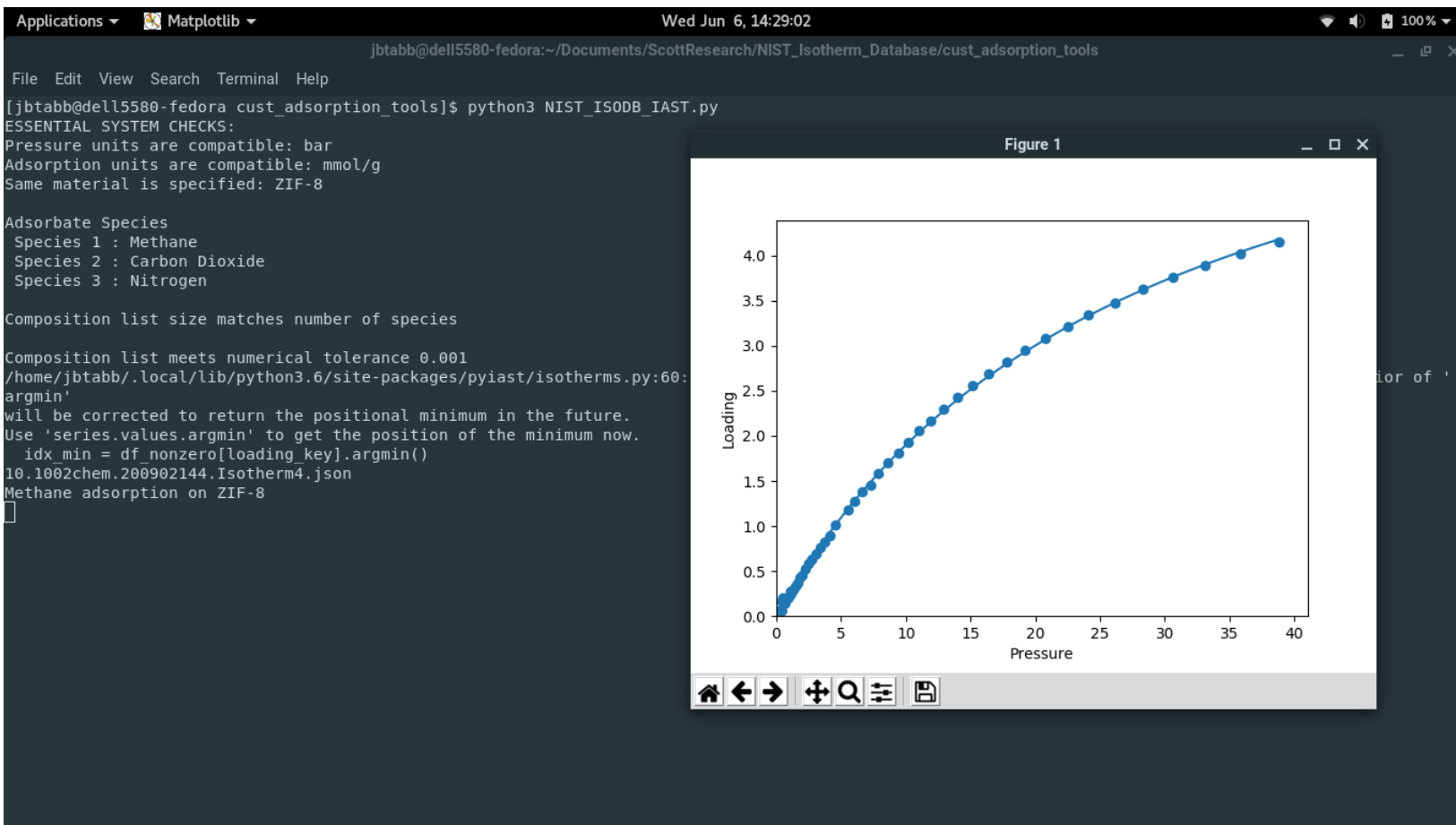
How to Use Results

- Print results and manually look at them (see image below and the “results” file)
- Continue to use JSON data within the program (i.e. NIST’s tool)

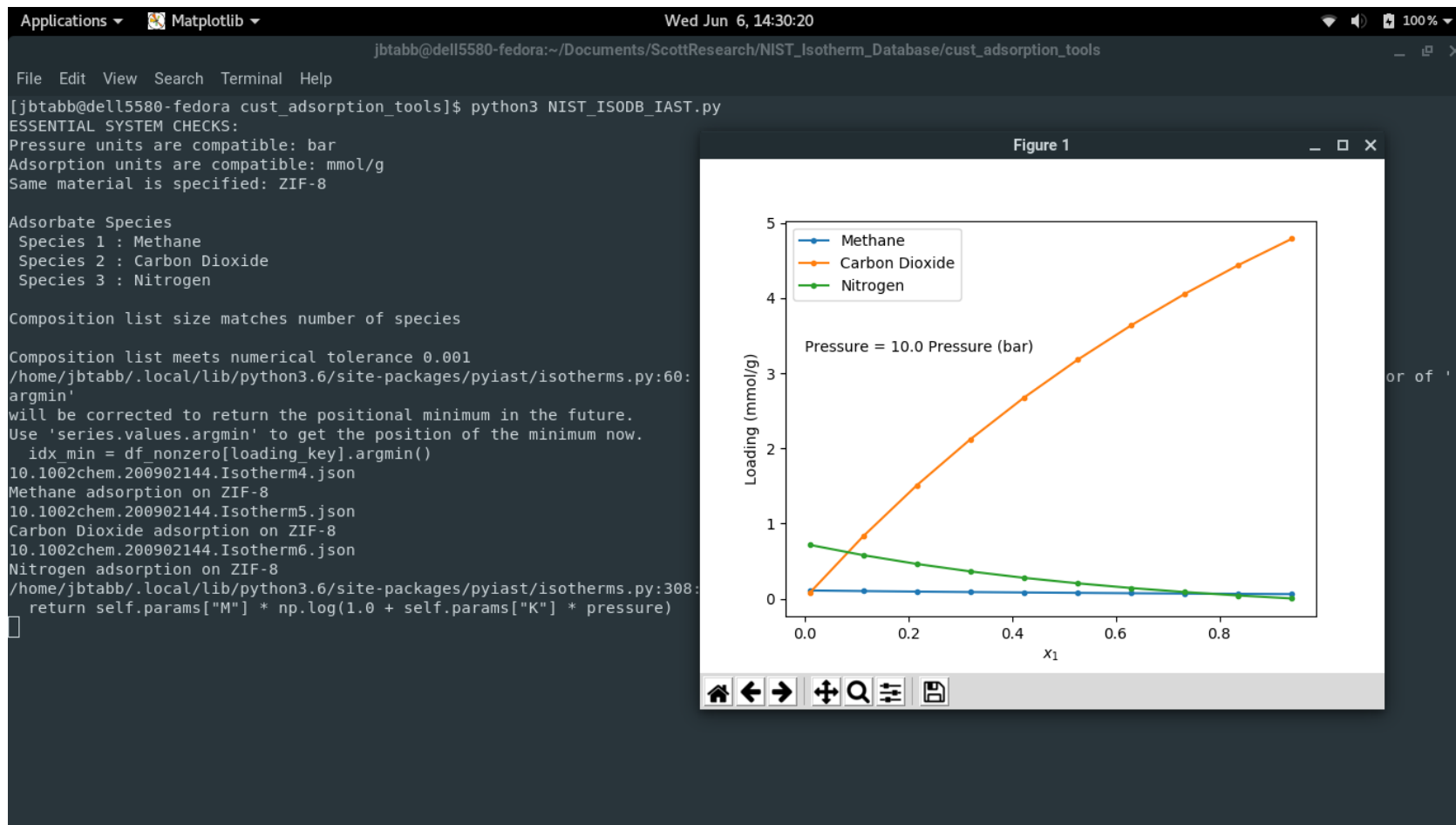
NIST ISO-DB Tool

- NIST tool written in Python Jupyter Notebook gets data from their database, performs operations on it, and plots the results.
 - Uses pyIAST package to apply "Ideal Adsorbed Solution Theory" (IAST)
 - Uses ISO-DB API
 - <https://adsorbents.nist.gov/isodb/index.php#tools>

NIST Tool Demo Results



NIST Tool Demo Results



“And”-Search Tool Inner-Workings Overview

- Get adsorbates from user
- Check user-specified adsorbates against NIST database listing of adsorbate synonyms to get a key for that adsorbate that can be used to access other data for that adsorbate.



JSON Raw Data Headers

Save Copy Pretty Print

```
[
  {
    "InChIKey": "XSTXAVWGXDOKEI-UHFFFAOYSA-N",
    "name": "1,1,2-Trichloroethene",
    "synonyms": [
      "1,1,2-trichloroethene",
      "1,1,2-trichloroethylene",
      "1,1,2-tris(chloranyl)ethene",
      "C2HCl3",
      "Trichloroethene",
      "Trichloroethylene"
    ]
  },
  {
    "InChIKey": "LGXVIGDEPROXKC-UHFFFAOYSA-N",
    "name": "1,1-dichloroethylene",
    "synonyms": [
      "1,1-dichloroethene",
      "1,1-bis(chloranyl)ethene",
      "1,1-DCE",
      "1,1-Dichloro-Ethene",
      "1,1-dichloroethylene",
      "1-C2H2Cl2",
      "Vinylidene chloride"
    ]
  }
],
```

- Iterate through the entire database list of research papers and set aside the ones that list only the user-specified adsorbates.

```
JSON  Raw Data  Headers
Save  Copy  Pretty Print

[
  {
    "DOI": "10.1002/adem.200500223",
    "title": "Improved Hydrogen Storage in the Metal-Organic Framework Cu3(BTC)2",
    "journal": "Advanced Engineering Materials",
    "year": 2006,
    "authors": [
      "P. Krawiec",
      "Markus Kramer",
      "M. Sabo",
      "R. Kunschke",
      "Heidrun Fröde",
      "Stefan Kaskel"
    ],
    "categories": [
      "exp"
    ],
    "adsorbents": [
      {
        "hashkey": "NIST-MATDB-991daf7313251e7e607e2bab2da57e33",
        "name": "CuBTC"
      }
    ],
    "adsorbentMaterial": [
      "CuBTC"
    ],
    "adsorbates": [
      {
        "InChIKey": "IJGRMHOSHXDMSA-UHFFFAOYSA-N",
        "name": "Nitrogen"
      },
      {
        "InChIKey": "UFHFLCQGNINRP-UHFFFAOYSA-N",
        "name": "Hydrogen"
      }
    ],
    "adsorbateGas": [
      "Nitrogen",
      "Hydrogen"
    ],
    "temperatures": [
      77
    ]
  }
]
```

- After iterating through the entire database list, extract the information we care about from the entries we set aside.

```
"temperatures": [
  77,
  87
],
"pressures": [
  0,
  1
],
"isotherms": [
  {
    "filename": "10.1002adem.200500223.isotherm1"
  },
  {
    "filename": "10.1002adem.200500223.isotherm2"
  },
  {
    "filename": "10.1002adem.200500223.isotherm3"
  }
]
},
{
  "DOI": "10.1002/adem.201000246",
  "title": "MOF Processing by Electrospinning for Functional Textiles",
  "journal": "Advanced Engineering Materials",
  "year": 2011,
  "authors": [
    "Marcus Rose",
    "Bertram Böhringer",
    "Marc Jolly",
    "Roland Fischer",
    "Stefan Kaskel"
  ],
  "categories": [
    "exp"
  ],
  "adsorbents": [
    {
      "hashkey": "NIST-MATDB-991daf7313251e7e607e2bab2da57e33",
      "name": "CuBTC"
    },
    {
      "hashkey": "NIST-MATDB-c86c6ddb29e17b5beb79e22bca90231a",
      "name": "MOF-5"
    }
  ]
}
```

Example Results

```
Find original research paper with DOI at http://dx.doi.org/{DOI}  
Example: http://dx.doi.org/10.1002/chem.200902144  
Access the isotherm data at: https://adsorbents.nist.gov/isodb/api/isotherm/{filename}.json  
You can also change the .json to .csv  
Example: https://adsorbents.nist.gov/isodb/api/isotherm/10.1002Aic.10306.Isotherm1.csv  
Below is a listing of all results that match your search parameters
```

```
DOI: 10.1007/s10934-011-9494-5  
title: Binary adsorption behaviour of methane and nitrogen gases  
journal: Journal of Porous Materials  
year: 2011  
authors: V. P. Mulgundmath, F. H. Tezel, F. Hou, T. C. Golden  
adsorbentMaterial: Silicalite MFI, Zeolite 13X, Alumina  
  
DOI: 10.1021/acs.iecr.5b01608  
title: Adsorption Equilibrium and Dynamics of Fixed Bed Adsorption of CH4/N2 in Binderless Beads of 5A Zeolite  
journal: Industrial & Engineering Chemistry Research  
year: 2015  
authors: José A. C. Silva, Alexandre F. P. Ferreira, Patrícia A. P. Mendes, Adelino F. Cunha, Kristin Gleichmann, Alírio E. Rodrigues  
adsorbentMaterial: Binderless Beads of Zeolite 5A  
  
DOI: 10.1021/Ie200652e  
title: Adsorption Measurements of Nitrogen and Methane in Hydrogen-Rich Mixtures at High Pressures  
journal: Industrial & Engineering Chemistry Research  
year: 2011  
authors: Moises Bastos-Neto, Andreas Moeller, Reiner Staudt, Jürgen Böhm, Roger Gläser  
adsorbentMaterial: Zeolite 5A
```

“AND”-Search Tool Details

- Sometimes the server is down. In this case, the program will get stuck at “Fetching JSON file from database...” or go past that and crash because it doesn’t have the data it needs.
 - You may be able to download the JSON on a day that you will be using it a lot to avoid the dependance on the server connection. You will miss any newly added entries after you use a downloaded JSON, but will have more reliable access to it.
 - The code does not support this, so you would have to change it.
- The program makes use of several functions. The main code that starts the program is at the bottom of the “and_search_multi_adsorbates.py” file. It makes use of the “relevant_biblio_entry.py” file. It names the results with the date and time and stores them in the folder named “results”.
- The demo for handling JSON is named “use_api_example.py”. It can be run independently or deleted.
- Read the comments in the files for more details.