

The NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials

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MATERIAL MEASUREMENT LABORATORY

Database Overview and Objectives

1. A “Data Informatics” complement to the NIST/ARPA-E **FACT Laboratory**
   - Database of **adsorbent materials** and their **adsorption characteristics**
   - NIST Standard Reference Data Product (avoid costly SRM)

2. External Guidance from “Data Task Force”

3. Draw data contents from existing scientific literature

4. On-line tools, including isotherm plotting and comparison, analysis tools (not yet)

NIST / ARPA-E Database of Novel and Emerging Adsorbent Materials

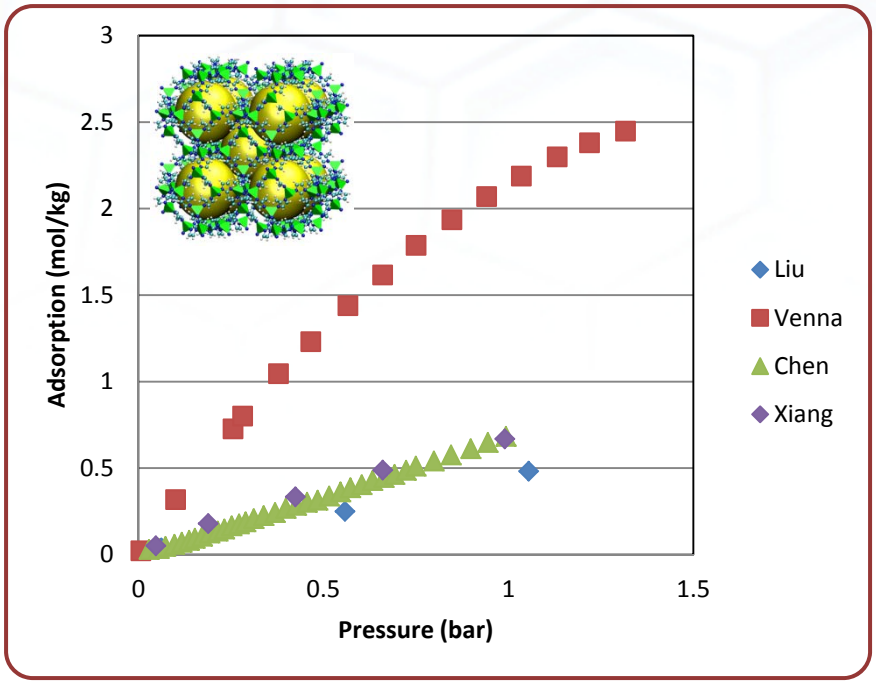
http://adsorbents.nist.gov

NIST SRD-205

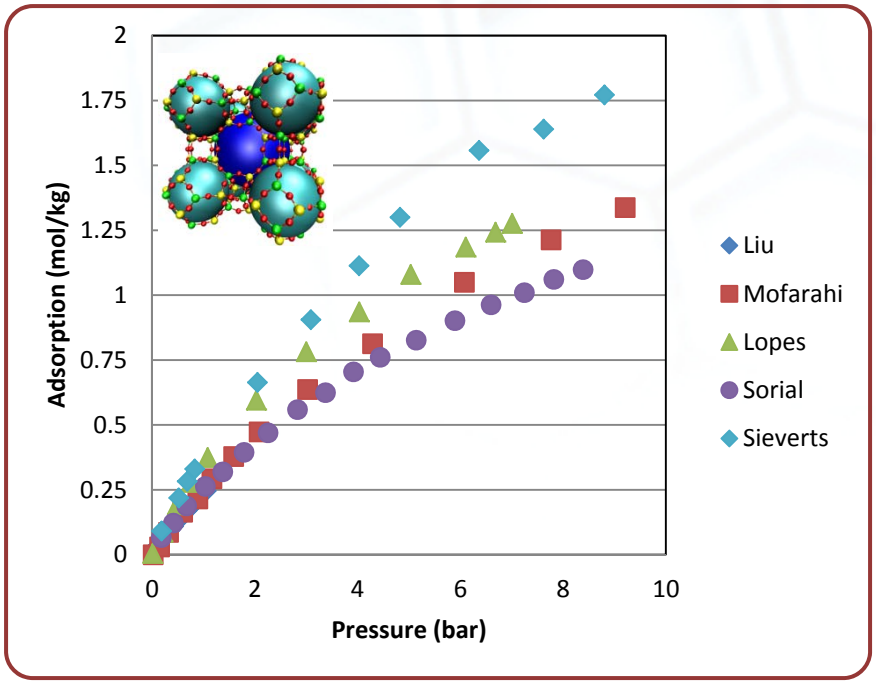
NIST / ARPA-E Database of Novel and Emerging Adsorbent Materials

Example Virtual Interlaboratory Studies:
Direct comparison of isotherms harvested from literature

CO_2 Sorption by ZIF-8 @ 298K



N_2 Sorption by Zeolite 5A @ 303K



Note outlier isotherm for ZIF-8, inconsistency even for an industrial material like Zeolite 5A.

Demonstration – http://adsorbents.nist.gov

1. Site Geography and Search Fields

2. Example Searches:
   a) Material: ZIF-8
   b) Material: ZIF-8 and Gas: CO_2
   c) Measurement Conditions (T range, P range, Type)
   d) Bibliography
   e) Progressive Search
   f) Restrict to entries with associated isotherms

3. Isotherm Comparison (use “Demo Zeolite 5A / N2” or “Demo ZIF-8 / CO2”)

NIST / ARPA-E Database of Novel and Emerging Adsorbent Materials

- Database Statistics:
  - 2578 Papers
  - 19628 Adsorption Isotherms
  - 280 Adsorbates ; 3906 Adsorbent Materials

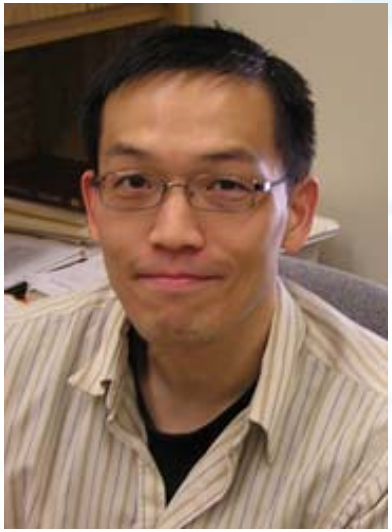
- Pitfalls:
  - Lack of uniformity in MOF names
  - Inconsistencies in units (mmol/g, N/uc, etc.)
  - Thermodynamic Errors

- Opportunities for new Data Standards (break-out sessions?):
  - Isotherm reporting standards (IUPAC recommendations?)
  - JSON isotherm format (community standard…)
  - MOF / Adsorbent Index (catalog ID vs name?)
  - Database as a **Adsorption Data Repository** (direct submission with paper)
  - Direct data output from commercial instruments

Personnel and Acknowledgments

Daniel W. Siderius

Russell D. Johnson, III



Vincent K. Shen

Data Task Force – Phil Barrett, Charles Coe, Karl Johnson, Alex Neimark, Peter Ravikovitch, Randy Snurr, Orhan Talu

Many thanks to past/present students and associates:

SURF: Jaime Santillan Mercado

SHIP: Emily Yang, Nicholas Kibbey, Alex Fairhall

MCI: Josh Hong

Guest Researchers: Qi Gan, Brittany Blunt

Objectives – An Adsorption Data Informatics Resource

1. As a complement to the NIST/ARPA-E **F**acility for **A**dsorbent **C**haracterization and **T**esting, design and introduce a web-based database of adsorbent materials and the adsorption characteristics of those materials.
    - NIST Standard Reference Data Product (avoid costly SRM)

2. The production database will be built on data drawn from the existing scientific literature and measurements from the FACT Laboratory. Jointly bibliographic and data-centric; includes article reference information and digitized adsorption isotherm data.

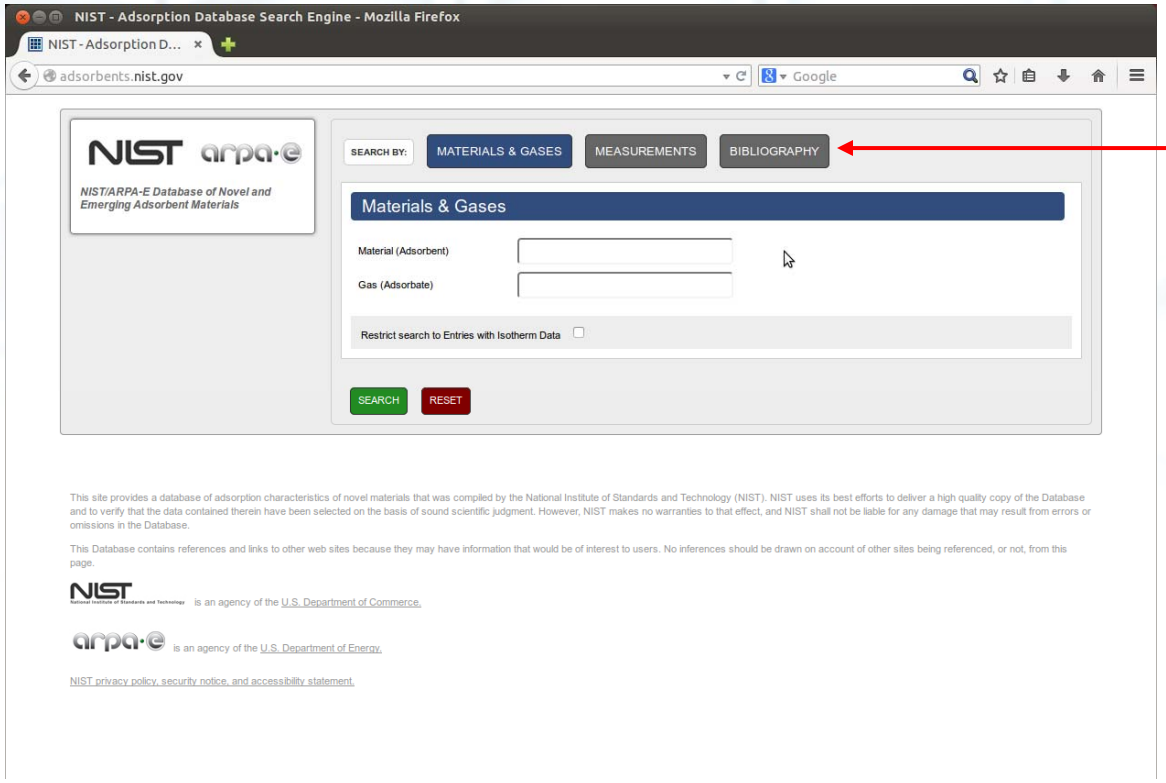
3. Production database allows for on-line plotting of adsorption isotherms, users may conduct "virtual interlaboratory studies" by comparison of results in the database. Plan to include data analytic tools.

NIST / ARPA-E Database of Novel and Emerging Adsorbent Materials

http://adsorbents.nist.gov

NIST SRD-205

Example Search



Search Categories
(any or all)

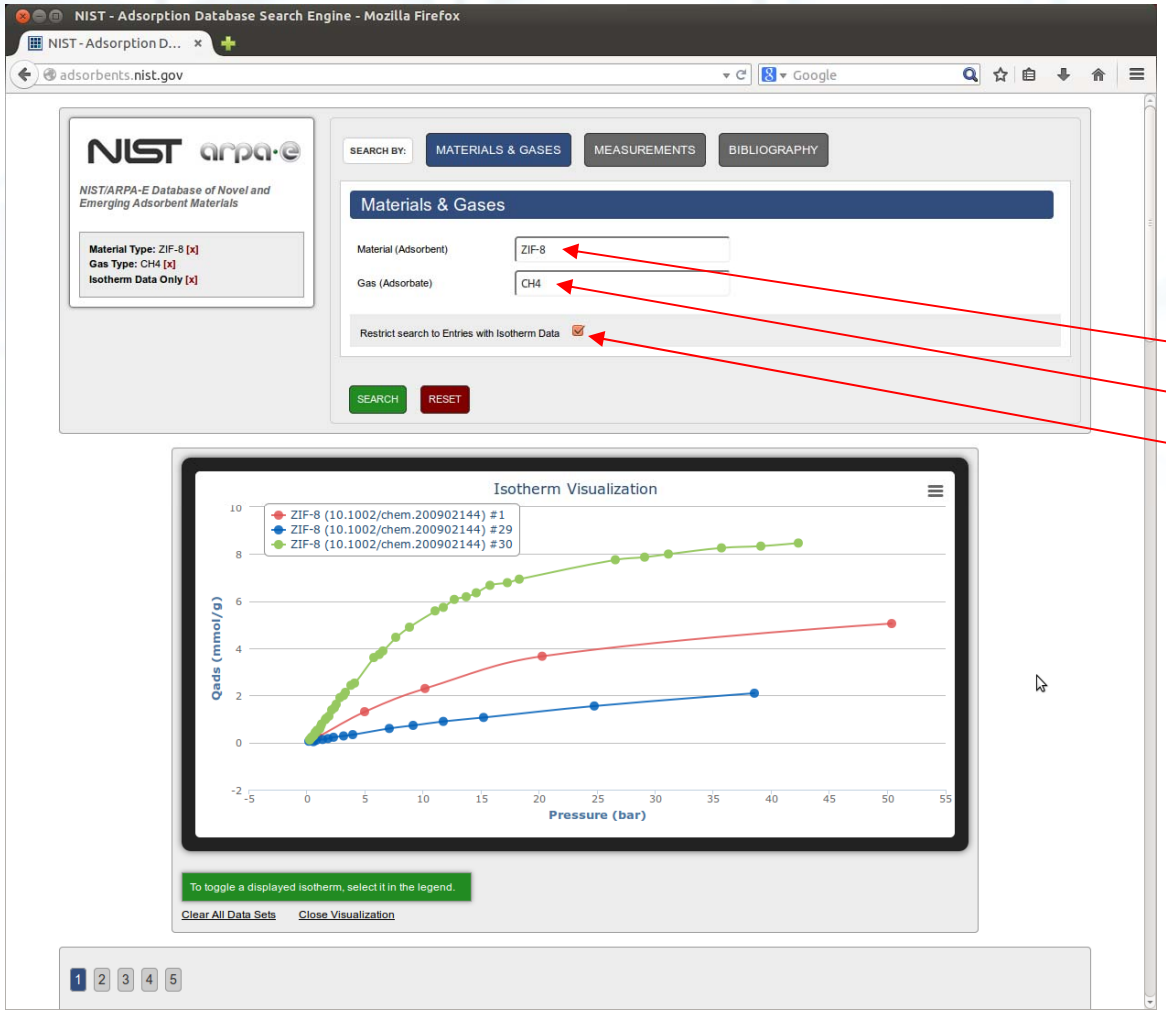
Search via:

1. Adsorbent Material
2. Adsorbate Gas
3. Measurement Type
4. Thermodynamic Conditions (Temperature / Pressure)
5. Bibliographic: Author/Journal/Title Keywords

Restrict Search to entries with associated isotherm

Progressive search – can add search constraints one by one

Example Search



Basic Search:

1. ZIF-8 Adsorbent (MOF)
2. Methane Adsorbate
3. List results with isotherm data

Results plotted from first result: Comparison of Adsorption Isotherms of CH_4, CO_2, and N_2 on ZIF-8 at 303K

NIST / ARPA-E Database of Novel and Emerging Adsorbent Materials

- Current Database contains (as of 10/27/2014):
  - 2578 Papers (abstracted relevant adsorption metadata)
  - 19628 Adsorption Isotherms (digitization of graphical isotherms)
  - 280 Adsorbates (mostly gases, some liquids and metal ions)
  - 3906 Adsorbent Materials (MOFs, Carbon, Silicas, Zeolites, etc.)

- Uses JSON files to store/pass isotherm information (**J**ava**S**cript **O**bject **N**otation)
  - Human-readable file containing isotherm data points with explanatory metadata
  - **Extensible** format: includes mandatory metadata fields (material, gas, temperature, units, DOI reference) but allows for optional or user-defined fields
  - Broad use would facilitate isotherm data exchange
  - May be used by an in-development European database of isotherms
  - Add option to instruments for direct output to JSON?

Example Isotherm JSON File & Isotherm Plot


```
{
          "DOI" : "10.1080/01496395.2010.513360",
          "adsorbentMaterial" : "Zeolite 5A",
          "adsorbateGas" : "CO2",
          "temperature" : 303,
          "adsorptionUnits" : "mmol/g",
          "pressureUnits" : "bar",
          "isotherm_data" : [
            {"pressure": 0.0136807, "adsorption" : 1.27692 },
            {"pressure": 0.03316, "adsorption" : 1.80576 },
            {"pressure": 0.0618991, "adsorption" : 2.21498 },
            {"pressure": 0.0977185, "adsorption" : 2.45468 },
            {"pressure": 0.144977, "adsorption" : 2.62465 },
            {"pressure": 0.210349, "adsorption" : 2.79477 },
            {"pressure": 0.341329, "adsorption" : 2.99536 },
            {"pressure": 0.585515, "adsorption" : 3.19689 },
            {"pressure": 0.734828, "adsorption" : 3.26795 },
            {"pressure": 0.886422, "adsorption" : 3.32906 },
            {"pressure": 0.997296, "adsorption" : 3.36989 }
          ]
}
```

Additional Data Fields

1. Institution / Laboratory
2. Date (month/day/year data was collected)
3. Gas Law (i.e. ideal or other, including relevant parameters)
4. Operator
5. Sample Holder (Why? “ … something I’ve found very important to track in previous jobs.” “Tricky to have standard nomenclature for all instruments.”)

Necessary for widespread use: Write a file specification

Pitfalls & Opportunities

- Major pitfalls encountered while gathering data:
  - Lack of uniformity in adsorbent names, particularly MOFs:

    e.g., **HKUST-1** (place-name), **CuBTC** (common name), **Basolite® C300** (commercial), **Copper (II) benzene-1,3,5-tricarboxylate** (IUPAC)

    e.g., **$[Ru^{(II)}(bpy)_2(dcbpy)]Cl_2$**, **$C_{26}H_{24}N_2O_4Zn$**

    Other synonyms in adsorbent list? (probably, but nary impossible to track down)
  - Inconsistencies in units: **mmol/g** (preferred), **cm^3(STP)/g** (acceptable, but prone to errors), **Molecules/Cavity** (informative, but not useful for comparisons), **Fractional Occupancy**
  - Thermodynamic Errors: Reducing pressure by p^{sat} for $T>T_c$; Absolute vs. Excess

- Opens opportunities for new reporting standards:
  - Standard units for gas loading (and pressure? – not necessary)
  - Require specification of isotherm type (excess vs. absolute)
  - Community could adopt JSON format as de facto standard format

- MOF Material Catalog: An index of MOFs for improved tracking and cross-referencing

NIST / ARPA-E Database of Novel and Emerging Adsorbent Materials

- Future Goals:
  - Additional Data: 200 papers, 1200 isotherms/year
  - Include of data from FACT Lab analyses
  - Online data analysis of isotherm data: Fits to isotherm model, BET Surface Area

- Repository of data for Adsorption / Porous Materials User Community:
  - Users could directly submit data from published articles to be added to the NIST/ARPA-E Database. Procedure would require certain article metadata and annotated isotherm data.
  - Similar to publication requirements for crystallographic data (CIF).