User Guide and Search Tutorial for the

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

NIST SRD-205

http://adsorbents.nist.gov

Version 1.0
30 September 2015

Table of Contents

Introduction

The following document is a User Guide and Search Tutorial for the **NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials**. This database is a standard reference database compiled by the National Institute of Standards and Technology (NIST, an agency of the U.S. Department of Commerce) in cooperation with the Advanced Projects Research Agency-Energy (ARPA-E, an agency of the U.S. Department of Energy). It is cataloged as NIST Standard Reference Database 205, i.e., NIST SRD-205, and is accessible through the HTML link http://adsorbents.nist.gov.

NIST SRD-205 is a free, web-based catalog of adsorbent materials and measured adsorption properties of numerous materials obtained from article entries from the scientific literature. The database also contains adsorption isotherms digitized from the cataloged articles, which can be compared visually online in the web application, analyzed online with available tools, or exported for offline analysis.

As a standard reference data product of NIST, SRD-205 is subject to copyright under the Standard Reference Data Act of 1968 (Public Law 90-396, U.S. § 290-290f), though this copyright has not been exercised as of 30 September 2015. For inquiries regarding licensing or reproduction of the data contents of SRD-205, please consult the list of database contacts on Page 14.

Database Engine Structure and Layout

The following section describes the structure of the database engine, the layout of the web application, and the attribute categories for searches within the database.

Primary Database Index

NIST SRD-205 is a database of adsorbent materials, cataloged according to the literature sources of information and/or data about a material and or materials. Structurally, database records in SRD-205 are the literature sources (including journal articles, reports of analysis, or other technical reports) and are uniquely identified by a persistent identifier known as a **Digital Object Identifier** (DOI, http://www.doi.org). The DOI serves as the primary key for the relational database that serves data to the web application at http://adsorbents.nist.gov. A DOI is formatted as:

> **10.1000**/**ABCDEF**

in which "**10.**" is the DOI prefix, **1000** is the registry index and **ABCDEF** is the DOI suffix. DOIs are resolved to the original source (not a reference to the source) by linking to

> http://dx.doi.org/**10.1000**/**ABCDEF**

SRD-205 is designed to be compatible with other implementations of the Handle System (http://www.handle.net) and, as such, future records in the database may substitute handles for DOIs

without loss of functionality.

Search Engine Layout

The database search engine has three panels, the Search panel, the Results panel, and the Visualization panel. Each will be discussed in sequence.

Figure 1: Default view of NIST SRD-205, showing the "Materials & Gases" tab of the Search panel.

Figure 1 shows the Search panel, which is the initial view of SRD-205 shown after loading or reloading the main webpage. Three tabs are part of the Search panel, "Materials & Gases" (blue), "Measurements (gray), and "Bibliography (gray). Each tab contains different search criteria, which are discussed below. The active tab is highlighted in blue; another tab may be activated by a mouse click on the tab of interest.

Figure 2: Example results for a search in NIST SRD-205, shown in the Results panel.

Figure 2 shows the Results panel for an example of results for a successful search, which is located below the Search panel. The results panel is shown after a successful serach. Each result (i.e., a record identified by its DOI) is allocated a row to summarize results for that record. The columns are, from left to right, the title (also shows the DOI, which links directly to the record source document, and a link for isotherm data in green), the categories attributed to the record, the adsorbents, the adsorbates,

the temperatures, the pressure range in the paper, the authors, the publication journal, and the year of publication. All columns except the year correspond to attributes of the database record that may be searched (see the following subsection).
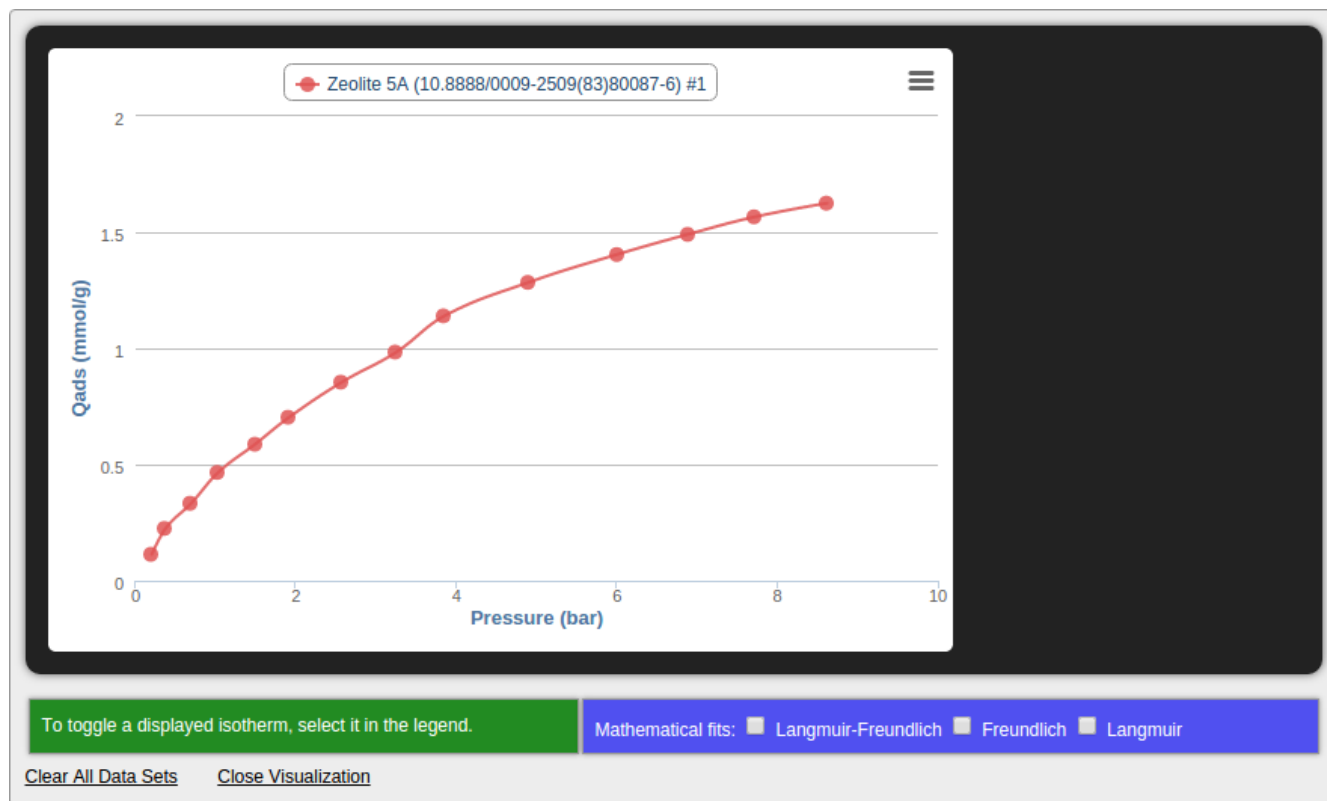
Figure 3: Example isotherm visualization, shown in the Visualization panel.

Lastly, Figure 3 shows the Visualization panel, which includes an example isotherm from the search results shown in Figure 2. The Visualization panel is placed between the Search and Results panels, after an isotherm is plotted. The panel may be closed by the "Close Visualization" link. Options for isotherm fitting (discussed in "Plotting Isotherm Data" on Page 9) are listed in the blue bar.

To return the search engine application to its default state, click or touch the red "Reset" button in the Search panel.

Search Criteria

In NIST SRD-205, search criteria correspond to attributes of records in the database. The criteria are grouped together in the aforementioned tabs, "Materials & Gases," "Measurements," and "Bibliography." One or more tabs may be searched in sequence (see "Example Search 4: Sequential Search" on Page 8).

The "Measurements & Gases" tab contains two criteria, **Material (Adsorbent)** and **Gas (Adsorbate)**.

These fields describe the the **adsorbent material** (the host material) and the **adsorbate gas (**the **guest species**), respectively. The list of adsorbent materials and adsorbate gases in the NIST SRD-205 database can be viewed by clicking the "List All Adsorbents" and "List All Adsorbates" links in the "Materials & Gases" tab. The lists will be automatically generated from the underlying relational database and then shown in a new browser tab or window.

The "Measurements" tab contains three criteria, **Measurement**, **Temperature Type**, and **Pressure Range**. The Measurement criteria describes the type of Measurement, classified as experiment (a real laboratory measurement), simulation (measurements derived from molecular simulations), Quantum/Ab Initio/DFT (measurements derived from first principles or quantum mechanical methods), or modeling (a catch-all category comprising non-experimental adsorption measurements that are based on neither molecular simulation nor quantum mechanics). The Temperature Type criteria is divided into two options: a single temperature or a temperature range, but with both in Kelvin units. Likewise, the Pressure Range is divided into two options: a single pressure or a pressure range, but with both in bar units. Both the Temperature and Pressure criteria are matched to database records via an *inclusive* boolean search. Since records in the database are categorized by individual temperatures, searching by "Single Temperature" will locate all records that include the specified temperature in their temperature attribute field. Searching by "Temperature Range" will locate all records whose temperature attributes fall within the specified temperature range. Database records are categorized by a pressure range, i.e., the minimum and maximum pressures noted in the record. Searching by "Single Pressure" will locate all entires whose pressure range contains the specified pressure. Searching by "Pressure Range" will locate all entires whose pressure range overlaps the specified pressure range.

The "Bibliography" tab contains three criteria: **Author**, **Title**, and **Journal Name**. The author criteria allows a user to search again author surnames. The title criteria allows for searches against keywords in the title of database records. The journal name criteria allows for searches against the journal name; journal names may be abbreviated in the database.

Lastly, in the "Materials & Gases" Tab, there is the checkbox to "Restrict search to Entries with Isotherm Data." This option, when active, restricts the search to database records that have associated isotherm data.

Search Tutorials

The following section provides several tutorials for searching through records in NIST SRD-205.

Example Search 1: Adsorbent Material Only

1. Load http://adsorbents.nist.gov
2. In the "Material (Adsorbent)" entry box, type "demo." A drop-down list of suggestions will be provided.
3. Touch or click "Demo ZIF-8" in the drop-down menu.
4. Touch or click "SEARCH."
5. Four results will appear in the Results panel.

The four results are the four database records whose "Adsorbent" attribute field matches "Demo ZIF-8." A similar search with a different material name would return all database records matching the specified material name. The drop-down menu of suggested material names contains up to 30 adsorbent material names matching the text entered in the entry box. The user may either select a material from the drop-down menu or type a material name manually.

This same procedure may be used to search by Adsorbate Gas only, using the "Gas (Adsorbate)" entry box and typing a gas name in step 2.

Example Search 2: Adsorbent Material and Adsorbate Gas

1. A) Load http://adsorbents.nist.gov OR B) click "RESET" in the Search panel and then click the "MATERIALS & GASES" tab.
2. In the "Material (Adsorbent)" entry box, type "demo." Select "Demo Zeolite 5A" or type the full string.
3. In the "Gas (Adsorbate)" entry box, type "co2" and either select "CO2" from the drop-down menu or type the full string.
4. Touch or click "SEARCH."
5. Two results will appear in the Results panel.

This is an example of a successful search using both the adsorbent material and adsorbate gas attributes. The results are the set of database records that include both "Demo Zeolite 5A" in the Adsorbent attribute field and "CO2" in the Adsorbate attribute field.

Example Search 3: Adsorbent Material and Temperature

1. A) Load http://adsorbents.nist.gov OR B) click "RESET" in the Search panel and then click the "MATERIALS & GASES" tab.
2. In the "Material (Adsorbent)" entry box, type "demo." Select "Demo Zeolite 5A" or type the full string.
3. Click the "MEASUREMENTS" Tab.
4. From the "Select Temperature Criteria" menu, select the "Single Temperature (K)" option.
5. Enter "303" in the "Single Temp:" entry box.
6. Touch or click "SEARCH."
7. Four results will appear in the Results panel.

This is an example of a successful search using both the adsorbent material and temperature attributes. The results are the set of database records that include both "Demo Zeolite 5A" in the 303 K in the Temperature attribute field. NOTE: this does not guarantee that the article record contains an isotherm of "Demo Zeolite 5A" material at 303 K, only that the records contain both of those attributes.

This procedure can be re-used to search by adsorbent material, gas, measurement conditions and type, and bibliographic information, by changing the search criteria in steps 2-5 and by adding additional criteria prior to step 6.

Example Search 4: Sequential Search

The search engine in NIST SRD-205 may be used in a sequential manner, that is, by a procedure that sequentially adds or removes new search criteria:

1. A) Load http://adsorbents.nist.gov OR B) click "RESET" in the Search panel and then click the "MATERIALS & GASES" tab.
2. In the "Material (Adsorbent)" entry box, type "demo," then select "Demo Zeolite 5A".
3. Touch or click "SEARCH."
4. Five records will appear in the Results panel.
5. Click the "MEASUREMENTS" Tab, then select the "Single Temperature (K)" option from the "Select Temperature Criteria" menu, and finally enter 303 in the "Single Temp:" entry box.
6. The results panel automatically updates itself, reducing the results to four records.
7. Click on the "MATERIALS & GASES" tab.
8. In the "Gas (Adsorbate)" entry box, type "CH4," then select CH4 from the drop-down menu.
9. The results panel automatically updates itself, reducing the results to two records.
10. Click on the "MEASUREMENTS" tab.
11. Select "Modeling" from the "Select Measurement Category" menu.
12. The results panel automatically updates itself, reducing the results to a single record.
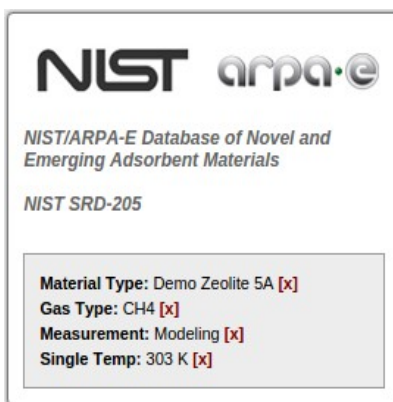

Figure 4: Search panel showing the search criteria for the sequential search in Example Search 4.

13. In the Search panel, the right panel holds a list of search criteria, as shown in Figure 4. Click the red "X" next to "**Material Type:** Demo Zeolite 5A" in the search criteria list.
14. The results panel automatically updates itself, increasing the results to (as of 30 September 2015) to 24 records, arranged in five pages.

The sequential search procedure accomplished, in order:
1. A search for all records matching "Demo Zeolite 5A" in the adsorbent material attribute field.
2. Restricted the results of #1 to records with 303 K in the temperature attribute field.
3. Restricted the results of #2 to records with CH4 in the adsorbate gas attribute field.
4. Restricted the results of #3 to records with Modeling in the Measurement type attribute field.
5. Expanded the results of #4 to records matching 303 K in the temperature attribute field AND CH4 in the adsorbate gas attribute field AND Modeling in the Measurement type attribute field.

By using the procedure in Example Search 4 as a template, a user can modify a previous search by adding or subtracting new criteria sequentially, using any of the search criteria fields.

Plotting Isotherm Data

After a successful search, a user has the option of plotting adsorption isotherm data in the NIST SRD-205 web application. First, after a successful search, a user must click or touch the "XX isotherms" link (green) in the results panel for a particular record, where XX is the number of isotherms associated with the record. After selecting the green link, a menu of isotherms will appear in the results panel, as shown in Figure 5.

Title	Category	Adsorbent	Adsorbate	Temperature (K)	Pressure Range (bar)	Authors	Journal	Year
10.8888/0009-2509(83)80087-6 **Adsorption Equilibria for Oxygen and Nitrogen Gas-Mixtures on 5a Molecular-Sieves** Uploaded: 2/6/2014 4 isotherms	exp, model	Demo Zeolite 5A	O2 N2	278.15, 293.15, 303.15	[0, 9]	G. A. Sorial W. H. Granville W. O. Daly	Chemical Engineering Science	1983

Related Isotherms	Material	Gas	Temperature (K)		
Matching Isotherm #1	Zeolite 5A	N2	278	☐ Plot Values	Download Data
Matching Isotherm #2	Zeolite 5A	O2	303	☐ Plot Values	Download Data
Matching Isotherm #3	Zeolite 5A	N2	293	☐ Plot Values	Download Data
Matching Isotherm #4	Zeolite 5A	N2	303	☐ Plot Values	Download Data

Figure 5: Example results in the Results panel, with the Isotherms menu open.

Each line in the "Related Isotherm" list corresponds to an isotherm included in the source publication of the database record. Metadata for the isotherm is also listed, including the Adsorbent Material, the Adsorbate Gas, and the Temperature. Clicking the checkbox next to "Plot Values" will instruct the web application to plot that particular isotherm in the Visualization panel, as shown in Figure 3. Additional isotherms may be added to the Visualization panel by click the checkbox for that isotherm. The web application will only allow multiple isotherms to be plotted if the y-axis (Adsorption) units are identical; otherwise an error is reported and the additional isotherm will not be plotted. Isotherms from other database records may be plotted by clicking the "XX isotherms" link for other records, then selecting the checkbox for the isotherm of interest. Isotherms in the Visualization panel may be toggled on or off by clicking the DOI/isotherm identifier in the top of the Visualization panel.

Fitting Isotherm Data

Users of NIST SRD-205 also have the option of fitting adsorption isotherm data to certain isotherm models. After plotting an isotherm, the Visualization panel include several "Mathematical fits" in the blue bar, as shown in Figure 3. Selecting the checkbox for one or more isotherm models will activate the mathematical fit of all isotherms currently in the Visualization panel for the selected models. As of 30 September 2015, the available models are the Langmuir, Freundlich, and Langmuir-Freundlich

isotherms. An example of two isotherm fits is shown in Figure 6, labeled as "La" for the Langmuir isotherm fit and "LaFr" for the Langmuir-Freundlich isotherm fit. "Fr" is the abreviation for the Freundlich isotherm.
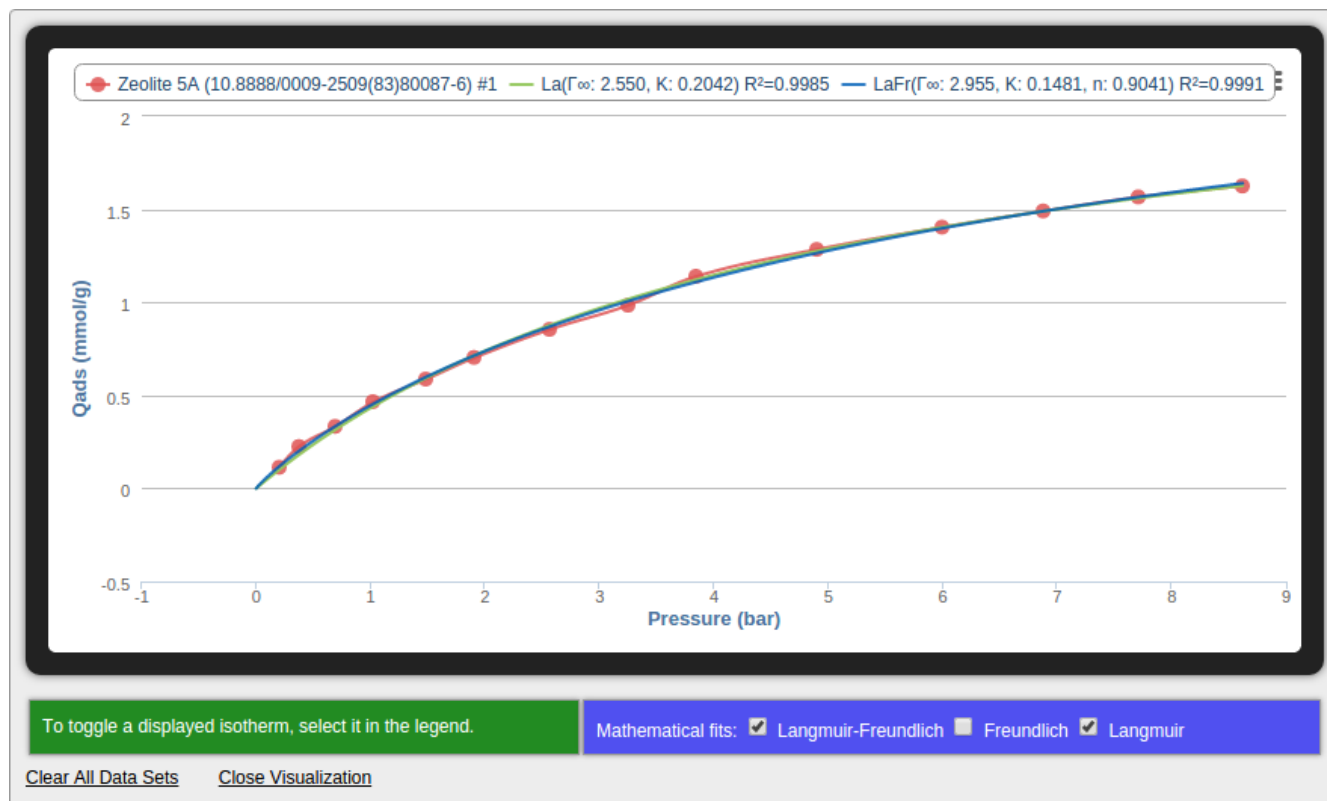
Figure 6: Example isotherm visualization, shown in the Visualization panel, with the Langmuir and Langmuir-Freundlich fitting options active.

Fitting parameters for each model are reported in the top bar of the Visualization panel. Additionally, the R^2 (coefficient of determination) metric of the mathematical fit is reported.

The Langmuir isotherm model is given by:

$$\Gamma(p) = \Gamma_\infty \frac{Kp}{1 + Kp} \tag{1}$$

and has two fitting parameters: K and Γ_∞.

The Freundlich isotherm model is given by:

$$\Gamma(p) = k \, p^{1/n} \tag{2}$$

and has two fitting parameters: k and n.

The Langmuir-Freundlich isotherm model is given by:

$$\Gamma(p) = \Gamma_\infty \frac{(Kp)^n}{1 + (Kp)^n} \qquad (3)$$

and has three fitting parameters: K, n, and Γ_∞.

As for the plotted isotherm data, isotherm fits may be toggled on/off by clicking the fit identifier in the top of the Visualization panel.

The units for the reported for the isotherm fits depend on both the selected model and the axis units of the isotherm itself. The user is responsible for determining the units from both the isotherm model equation and the axis labels. For example, since the x- and y-axes units in Figure 6 are bar and (mmol/g), respectively, and using equation (1) the units of K are (bar^{-1}) and the units of and Γ_∞ are (mmol/g). Similarly, for the the Langmuir-Freundlich fit, the units of K are (bar^{-1}), the units of Γ_∞ are (mmol/g), and n is dimensionless. For a Freundlich isotherm with the same axes units, the units of k would be [(mmol/g) bar^n] and n would be dimensionless.

The isotherm fits are done using either 1) linear regression for isotherms that can be linearized or 2) a numerical regression. Currently, the linearizable isotherm models are the Langmuir and Freundlich options. All other isotherms are fit using numerical regression. The isotherm fit for the numerical regressions is necessarily non-unique, since it is ultimately an optimization scheme that depends on the initial guess for the fitting parameters.

Downloading Isotherm Data

Isotherm data associated with database records in NIST SRD-205 may be downloaded for offline use. After a successful search, the user opens the list of isotherms for a record (as described in Section "Plotting Isotherm Data" on page 9), then clicks the "Download Data" link for the isotherm of interest. The user's web browser will download a file entitled "isotherm_export.xls." This data file is a spreadsheet in the MS Excel format, which can be opened with most spreadsheet applications. In the spreadsheet file are the isotherm metadata as well as the isotherm data itself.

The metadata are in Rows 1-6:

  Row 1: DOI
  Row 2: Adsorbent Material Name
  Row 3: Adsorbate Gas Name
  Row 4: Temperature (Kelvin)
  Row 5: Adsorption (vertical) axis units
  Row 6: Pressure (horizontal) axis units

The seventh line is purposely blank. Rows 8 and above contain the tabular isotherm data. The first (A) column contains the pressure abscissas and the second (B) column contains the values of adsorption measurements the pressure in the same row.

Linking to Articles and Data

Article records in NIST SRD-205 may be directly accessed via an HTML link:

>   http://adsorbents.nist.gov/doi.php?urldoi=**DOI**

where **DOI** is the DOI or Handle of the article. For example, the HTML link

>   http://adsorbents.nist.gov/doi.php?urldoi=10.1016/j.colsurfa.2013.03.025

will open the record in SRD-205 for the article whose DOI is "10.1016/j.colsurfa.2013.03.025".

User Feedback

Users of NIST SRD-205 may provide feedback to the database maintainers via the form located at http://adsorbents.nist.gov/feedback.php. This form is accessible through the SRD-205 website via the "Submit feedback, comments, or corrections" link in the webpage footer. User feedback is sent to the email address **isotherm@nist.gov**.

Citation Guide

To cite this database, we suggest use of a citation format appropriate to that of an edited book:

>   Siderius, D.W., Shen, V.K., Johnson III, R.D. and van Zee, R.D., Eds., NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials, NIST Standard Reference Database Number 205, National Institute of Standards and Technology, Gaithersburg MD, 20899, http://adsorbents.nist.gov, (retrieved [date of access]).

Troubleshooting

Web Browser: NIST SRD-205 utilizes elements of HTML5 and, consequently, may not operate correctly in older web browsers. For best performance we recommend the use of a HTML5-compliant browser, including Chrome (version 28 and newer), Firefox (version 3.5 and newer), Safari (version 5 and newer), and Internet Explorer (version 9 and newer).

Search Difficulties: Users have reported occasional "lockup" of the NIST SRD-205 web application, where it will not respond to search queries. To restore search functionality, simply reload the main http://adsorbents.nist.gov page and repeat the desired database search.

Disclaimer Statement

This user guide describes a database of adsorption characteristics of novel materials that was compiled by the National Institute of Standards and Technology (NIST). NIST uses its best efforts to deliver a high quality copy of the Database and to verify that the data contained therein have been selected on the basis of sound scientific judgment. However, NIST makes no warranties to that effect, and NIST shall not be liable for any damage that may result from errors or omissions in the Database.

Certain commercial equipment, instruments, suppliers, software, or materials are identified in the Database to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials, equipment, or software identified are necessarily the best available for the purpose.

The Database contains references and links to other web sites because they may have information that would be of interest to users. No inferences should be drawn on account of other sites being referenced, or not, from this page.

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NIST Staff and Associates

     Brittany Blunt

     Eric Boesch

     Jasmine Chang

     Laura Espinal

     Alex Fairhall

     Qi Gan

     Seung Joo Hong

     Russell Johnson

     N. Andrew Kalra

     Nicholas Kibbey

     Jaime Santillan Mercado

     Vincent Shen

     Daniel Siderius

     Roger van Zee

     Emily Yang

NIST SRD-205 Data Task Force

     Phillip Barrett

     Charles Coe

     J. Karl Johnson

     Alexander Neimark

     Peter Ravikovitch

     Randall Snurr

     Orhan Talu

Contact Information

General Editor and Maintainer: Daniel W. Siderius [**daniel.siderius@nist.gov**].

Project Manager: Vincent K. Shen [**vincent.shen@nist.gov**].

Deputy Division Chief: Roger D. van Zee [**roger.vanzee@nist.gov**]

Division Chief: Carlos Gonzalez [**carlos.gonzalez@nist.gov**]