About OMICS Group

OMICS Group International is an amalgamation of Open Access publications and worldwide international science conferences and events. Established in the year 2007 with the sole aim of making the information on Sciences and technology 'Open Access', OMICS Group publishes 400 online open access scholarly journals in all aspects of Science, Engineering, Management and Technology journals. OMICS Group has been instrumental in taking the knowledge on Science & technology to the doorsteps of ordinary men and women. Research Scholars, Students, Libraries, Educational Institutions, Research centers and the industry are main stakeholders that benefitted greatly from this knowledge dissemination. OMICS Group also organizes 300 International conferences annually across the globe, where knowledge transfer takes place through debates, round table discussions, poster presentations, workshops, symposia and exhibitions.

About OMICS Group Conferences

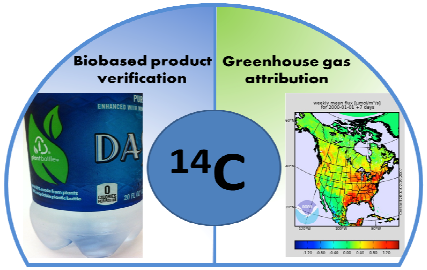
OMICS Group International is a pioneer and leading science event organizer, which publishes around 400 open access journals and conducts over 300 Medical, Clinical, Engineering, Life Sciences, Phrama scientific conferences all over the globe annually with the support of more than 1000 scientific associations and 30,000 editorial board members and 3.5 million followers to its credit.

OMICS Group has organized 500 conferences, workshops and national symposiums across the major cities including San Francisco, Las Vegas, San Antonio, Omaha, Orlando, Raleigh, Santa Clara, Chicago, Philadelphia, Baltimore, United Kingdom, Valencia, Dubai, Beijing, Hyderabad, Bengaluru and Mumbai.

Strategies for the Effective Integration of Reference Data and Reference Materials

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Material Measurement Laboratory

Standard Reference Materials (SRMs)

- **Standard Reference Materials® (SRMs) are Certified Reference Materials (CRMs) issued by the National Institute of Standards and Technology (NIST)**

- **Homogeneous, stable materials well-characterized for one or more chemical and/or physical properties**

- **Assist laboratories worldwide in validating analytical measurements of chemical composition**

NIST supplies industry, academia, government, and other users with about 1,300 reference materials of the highest quality and metrological value, supporting a wide variety of disciplines ranging from advanced materials to manufacturing, health and environment.

(http://www.nist.gov/srm)

NIST's Categories of Assigned Values

- **Certified value:** NIST has the highest confidence in its accuracy in that sources of bias have been investigated or taken into account.

- **Reference value:** Best estimate of the true value where sources of bias have not been fully investigated.

- **Information value:** A value that will be of interest and use to the SRM/RM user, but insufficient information is available to assess the uncertainty associated with the value.

Example: Deepwater Horizon Oil Spill



- **Interlaboratory studies (2011-2012)**
  - **Four matrices of interest: sediment, bivalve tissue, crude oil, and alligator blood**

	Sample (Unknown)	Control
Crude Oil	Deepwater Horizon source oil (NOAA; May 21, 2010) SRM 2779	SRM 1582 Petroleum Crude Oil
Mussel tissue	cryogenically homogenized mussel tissue (1990)	SRM 1974b Organics in Mussel Tissue (*Mytilus edulis*)
Sediment	fine particulate (<250 µm) fraction from SRM 1944	SRM 1941b Organics in Marine Sediment

Standard Reference Data

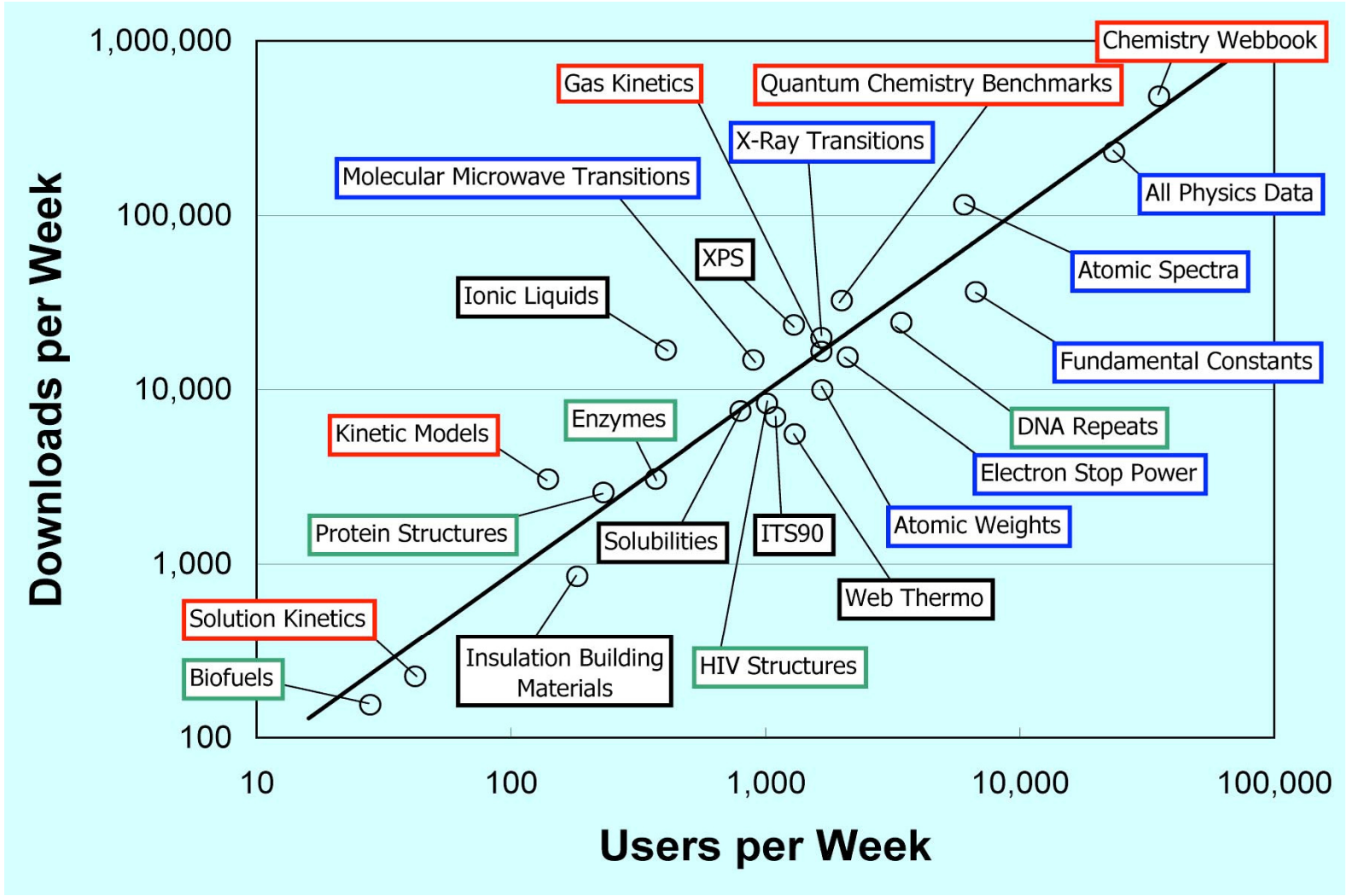
- For over 40 years, NIST has provided well-documented numeric data to scientists and engineers for use in technical problem-solving, research, and development.

- These recommended values are based on data which have been extracted from the world's literature, assessed for reliability, and then evaluated to select the preferred values.

- These data activities are conducted by scientists at NIST with a wide variety of technical expertise.

(http://www.nist.gov/srd)

NIST Data Online

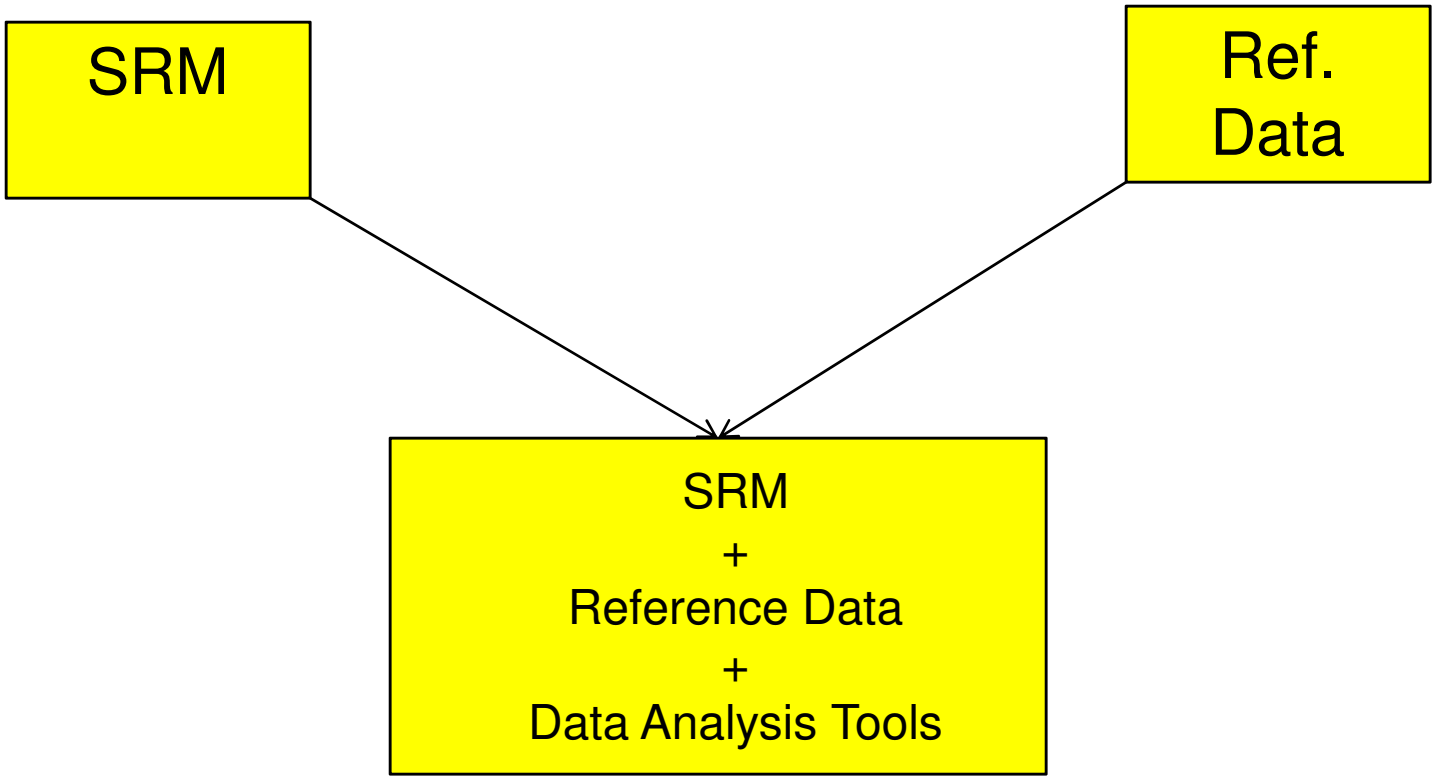


The New Challenges

- **Increased demand for more physical & chemical properties data for SRMs**
  - Particularly true in the case of complex advanced materials and biological mixtures.
- **No single institute/research group can provide all required measurements/data**
  - Resources limitations.
  - Hard to predict what new properties will be relevant to the scientific community.
- **Data should be reliable, and easily accessible.**
  - Seamless online access is a must.

The Solution

"The Integration of SRMs with Reference Data"



Implementation Requirements

- All information must be disseminated in the form a website
  - Effective and easy to use GUI.
- The website must be interactive
  - Users must be able to upload/download data.
- Should include Certificate as we all other types of data
  - Proper data annotation and meta-data.
- Most provide computational tools that help in the analysis and visualization of the data
  - Tools must be properly documented (manuals &tutorials).
- Site must be extensible and provide links to other sources of relevant information as necessary.

The Vision

- **Foster the creation of scientific communities/environs behind SRMs and Reference Data that will enable advances in science and technology**

- **Become "information brokers" rather than just "data providers"**

A Protopype: Metabolomics Data Quality

- **qMet - The NIST Data Quality System for Metabolomics**
  - ***A trusted, unbiased metabolomics quality data repository***
    - *Easy in, easy out*
    - *Data analytics*
    - *Metadata consistency*

qMet Website



Home | Data | Download | Upload | Sign Up

Welcome nik79

File Upload

Data Type: LC-MS

Add file | identifiers2.sdf | Upload

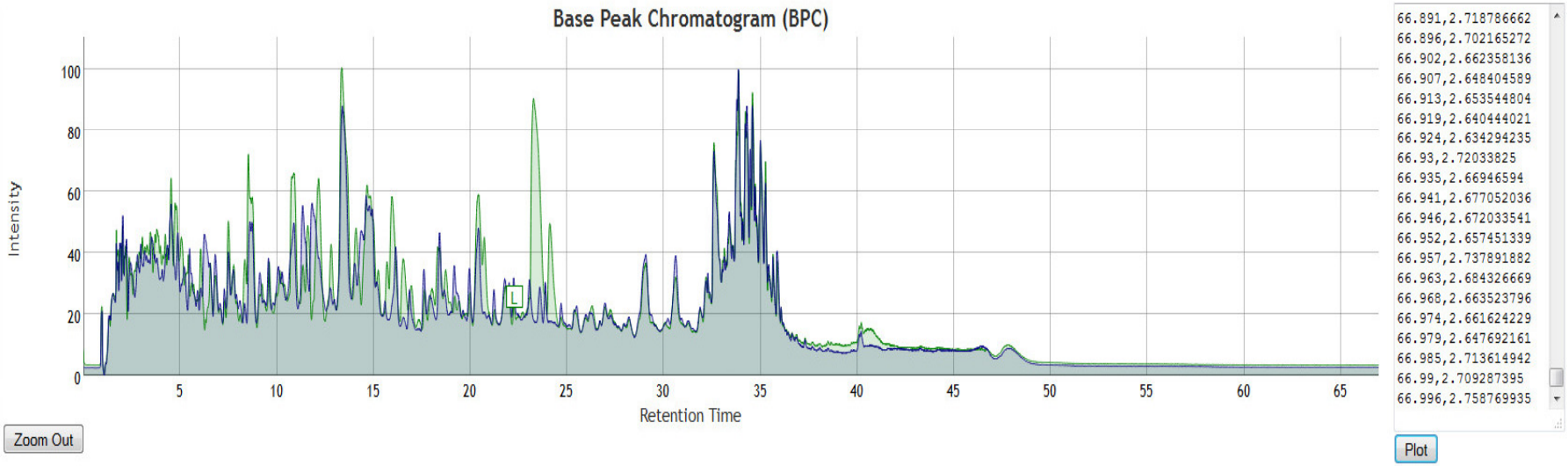
Uploading...27%

Chromatogram Comparison

User chromatogram

NIST chromatogram

X,Y coordinates of a chromatogram to compare against the NIST chromatogram



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

An Adsorption Data Informatics Resource

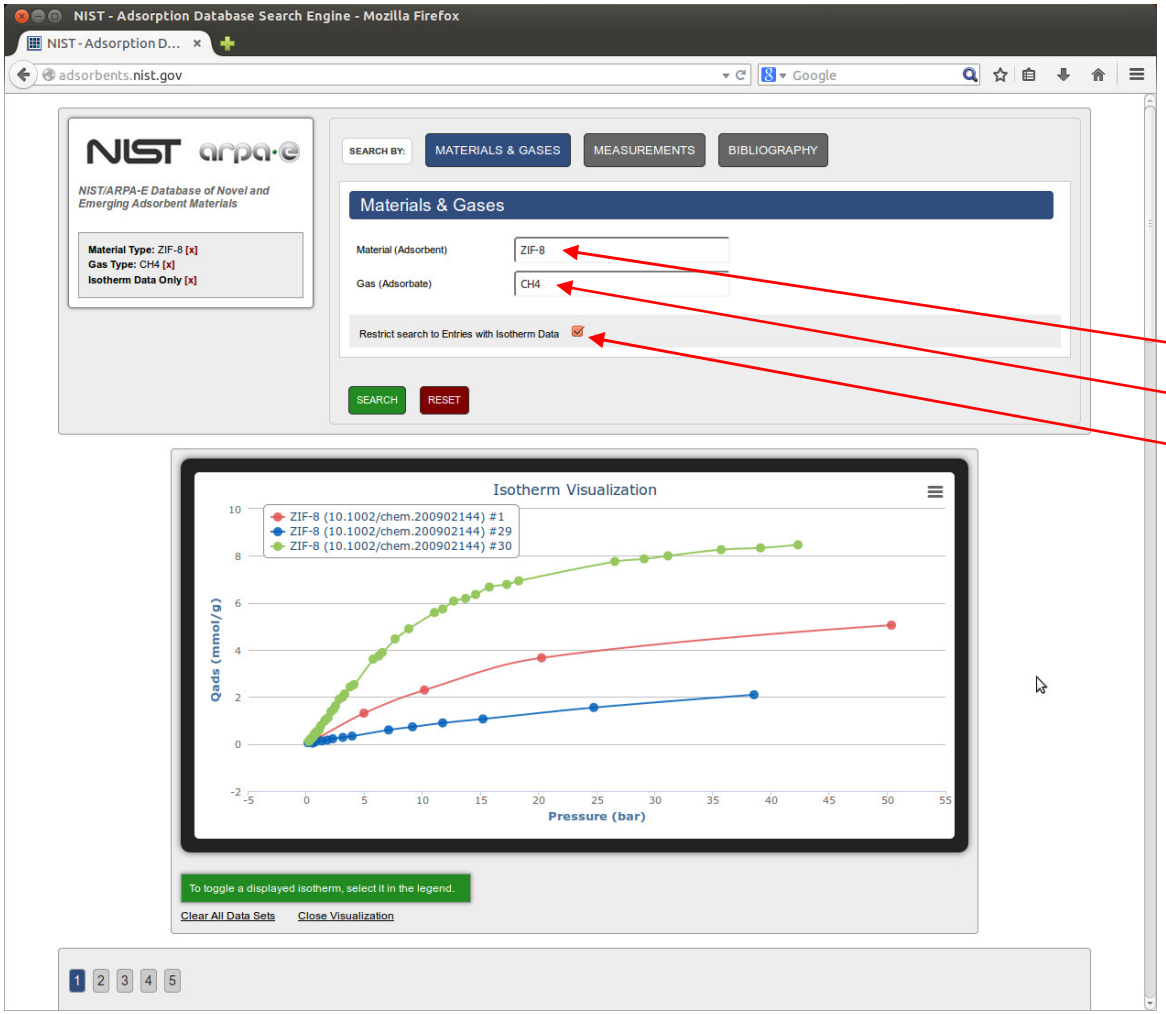
1. **As a complement to the NIST/ARPA-E Facility for Adsorbent Characterization and Testing (FACT), design and introduce a web-based database of adsorbent materials and the adsorption characteristics of those materials.**
   - **NIST Standard Reference Data Product**

2. **The production database is 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.**

- **http://adsorbents.nist.gov**

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:**
  - **2578 Papers (abstracted relevant adsorption metadata)**
  - **19842 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 (JavaScript Object Notation)**
  - **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**

Data Issues

- **Classification of data.**
- **Interoperability and integration of Databases.**
- **Culture.**

But, “Data” means different things to different people !

What is Data?

"Data is defined as Information (e.g. measurements, calculations, estimates, or statistics) obtained from investigation"

- **Collection:** The gathering of data, including documentation of source
- **Compilation**: The organization and adaptation of a collection of data in a manner suitable for its nature and intended use
- **Critical Evaluation**: The assessment of data by suitable and documented methods based on quality and fitness for use
- **Publication**: The preparation of articles, books, databases, or other media in order to provide data to the public
- **Dissemination**: The distribution of data in any format

Data Issue 1: Data Classification

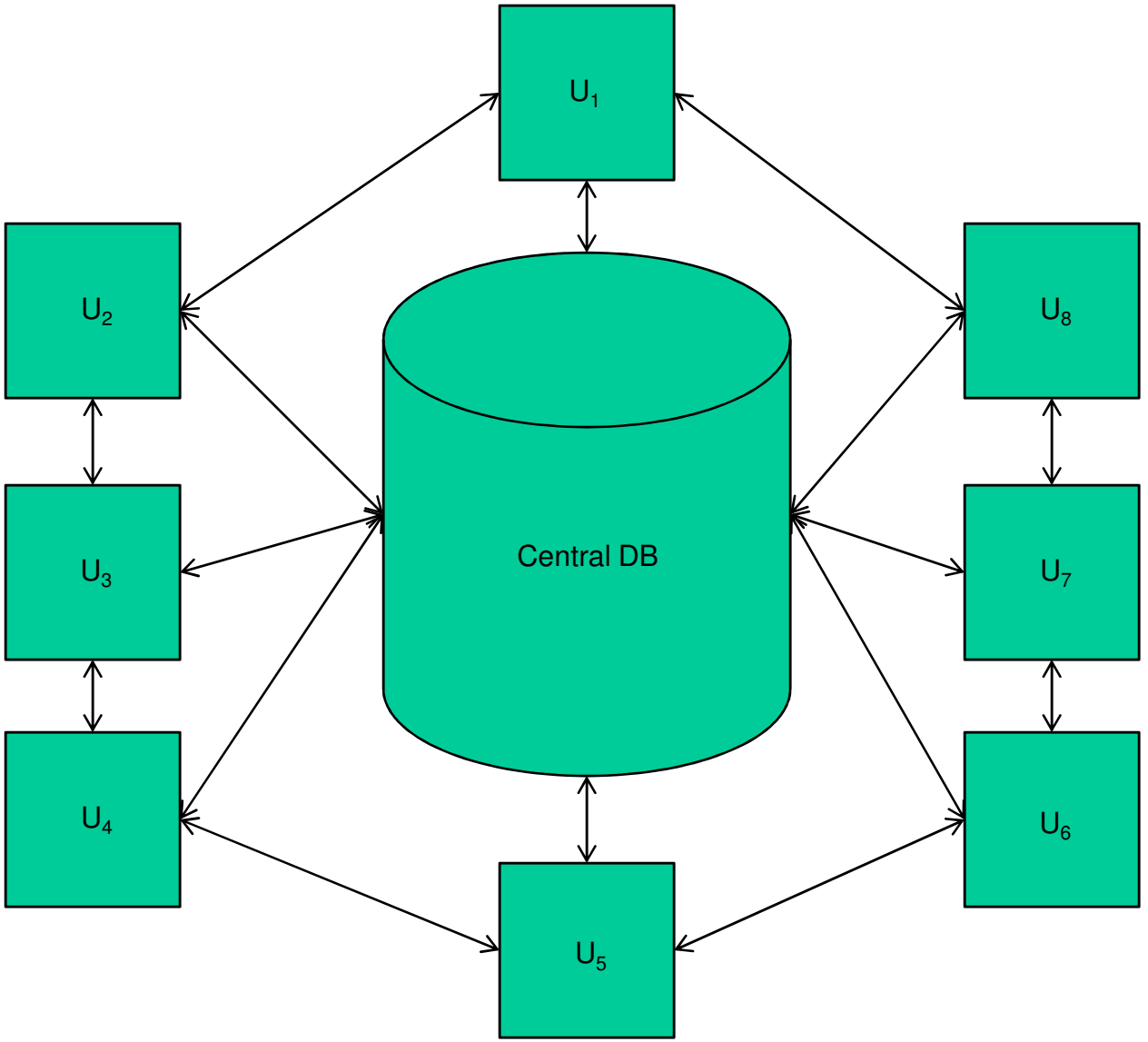
- **Standard Reference Data (SRD)**
  - Data that has been collected from documented sources, organized, evaluated by documented procedures and distributed under the requirements of the Standard Reference Data Act.
- **Reference Data**
  - Similar to SRD, but not distributed under the requirements of the SRD Act.
- **Compiled Data**
  - Data that has not been evaluated, but has been organized into a data product.
- **Archival Data**
  - Data appropriate for long term storage and re-use.
  - It is documented with respect to its source but has not been developed into an organized data product.
- **Non-archival Data**
  - Data which is intended for temporary use .
  - It may, for example, include data produced in development of experimental and/or computational techniques or testing of new equipment.

NIST

Data Issue 2: Interoperability and Integration of Databases

- **Data accessibility**
  - GUIs, data portals, mobile devices, user notifications.
- **Data formats standards**
  - Universal vs specific standards.
- **Semantic & ontology standards**
  - Flexible and extensible languages.
- **Meta-data standards**
  - Universal but extensible.
- **Data security**
  - IP issues, data encryption.
- **Big Data**
  - Moving data vs moving data analysis tools.

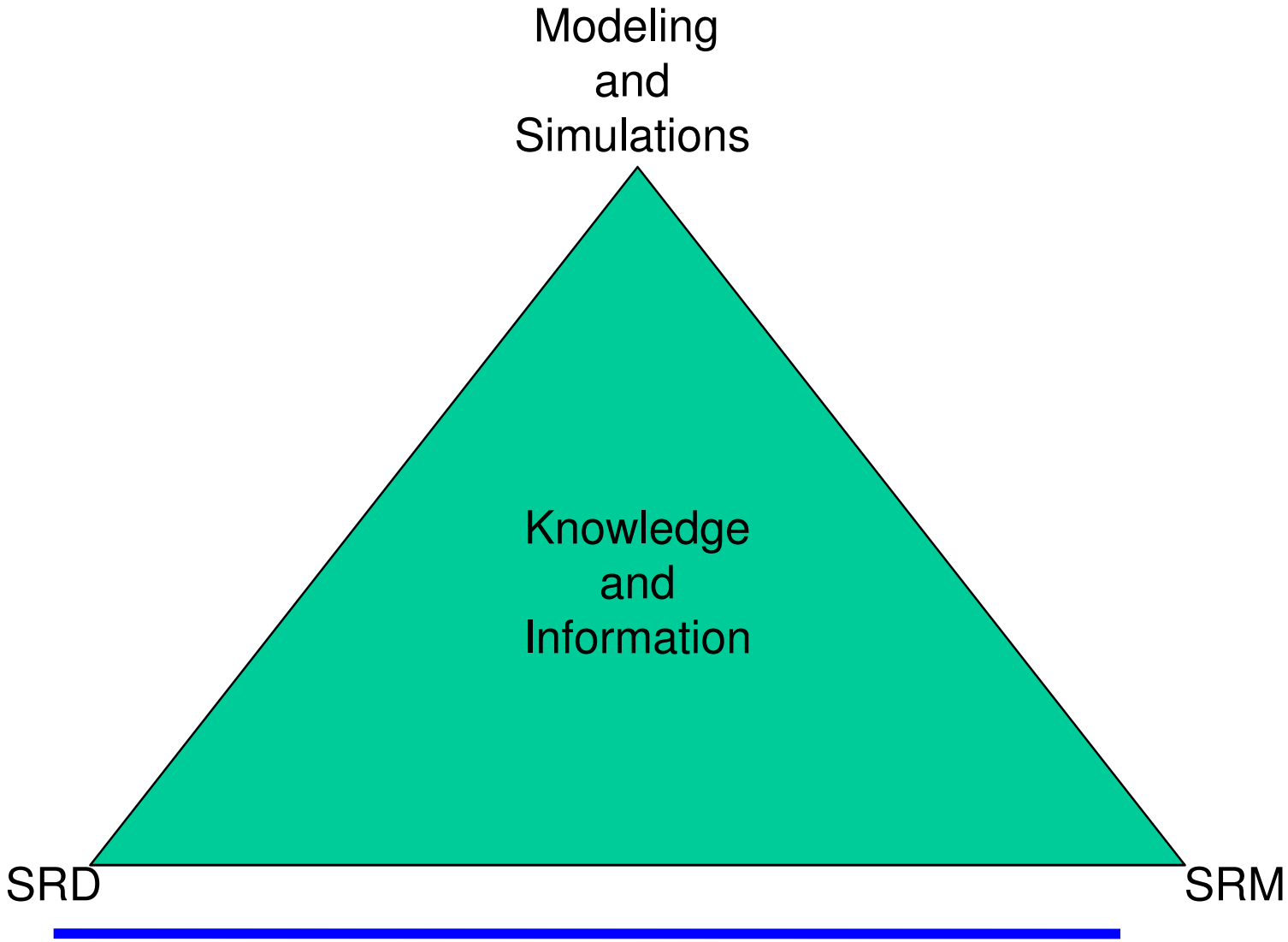
Data Accessibility: Data Federation



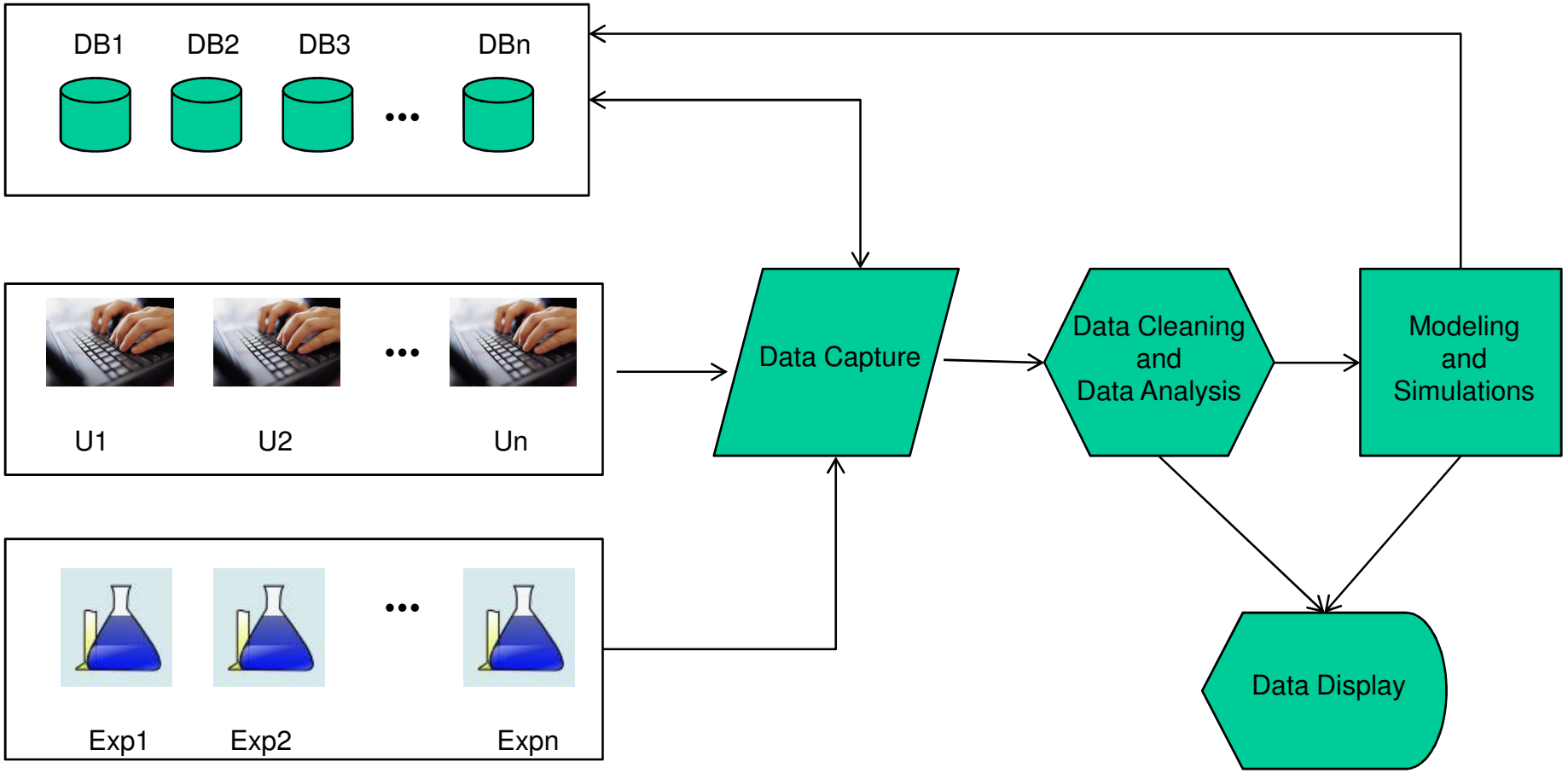
Data Issue 3: Culture

- Breaking barriers across disciplines.
- Adopting data management standards.
- Coping with new technology.
- Data sharing: “It is my data”.
- Understanding the benefits: “What’s in it for me”.

Going Forward: Beyond Data



One Approach: Scientific Workflows



Conclusions

- A new paradigm-shift involving the seamless integration of reference materials and reference data seems to be the logical way forward for information providers and metrology laboratories .
- Most of the current scientific and technological activities have become information-driven and data centric endeavours.
- Novel dissemination models (such as modern interactive databases and scientific workflows) as well data information tools must be implemented.
- These tools should be interactive so that scientists could submit data related to new properties not originally contained in the databases.
- Entire scientific communities/environs supporting particular reference materials will be created making the metrology laboratories supporting these activities scientific information brokers rather than just data providers.
- Significant challenges (technical and cultural) still remain.

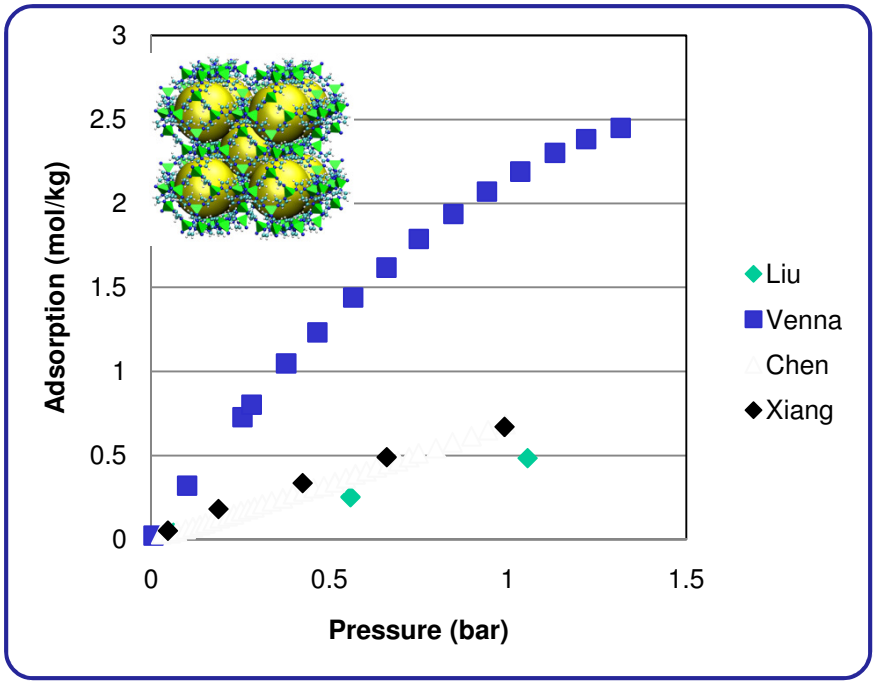
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- Specimen Bank Group
- Environmental Measurements Science Group

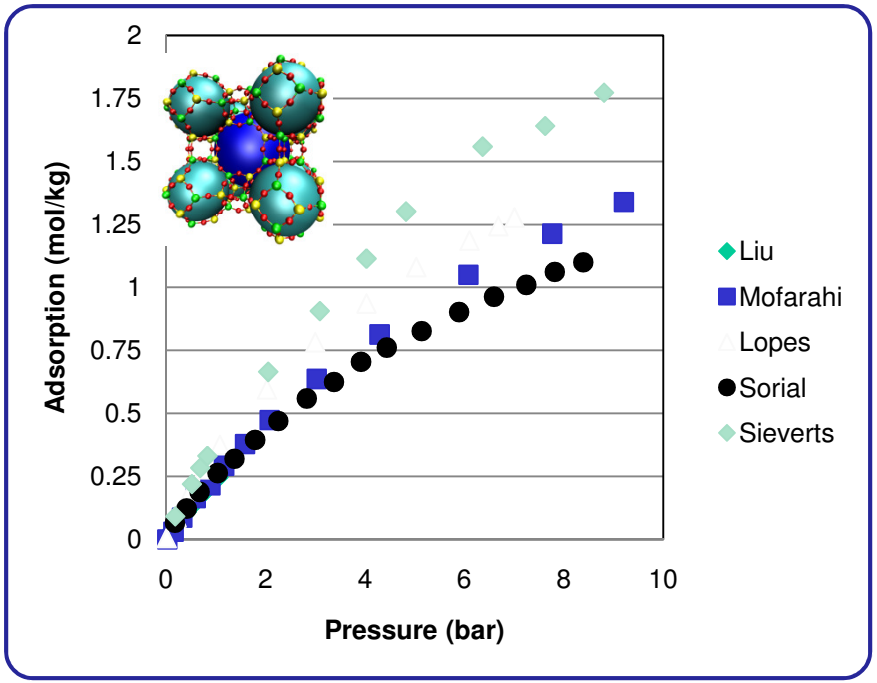
NIST / ARPA-E Database of Novel and Emerging Adsorbent Materials

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.

Let Us Meet Again

We welcome you all to our future conferences of OMICS Group International

Please Visit:

http://materialsscience.conferenceseries.com/

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