Fall 10-2-2012

NIST Databases for Materials Research

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NIST Databases for Materials Research

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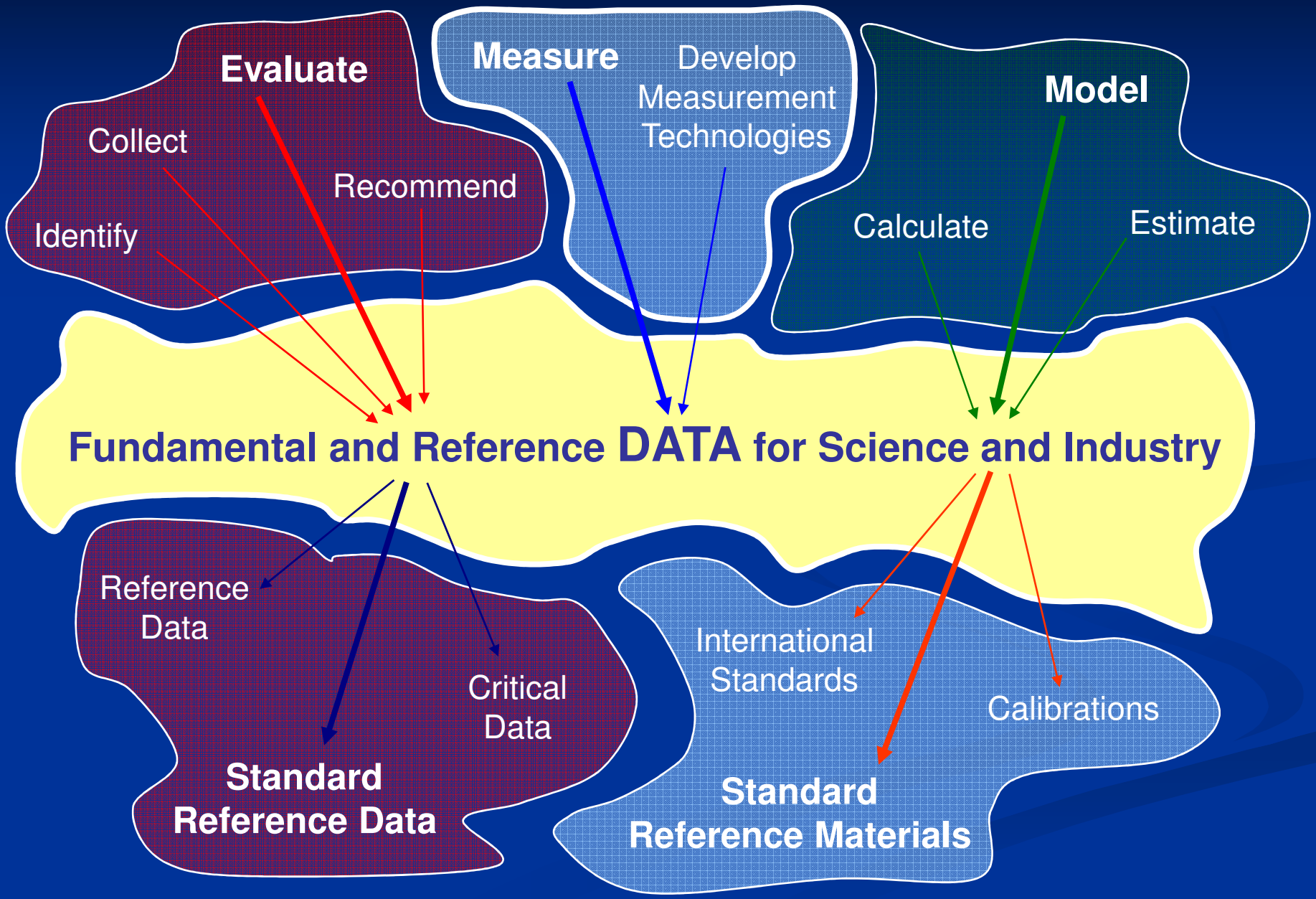
NIST Data Activities



NIST Role for Standards Setting Organizations

- **NIST is a research agency that provides critical data and measurement technologies for use in science and industry**
- **NIST is not a standards setting body, but provides reference data for "realizing" standards which are formally adopted by standards setting organizations**

- ***The* International Temperature Scale (for example)**
- **ITS-90 is realized, maintained and disseminated by NIST to provide a standard scale of temperature and was adopted by the International Committee of Weights and Measures (*CIPM*) as the official international temperature scale on January 1, 1990**
- **NIST reference tables of thermocouple electromotive force (emf) versus temperature have been adopted as standards by the American Society for Testing and Materials (*ASTM*)**

Standards Settings Bodies that Adopt NIST Realizations and Recommendations

- **International Association for the Properties of Water and Steam (*IAPWS*)**
- **International Commission on Radiation Units & Measurements (*ICRU*)**
- **International Union for Pure and Applied Chemistry (*IUPAC*)**
- **Committee on Data for Science and Technology (*CODATA*)**
- **International Union for Pure and Applied Physics (*IUPAP*)**
- **General Conference on Weights and Measures (*CGPM*)**
- **International Bureau of Weights and Measures (*BIPM*)**
- **International Organization for Standardization (*ISO*)**
- **American Society for Testing and Materials (*ASTM*)**
- **American National Standards Institute (*ANSI*)**
- **International System of Units (*SI*)**

NIST is a Primary Source of Reference Data

In addition to measuring, compiling, and evaluating critical reference data, NIST has published for over four decades much of the Standard Reference Data that is used in the physical and chemical sciences.

- ***National Standard Reference Data Series*** **(NSRDS): 1965-1987**
- ***Journal of Physical and Chemical Reference Data*** **(JPCRD): 1972-present**

Under the 1963 Standard Reference Data Act (Public Law 90-396) NIST has the primary responsibility in the Federal Government for providing reliable scientific and technical reference data.

CO…nts

NIST is…four years)

- Spee…
- Charg…
- Mass…
- Boltzm…
- Planc…
- Rydb…
- Avoga…
- Farad…
- Fine-…
- Gravi…
- Electr…
- Atomi…
- Electr…
- and o…

These c…odern *Physics*

Fundamental Physical Constants — Frequently used constants

Quantity	Symbol	Value	Unit	Relative std. uncert. u_r
speed of light in vacuum	c, c_0	299 792 458	m s^{-1}	(exact)
magnetic constant	μ_0	$4\pi \times 10^{-7}$	N A^{-2}	
		$= 12.566\,370\,614... \times 10^{-7}$	N A^{-2}	(exact)
electric constant $1/\mu_0 c^2$	ϵ_0	$8.854\,187\,817... \times 10^{-12}$	F m^{-1}	(exact)
Newtonian constant of gravitation	G	$6.674\,28(67) \times 10^{-11}$	m^3 kg^{-1} s^{-2}	1.0×10^{-4}
Planck constant	h	$6.626\,068\,96(33) \times 10^{-34}$	J s	5.0×10^{-8}
$h/2\pi$	$\hbar$	$1.054\,571\,628(53) \times 10^{-34}$	J s	5.0×10^{-8}
elementary charge	e	$1.602\,176\,487(40) \times 10^{-19}$	C	2.5×10^{-8}
magnetic flux quantum $h/2e$	Φ_0	$2.067\,833\,667(52) \times 10^{-15}$	Wb	2.5×10^{-8}
conductance quantum $2e^2/h$	G_0	$7.748\,091\,7004(53) \times 10^{-5}$	S	6.8×10^{-10}
electron mass	m_e	$9.109\,382\,15(45) \times 10^{-31}$	kg	5.0×10^{-8}
proton mass	m_p	$1.672\,621\,637(83) \times 10^{-27}$	kg	5.0×10^{-8}
proton-electron mass ratio	m_p/m_e	1836.152 672 47(80)		4.3×10^{-10}
fine-structure constant $e^2/4\pi\epsilon_0\hbar c$	α	$7.297\,352\,5376(50) \times 10^{-3}$		6.8×10^{-10}
inverse fine-structure constant	α^{-1}	137.035 999 679(94)		6.8×10^{-10}
Rydberg constant $\alpha^2 m_e c/2h$	R_∞	10 973 731.568 527(73)	m^{-1}	6.6×10^{-12}
Avogadro constant	N_A, L	$6.022\,141\,79(30) \times 10^{23}$	mol^{-1}	5.0×10^{-8}
Faraday constant $N_A e$	F	96 485.3399(24)	C mol^{-1}	2.5×10^{-8}
molar gas constant	R	8.314 472(15)	J mol^{-1} K^{-1}	1.7×10^{-6}
Boltzmann constant R/N_A	k	$1.380\,6504(24) \times 10^{-23}$	J K^{-1}	1.7×10^{-6}
Stefan-Boltzmann constant $(\pi^2/60)k^4/\hbar^3 c^2$	σ	$5.670\,400(40) \times 10^{-8}$	W m^{-2} K^{-4}	7.0×10^{-6}
Non-SI units accepted for use with the SI				
electron volt: (e/C) J	eV	$1.602\,176\,487(40) \times 10^{-19}$	J	2.5×10^{-8}
(unified) atomic mass unit $1\ \mathrm{u} = m_u = \frac{1}{12} m(^{12}\mathrm{C})$ $= 10^{-3}$ kg mol$^{-1}/N_A$	u	$1.660\,538\,782(83) \times 10^{-27}$	kg	5.0×10^{-8}

NIST Data Products and Activities

- Online Databases
- Electronic Databases (PC)
- Print Databases

- Standard Reference Materials
- Calibrations

- Measurement Technologies

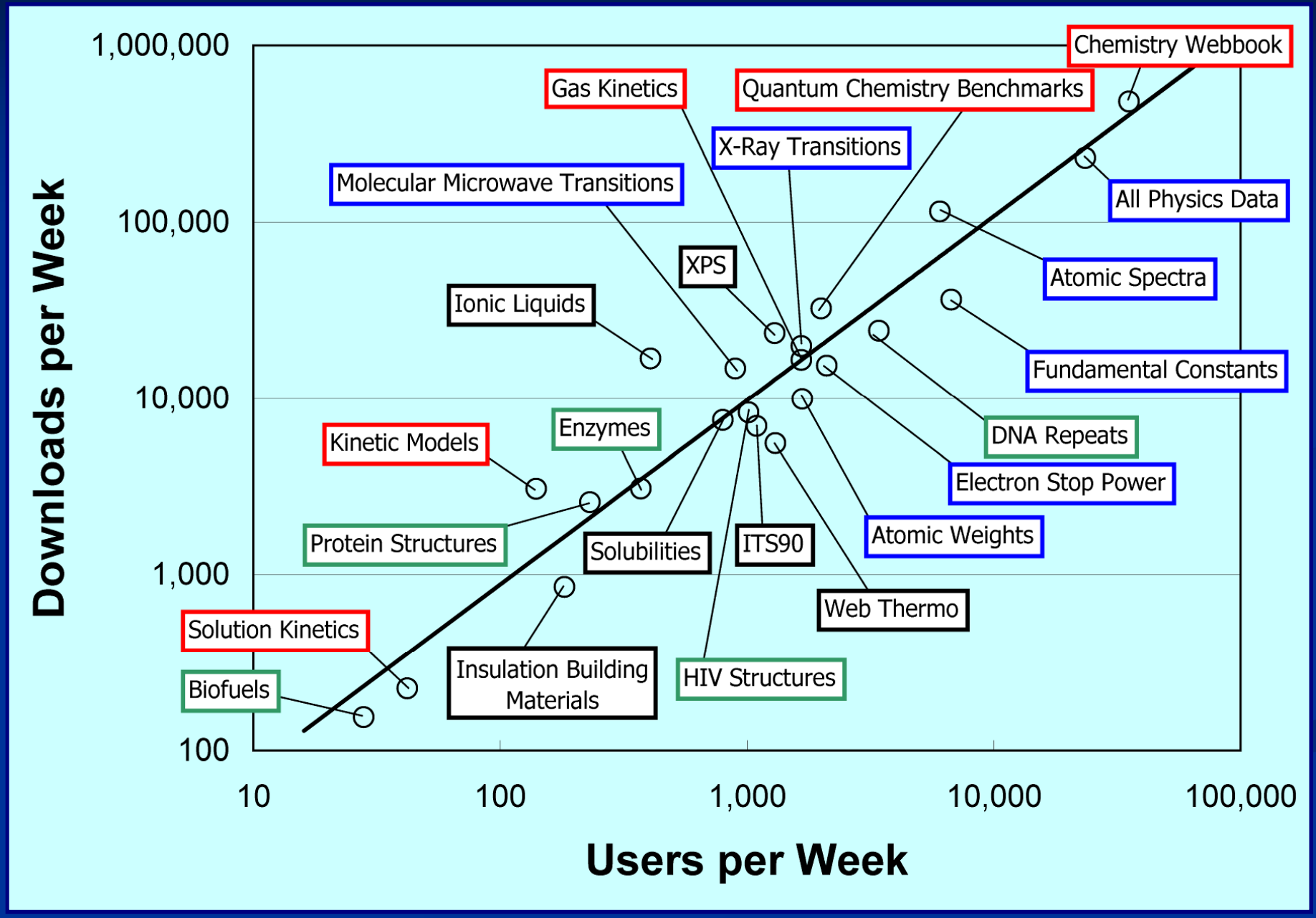
❑ Some for *FREE*

❑ Some for *FEE*

$ nominal costs for distributing databases (~$100-200)

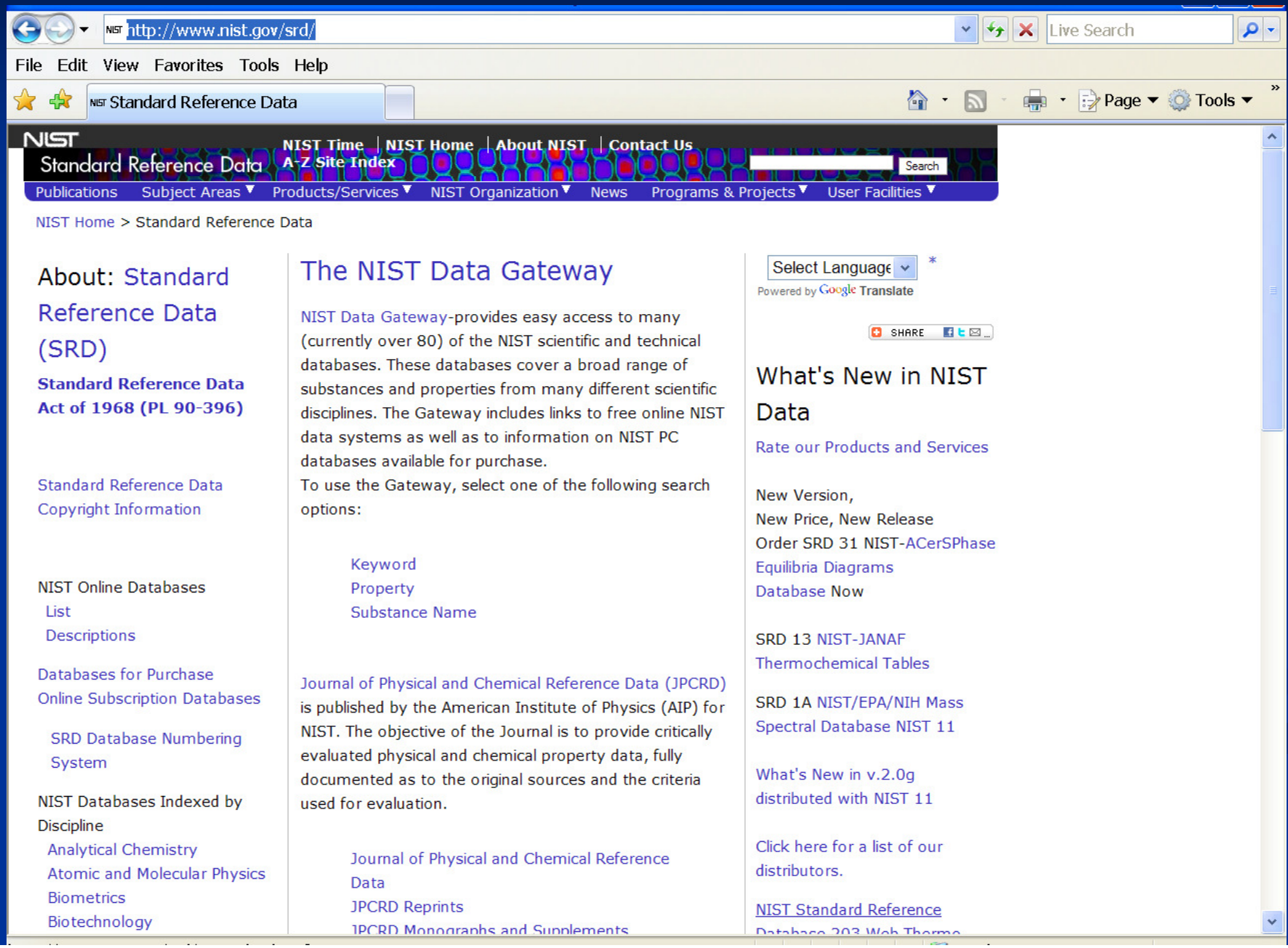
$$$ maintaining, expanding, and improving databases (~$1500-5000)

NIST Data Online



The NIST Data Gateway

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



Achieving the Vision

Next Steps

1. The DOE Office of Science and NSF will work together to enable the development, maintenance, and deployment of reliable, interoperable, and reusable software for the next-generation design of matter. The DOE, through its *Computational Materials and Chemistry by Design* program, and NSF, through aspects of its *Cyberinfrastructure Framework for 21st Century Science and Engineering*, will coordinate activities on the development of high quality production software toolkits that both incorporate new algorithms and allow for interoperability with existing software tools.
2. In support of their advanced software programs, both the DOE and NSF will also coordinate activity in the development of next-generation characterization tools that provide the fundamental basis for development of and validation of the algorithms and software tools.
3. An *Advanced Materials by Design* program led by NIST will target the development of standards infrastructure, reference databases, and centers of excellence that will enable reliable computer modeling and simulation for materials discovery and optimization. This activity will be coordinated closely with the DOE and NSF efforts on software and experimental tool design.

for rapidly verifying fitness of new materials for intended use.

6. NSF and DOD will play a lead role in addressing the next-generation workforce goals by: facilitating new partnerships between the relevant science and engineering communities in academia, government and industry to promote a culture supporting and embracing the use of the capabilities developed within this initiative; and engaging with students and colleagues to develop the culture and relevant training of the next-generation workforce.

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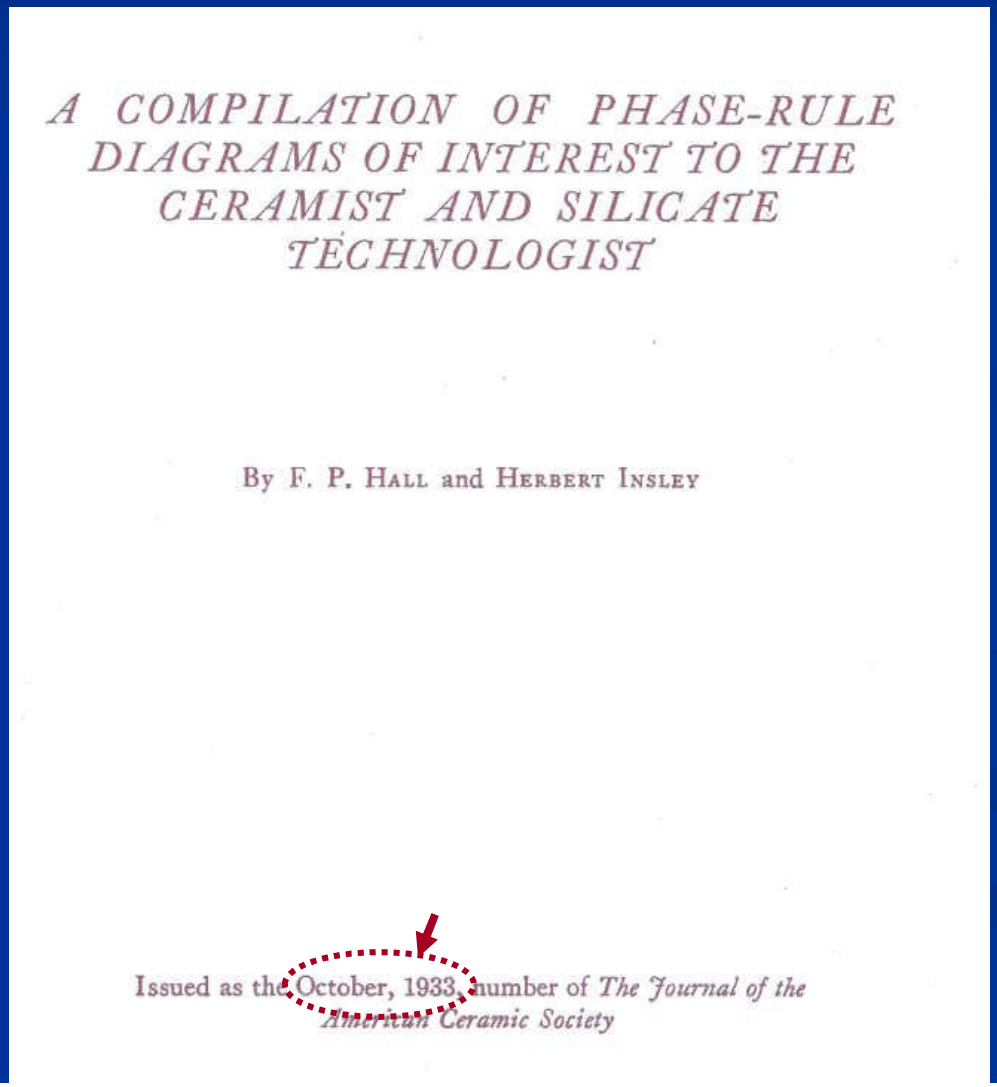
Phase Equilibria Diagrams Database

NIST SRD 31: http://www.nist.gov/srd/nist31.cfm

- **Began in 1933 via NIST-ACerS collaboration**



A COMPILATION OF PHASE-RULE DIAGRAMS OF INTEREST TO THE CERAMIST AND SILICATE TECHNOLOGIST

By F. P. Hall and Herbert Insley

Issued as the October, 1933, number of *The Journal of the American Ceramic Society*

Use of Phase Equilibria Diagrams

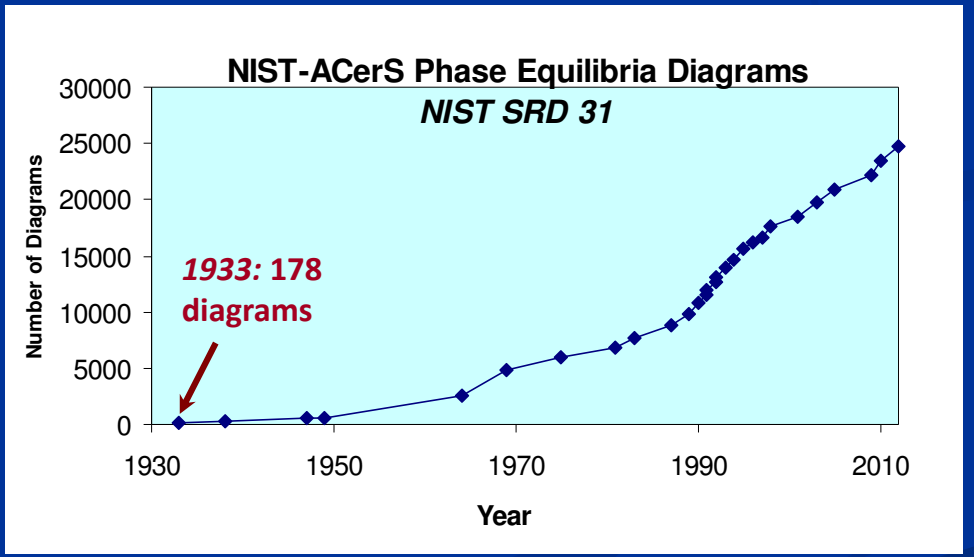
- **Phase equilibrium diagrams delineate the most fundamental properties of materials: *the conditions (temperature, pressure, composition) under which pure compounds and their mixtures are thermodynamically stable.***

- **Reliable data therefore provide essential thermo-chemical guidance for the technical exploitation of materials.**

Phase Equilibria Diagrams Database

NIST SRD 31: http://www.nist.gov/srd/nist31.cfm

- **Numerous material-system classes**
  - oxides
  - salts, halides
  - borides, carbides, silicides
  - pnictides: nitrides, phosphides, aresenides
  - chalcogenides, semiconductors: sulfides, selenides, tellurides
- **Continuous growth:**
  ~ 1,000 diagrams per year
- **Published data:**
  - 18,000 figures with ~ 26,000 diagrams
- **Unpublished data:**
  - ~ 25,000 entries with ~ 50,000 diagrams
  - sorted/searchable by chemical system
  - "INFO" file of ~ 6,000 literature references



contact: terrell.vanderah@nist.gov

Phase Equilibria Diagrams Database

NIST SRD 31: http://www.nist.gov/srd/nist31.cfm

Data Center Process

1. Search original literature
2. Identify, classify new entries
3. Enter citation and chemistry into database
4. Select material to be evaluated
5. Write critical evaluations/commentaries
6. Enter commentaries into database
7. Digitize evaluated diagrams
8. Edit commentaries and digitized diagrams
9. Publish content

http://www.nist.gov/srd/nist31.cfm

NIST Standard Reference Database 31 - Windows Internet Explorer

http://www.nist.gov/srd/nist31.cfm

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NIST Home > SRD > NIST Standard Reference Database 31

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- Analytical Chemistry
- Atomic and Molecular Physics
- Biometrics
- Biotechnology
- Chemical and Crystal Structure
- Chemical Kinetics
- Chemistry
- Communications
- Construction
- Environmental Data
- Fire
- Fluids
- International Trade
- Law Enforcement
- Materials Properties
- Mathematical Databases, Software and Tools
- Optical Character Recognition
- Personal Identity Verification

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Select Language

Powered by Google Translate

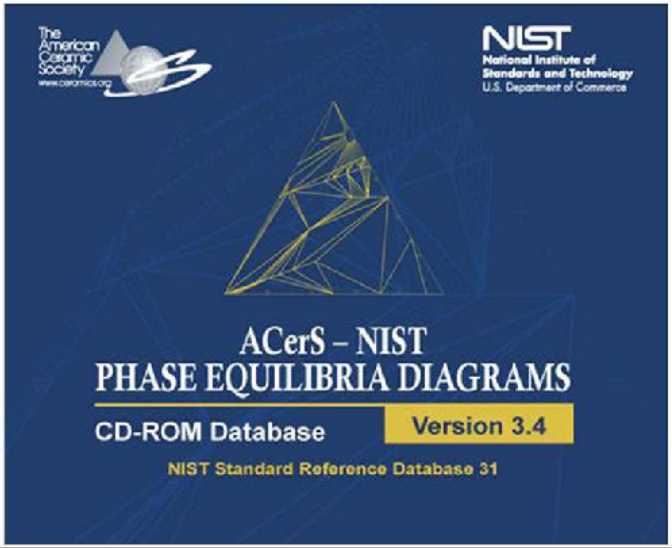
New release, Version 3.4

NIST Standard Reference Database 31

ACerS-NIST Phase Equilibria Diagrams Database:

(formerly known as *Phase Diagrams for Ceramists*)

Rate our Products and Services



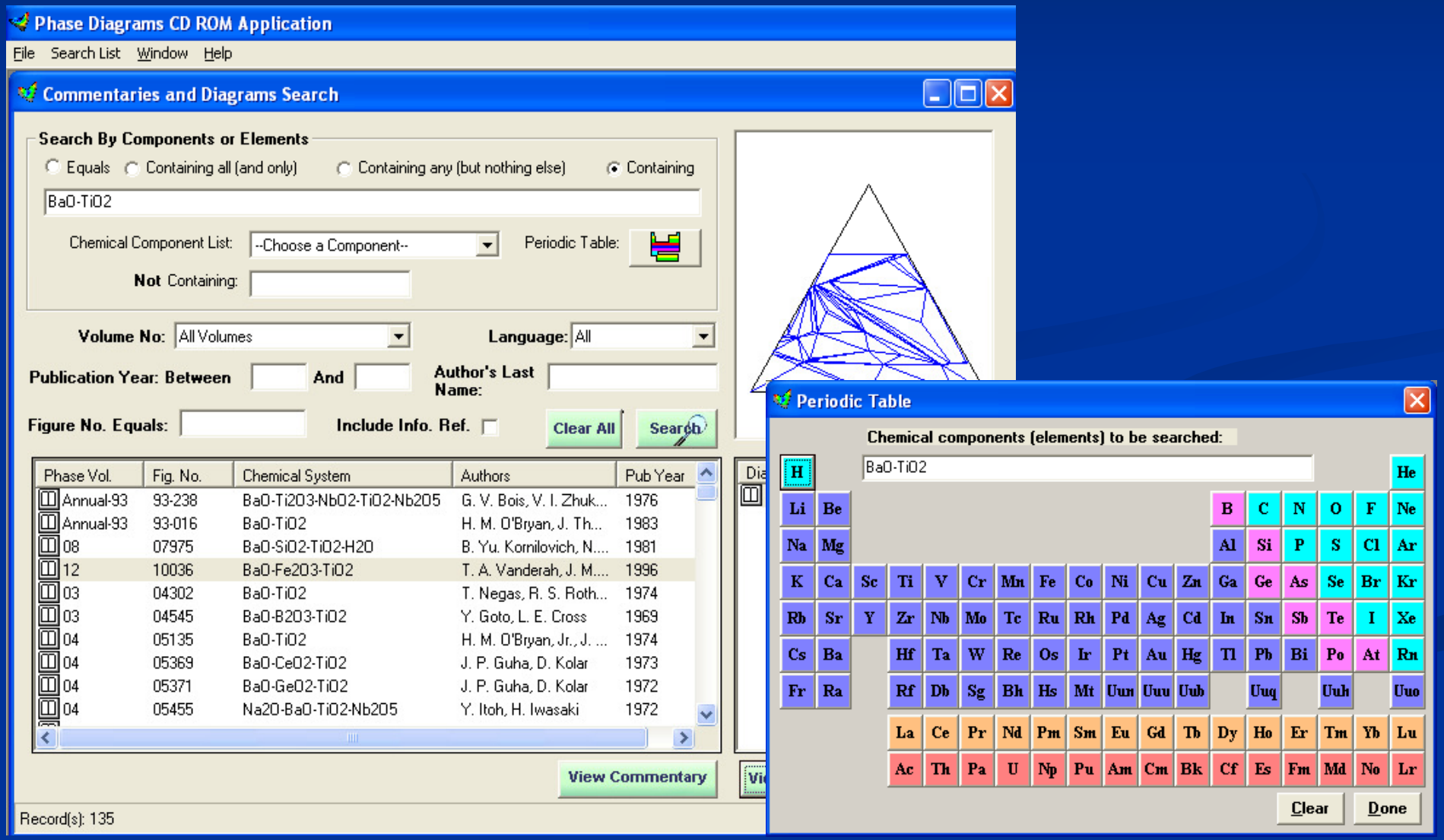
Done | Local intranet | 100%

start | Inbox - Micro... | Art Work+Ad... | Eudora | Microsoft Po... | NIST Standar... | 7:37 PM

Phase Equilibria Diagrams Database

NIST SRD 31: http://www.nist.gov/srd/nist31.cfm

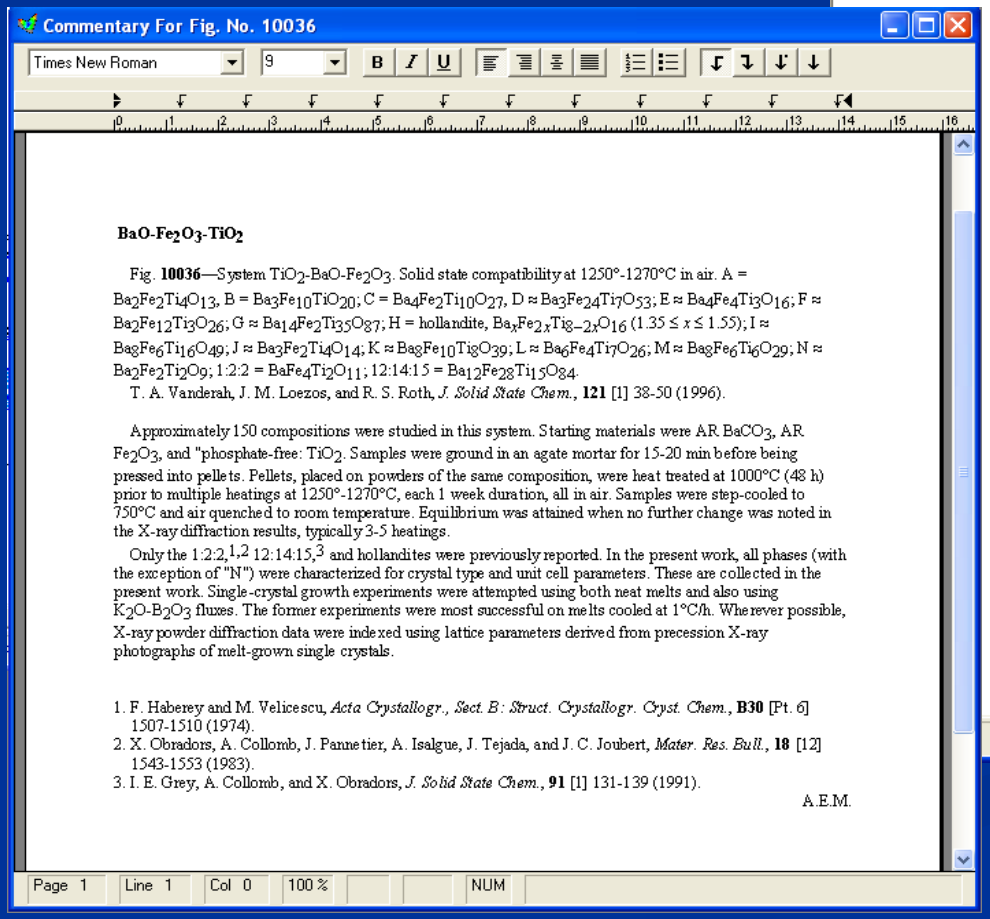
- ***Search interface:*** **by reference, element, component, figure no., volume**

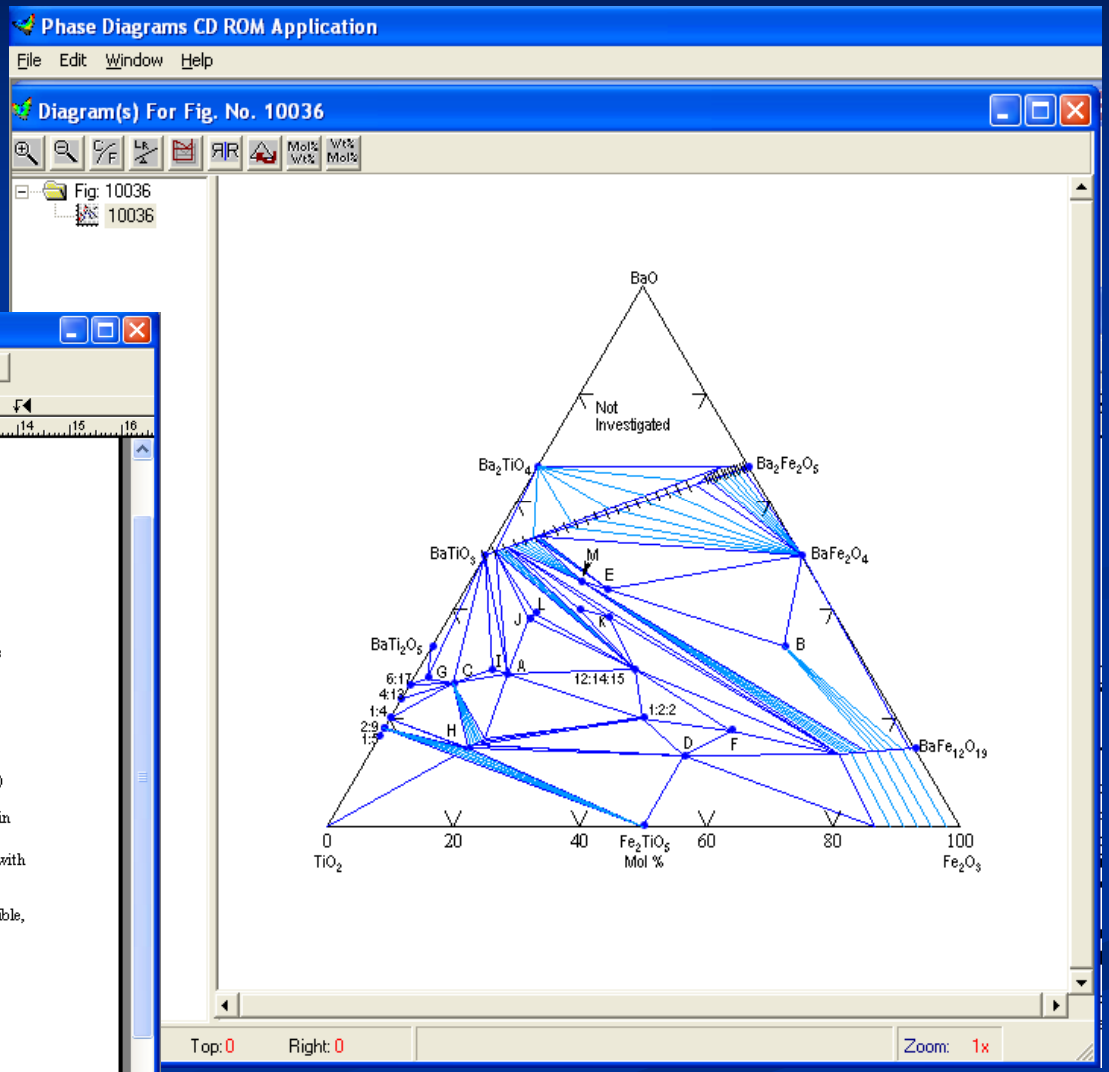


Phase Equilibria Diagrams Database

NIST SRD 31: http://www.nist.gov/srd/nist31.cfm

- ***Display:*** **Phase Diagram and Commentary data**



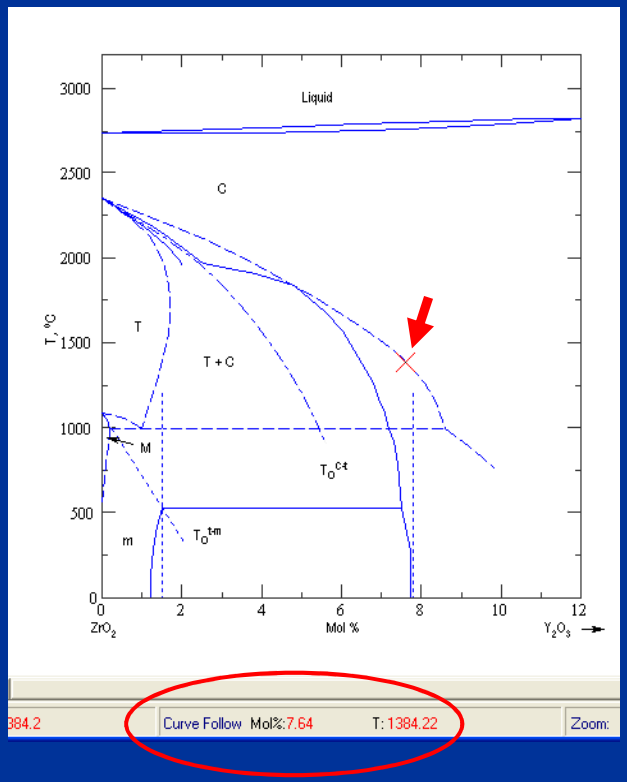


Phase Equilibria Diagrams Database

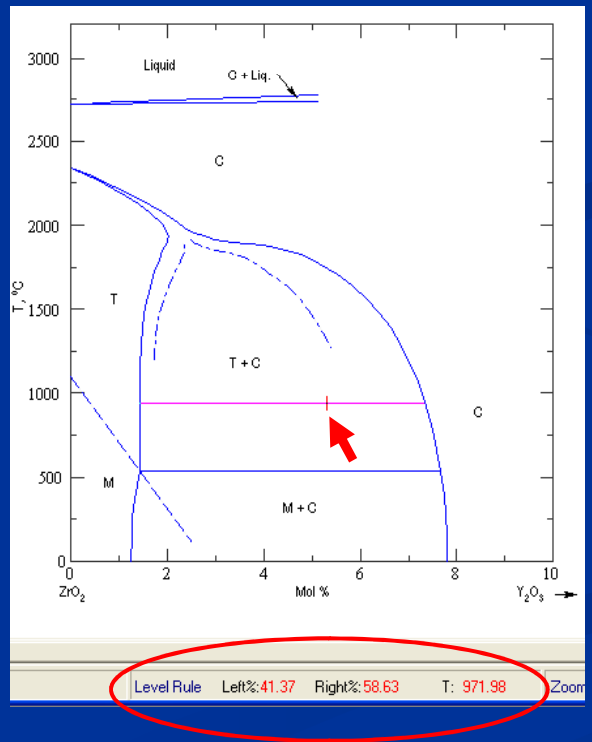
NIST SRD 31: http://www.nist.gov/srd/nist31.cfm

- **Built-in functions allow user to track coordinates, zoom, convert mol%↔wt%, use level rule, overlay diagrams, rotate ternaries**

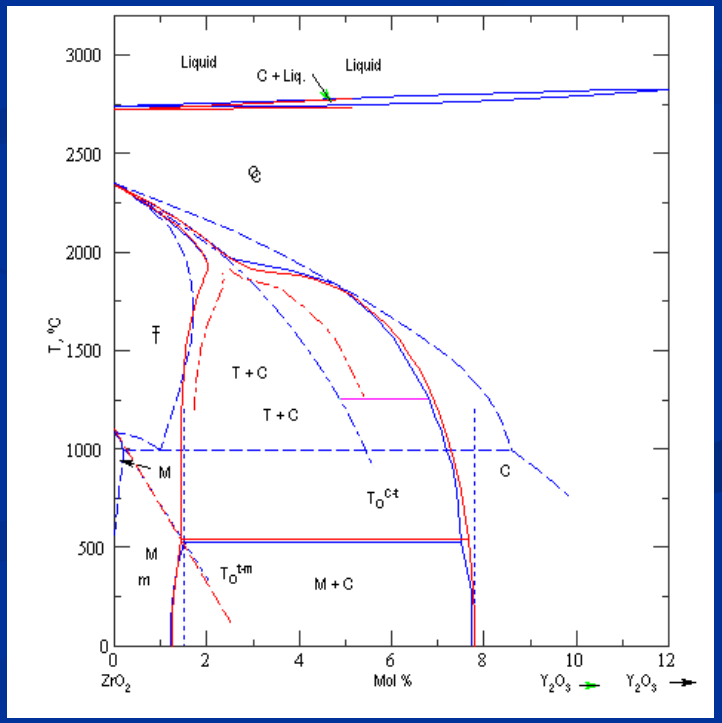
Curve Follow



Lever Rule



Overlay Diagrams



- Price recently reduced by ~2/3 ($3K → $950)
- Recent investments:

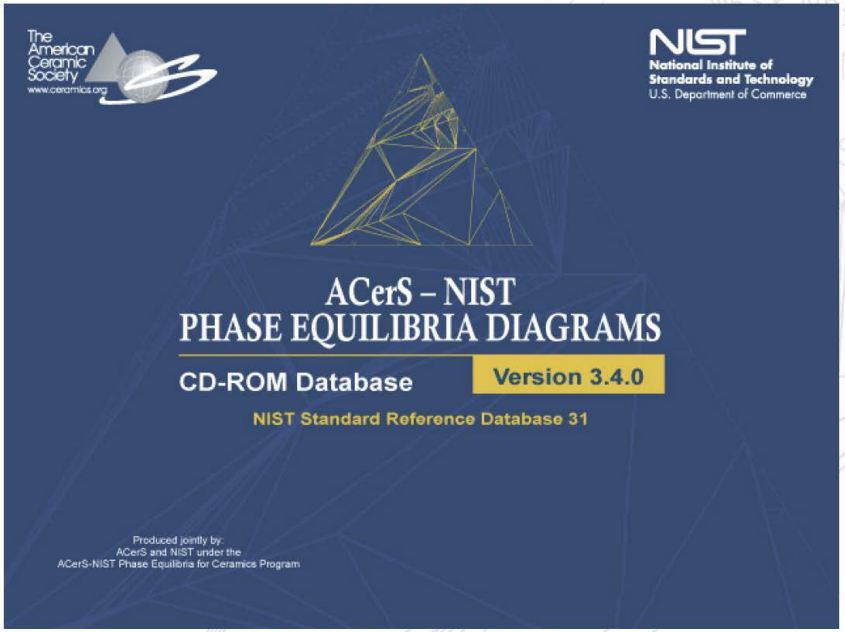
  >$0.5 M, all-new software, hardware, physical space

NIST Standard Reference Database 31

ACerS-NIST Phase Equilibria Diagrams Database

New Release, Version 3.4

New release
New, lower price



892 new entries

1,400 new diagrams

24,800 total diagrams

http://www.nist.gov/srd/nist31.cfm

ORDER NOW:

CD ROM Pricing:

Single User full version - $950.00
Single User annual upgrade - $250.00
Single User Upgrade from Version 3.2 - $500.00
Single User Upgrade from Version. 3.1 - $750.00
Multiple User full version - $1625.00
Multiple User annual upgrade - $425.00
Multiple User annual upgrade from Version 3.2 - $850.00
Multiple User annual upgrade from Version 3.1 - $1275.00

For more information, please contact:
National Institute of Standards and Technology
Standard Reference Data Program
(301) 975-2200
data@nist.gov

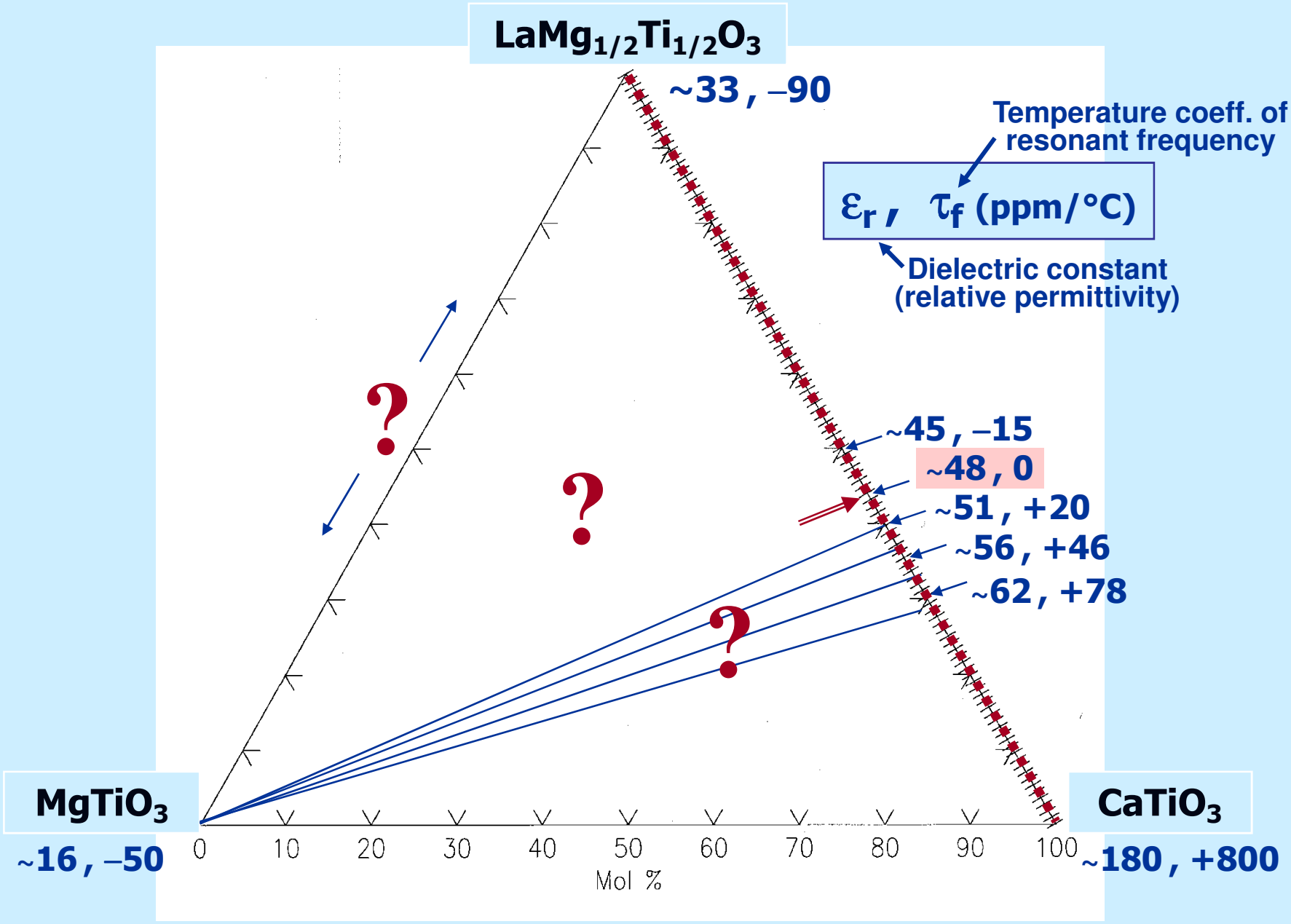
Rational Processing

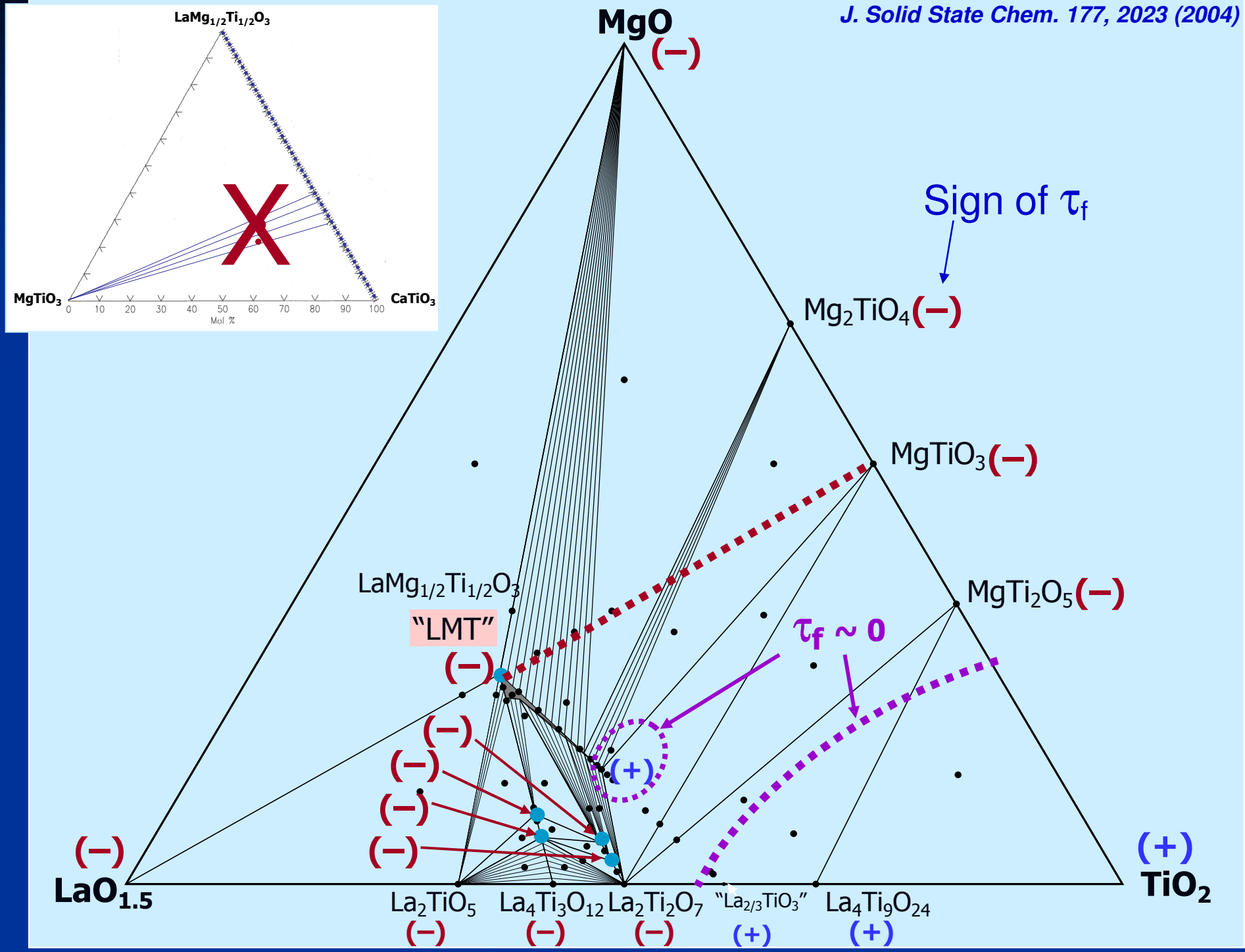
- **Reliable phase equilibrium diagrams are particularly useful when the exploitable properties are additive.**
- **Example: microwave dielectric ceramics**

$44LaMg_{1/2}Ti_{1/2}O_3$–$56CaTiO_3$ solid solution

- *of interest for resonators/filters*
- *dielectric constant ~48, temperature coefficient$_{(f)}$ ~0*
- *$\rightarrow$ need to improve dielectric loss*

$LaMg_{1/2}Ti_{1/2}O_3$–$CaTiO_3$ solid solution




J. Solid State Chem. 177, 2023 (2004)
MgO
(–)
Sign of τ_f
Mg_2TiO_4(–)
$MgTiO_3$(–)
$MgTi_2O_5$(–)
$LaMg_{1/2}Ti_{1/2}O_3$
"LMT"
(–)
$\tau_f \sim 0$
(+)
(–)
(–)
(–)
(–)
(–)
$LaO_{1.5}$
La_2TiO_5
$La_4Ti_3O_{12}$
$La_2Ti_2O_7$
"$La_{2/3}TiO_3$"
$La_4Ti_9O_{24}$
(–)
(–)
(–)
(+)
(+)
(+)
TiO_2
$LaMg_{1/2}Ti_{1/2}O_3$
X
$MgTiO_3$
$CaTiO_3$
0 10 20 30 40 50 60 70 80 90 100
Mol %

NIST Crystallographic Databases

- NIST Standard Reference Databases:
  - **SRD 3: NIST Crystal Data (~237,000 entries)**
    - **Inorganic and organic crystalline materials**
    - **Crystallographic information without atomic coordinates**
  - **SRD 83: NIST Structural Database (~60,000 entries)**
    - **Metals and inter-metallics**
    - **Atomic coordinates and structure types**
  - **SRD 84: FIZ/NIST Inorganic Crystal Structure Database (ICSD, ~150,000 entries)**
    - **Inorganic materials**
    - **Refined structure information**

contact: vicky.karen@nist.gov

FIZ-NIST Inorganic Crystal Structure Database

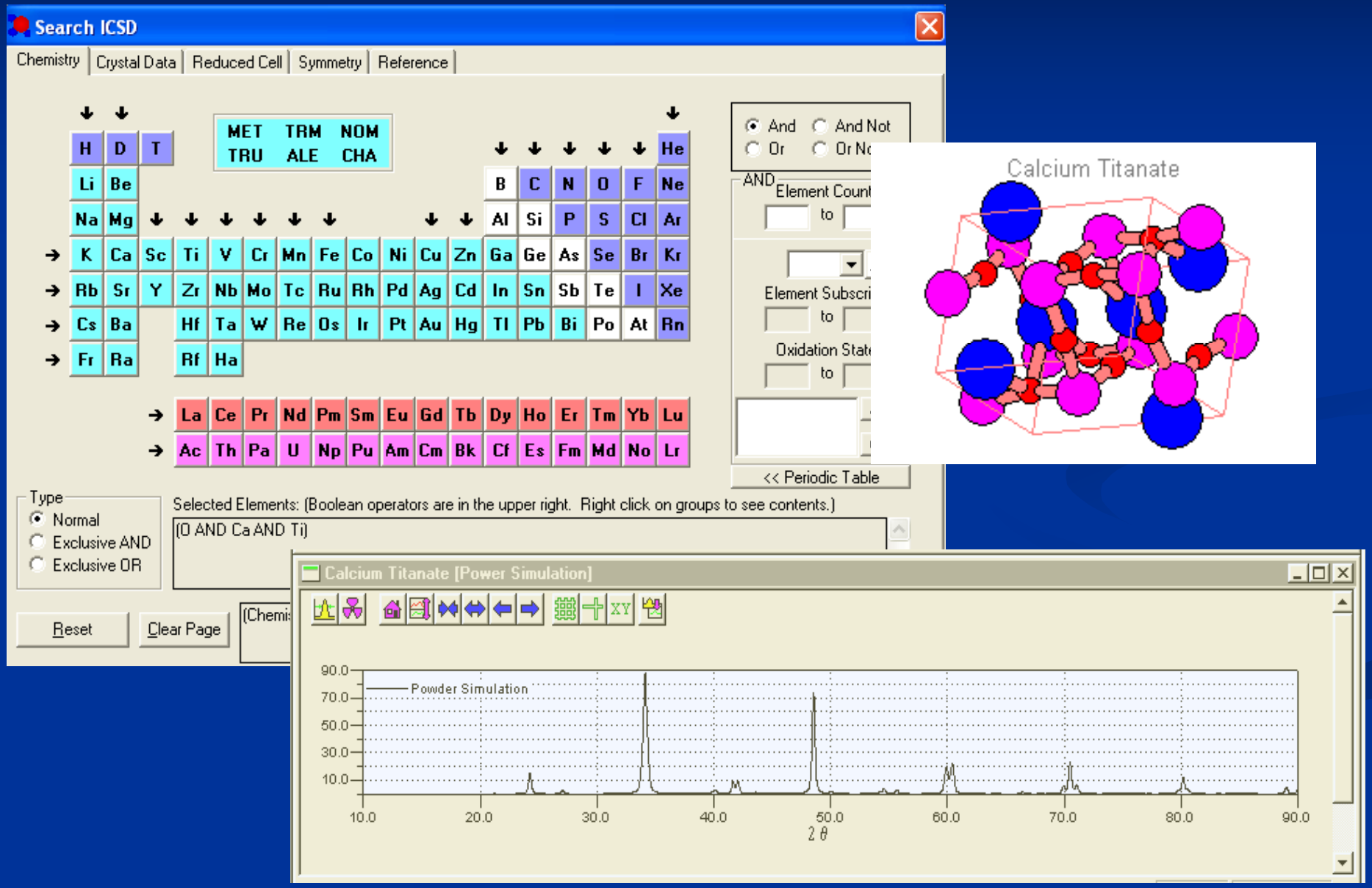
ICSD 150,042 entries, Release 2012-1

- **ICSD is a collection of crystal-structure data entries for non-organic compounds including inorganics, ceramics, minerals, pure elements, metals, and intermetallics.**
- **Data items added by experts or generated by computer programs include Wyckoff sequence, Pearson symbol, molecular formula and weight, calculated density, chemical valence, "ANX" formula, minimum interatomic distances, reduced and standard cells, mineral groups and names.**
- **The entries in the database are characterized by and can be retrieved by chemical, crystallographic, computational, and textual searches.**

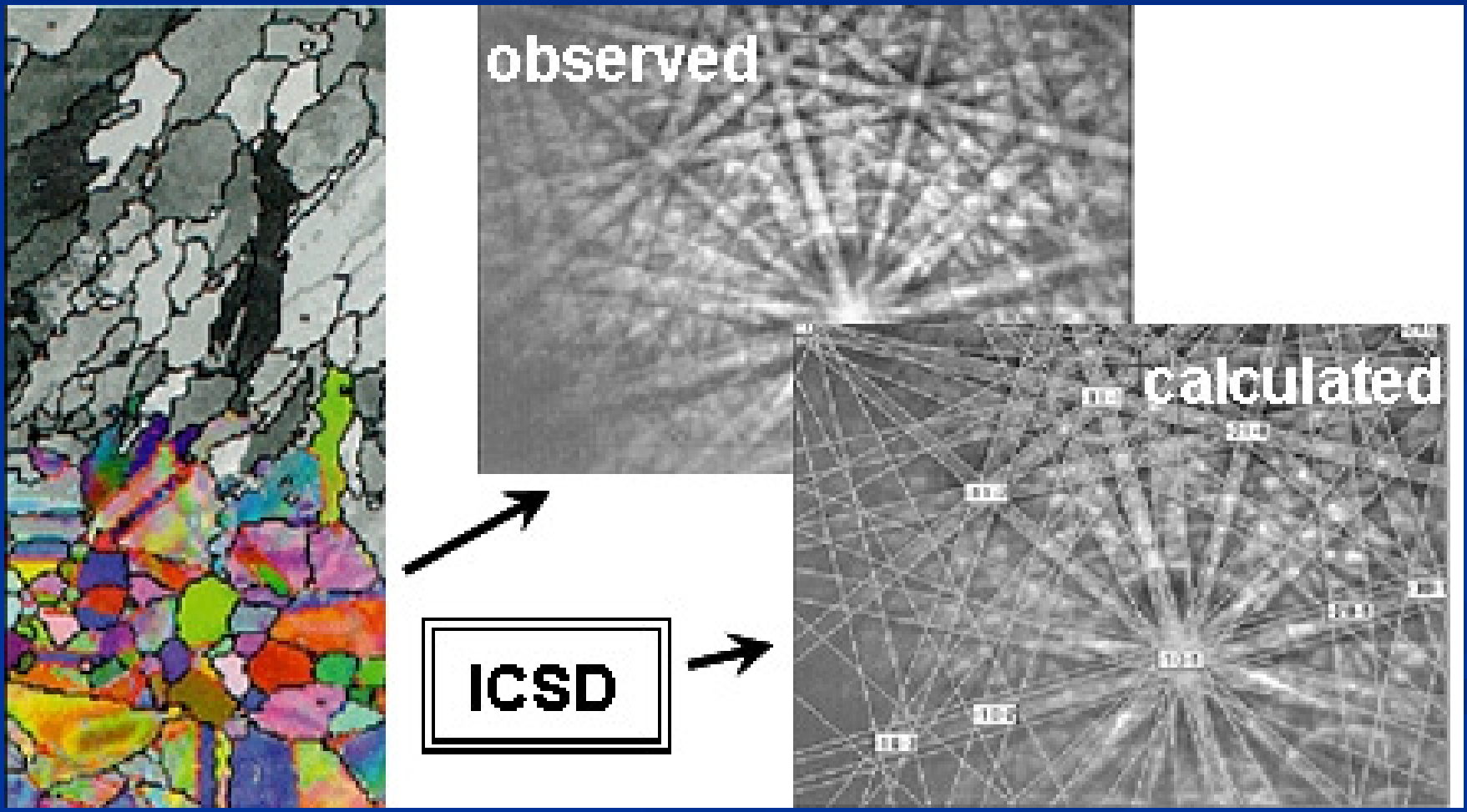
http://www.nist.gov/srd/nist84.cfm

contact: vicky.karen@nist.gov

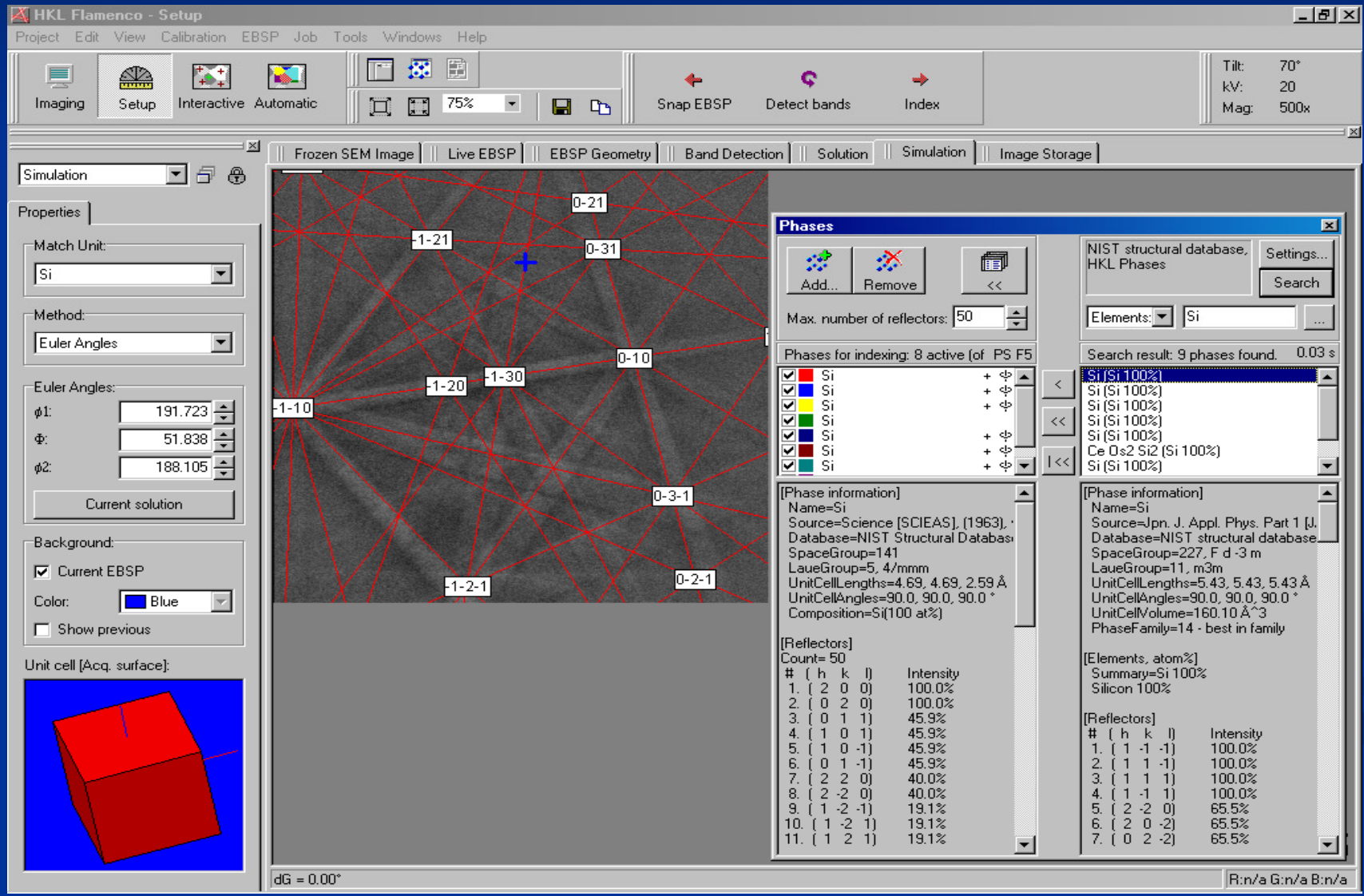
ICSD Database Applications



SRD 84 ICSD: Phase Identification by Electron Diffraction



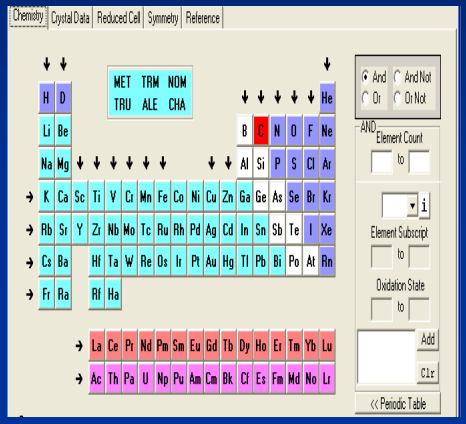
SRD 84 ICSD: Phase Identification by Electron Diffraction

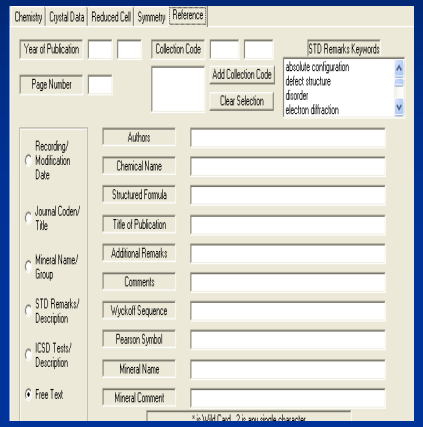


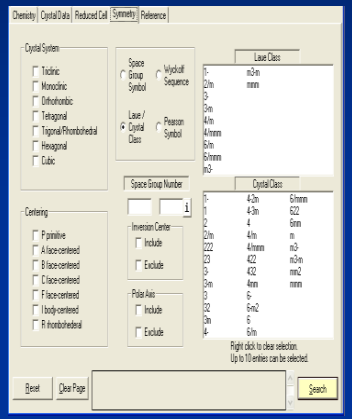
Vision of Crystallographic Database Applications in MGI

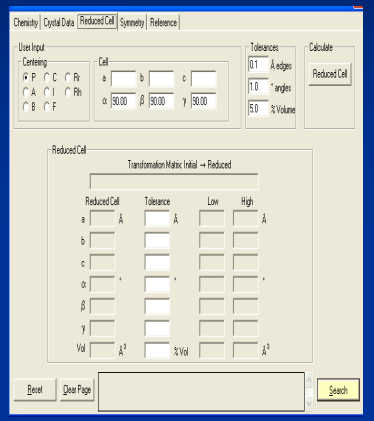
- **What can we do with the Crystallographic Databases:**
  - **Provide initial guidance in the designing stage**
    - Select materials based on known chemical/structural/symmetrical criteria.
    - *ab initio* calculation of properties using database information.
    - Data-mining and other methods for locating potential candidates.
  - **High-throughput phase identification in the experimental stage**
    - Lattice matching
    - Powder diffraction fingerprinting
    - Lattice-fringe fingerprinting
  - **Input for scientific simulation**, interfacing with other computational tools for data analysis and knowledge discovery.

New effort (2013): NIST Crystallographic Database Design to Accommodate MGI: *Intelligent Access to SRD 84*









More User Definable Views ....

Chemistry View

Literature View

Symmetry View

Application View

Relate Tables

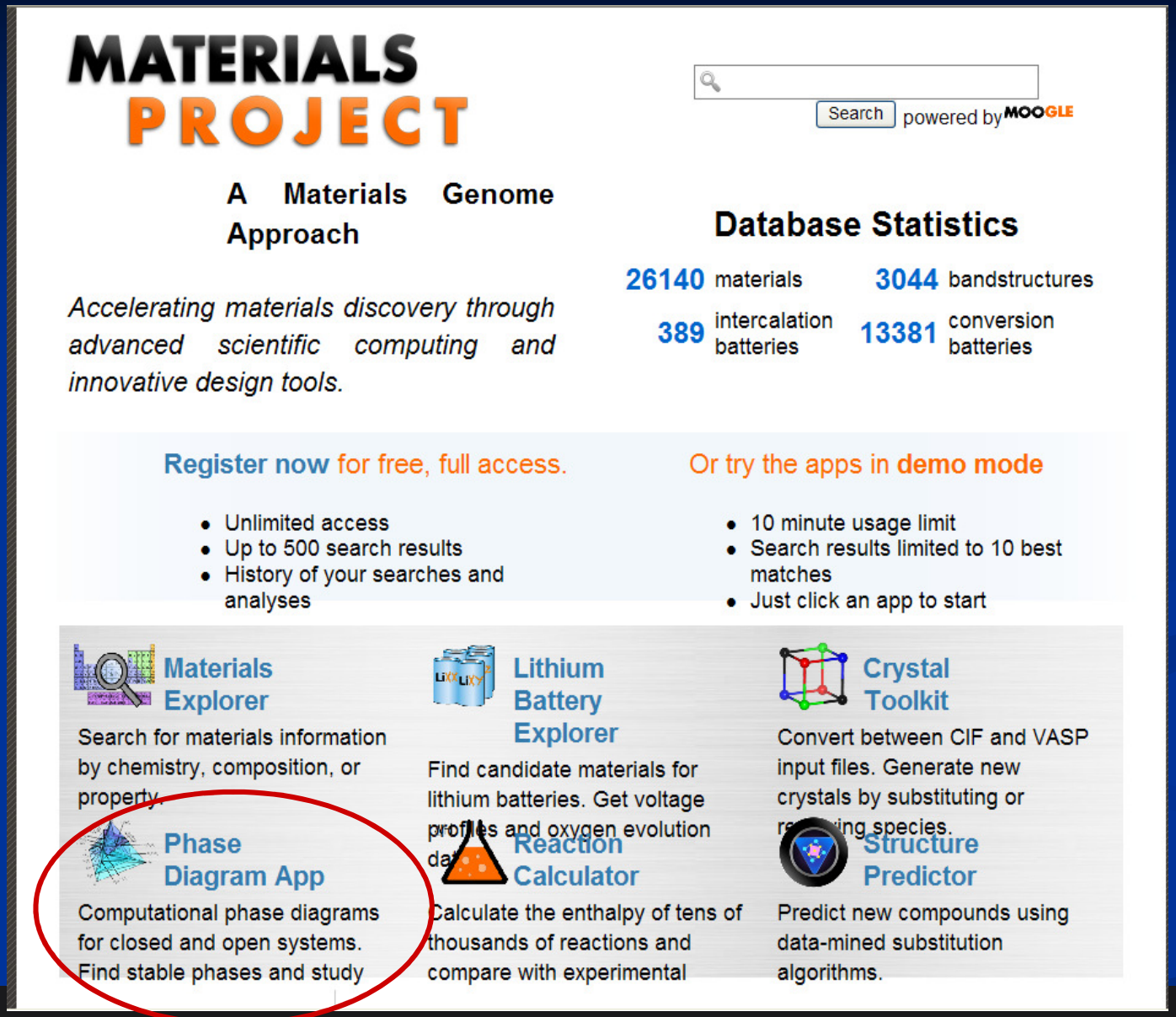
Chemistry | Reference | Density | Atomic Positions | Cell Parameters

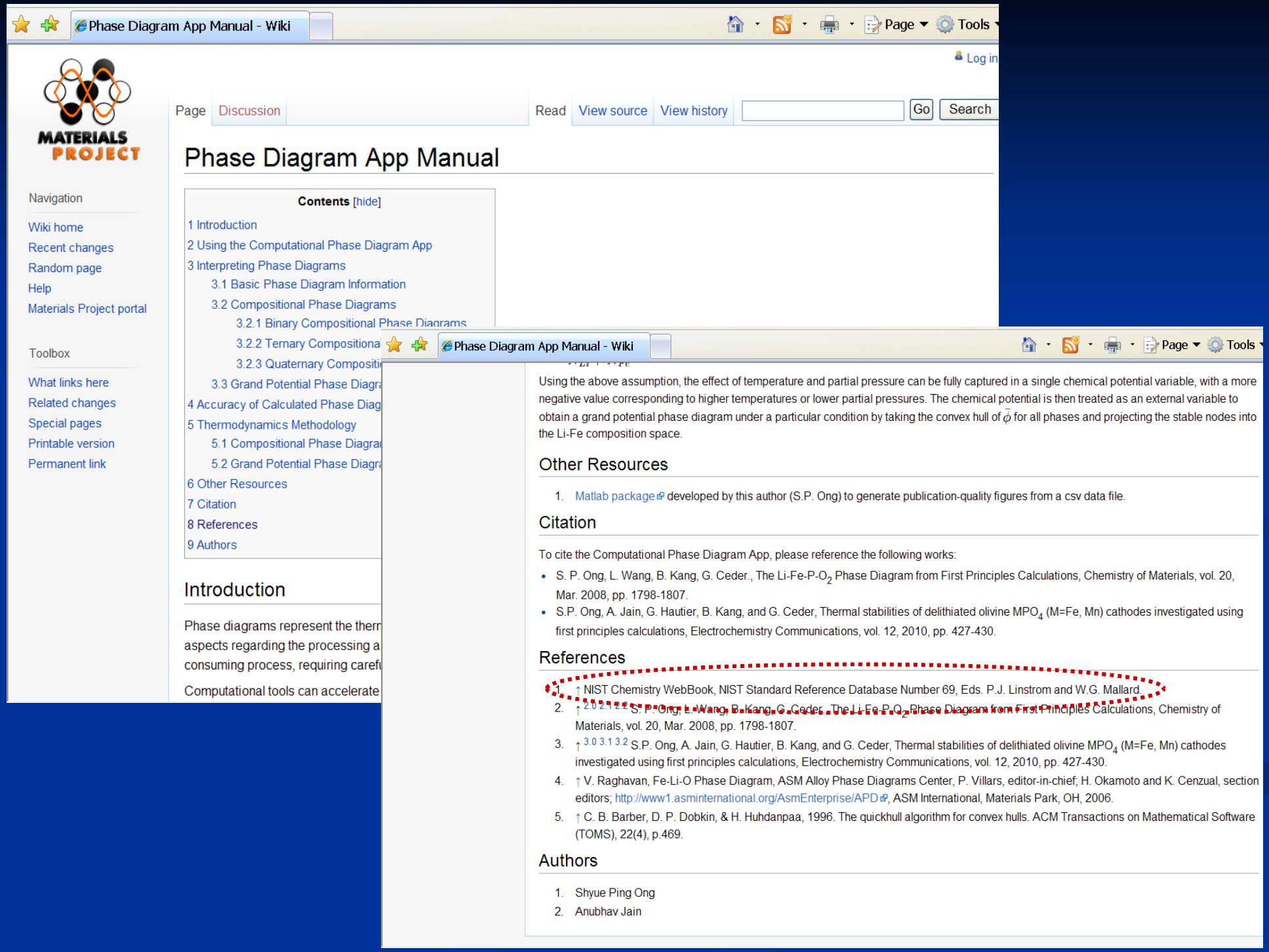
Literature Data

Reduced cell

Derived Data

http://www.materialsproject.org/

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Navigation
Wiki home
Recent changes
Random page
Help
Materials Project portal
Toolbox
What links here
Related changes
Special pages
Printable version
Permanent link
Contents [hide]
1 Introduction
2 Using the Computational Phase Diagram App
3 Interpreting Phase Diagrams
3.1 Basic Phase Diagram Information
3.2 Compositional Phase Diagrams
3.2.1 Binary Compositional Phase Diagrams
3.2.2 Ternary Compositiona
3.2.3 Quaternary Compositi
3.3 Grand Potential Phase Diagra
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Introduction
Phase diagrams represent the therr
aspects regarding the processing a
consuming process, requiring carefu
Computational tools can accelerate
Phase Diagram App Manual - Wiki
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Tools
Using the above assumption, the effect of temperature and partial pressure can be fully captured in a single chemical potential variable, with a more negative value corresponding to higher temperatures or lower partial pressures. The chemical potential is then treated as an external variable to obtain a grand potential phase diagram under a particular condition by taking the convex hull of $\bar{\phi}$ for all phases and projecting the stable nodes into the Li-Fe composition space.
Other Resources
1. Matlab package developed by this author (S.P. Ong) to generate publication-quality figures from a csv data file.
Citation
To cite the Computational Phase Diagram App, please reference the following works:
• S. P. Ong, L. Wang, B. Kang, G. Ceder., The Li-Fe-P-O2 Phase Diagram from First Principles Calculations, Chemistry of Materials, vol. 20, Mar. 2008, pp. 1798-1807.
• S.P. Ong, A. Jain, G. Hautier, B. Kang, and G. Ceder, Thermal stabilities of delithiated olivine MPO4 (M=Fe, Mn) cathodes investigated using first principles calculations, Electrochemistry Communications, vol. 12, 2010, pp. 427-430.
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1. ↑ NIST Chemistry WebBook, NIST Standard Reference Database Number 69, Eds. P.J. Linstrom and W.G. Mallard.
2. ↑ 2.0 2.1 2.2 S. P. Ong, L. Wang, B. Kang, G. Ceder., The Li-Fe-P-O2 Phase Diagram from First Principles Calculations, Chemistry of Materials, vol. 20, Mar. 2008, pp. 1798-1807.
3. ↑ 3.0 3.1 3.2 S.P. Ong, A. Jain, G. Hautier, B. Kang, and G. Ceder, Thermal stabilities of delithiated olivine MPO4 (M=Fe, Mn) cathodes investigated using first principles calculations, Electrochemistry Communications, vol. 12, 2010, pp. 427-430.
4. ↑ V. Raghavan, Fe-Li-O Phase Diagram, ASM Alloy Phase Diagrams Center, P. Villars, editor-in-chief; H. Okamoto and K. Cenzual, section editors; http://www1.asminternational.org/AsmEnterprise/APD, ASM International, Materials Park, OH, 2006.
5. ↑ C. B. Barber, D. P. Dobkin, & H. Huhdanpaa, 1996. The quickhull algorithm for convex hulls. ACM Transactions on Mathematical Software (TOMS), 22(4), p.469.
Authors
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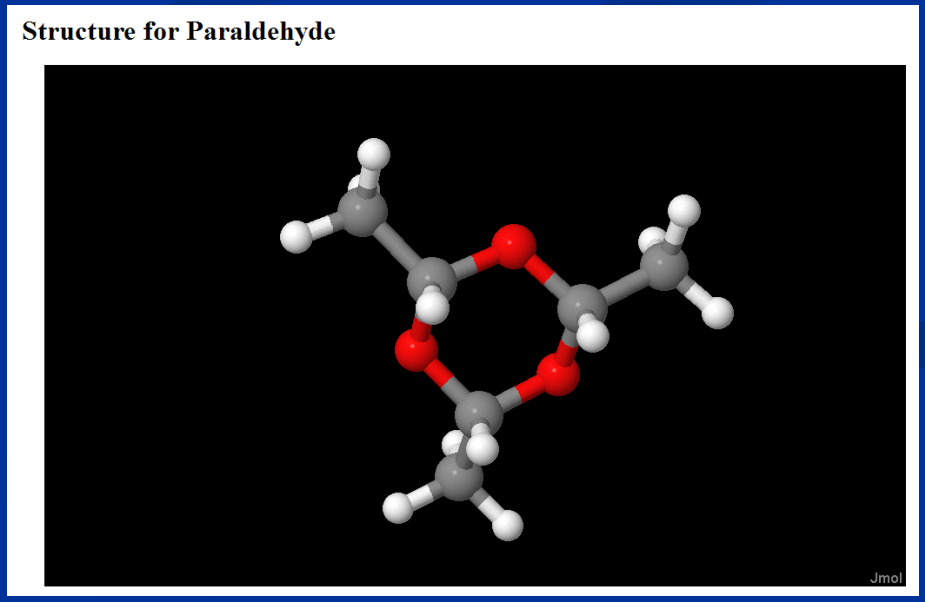
2. Anubhav Jain

The NIST Chemistry WebBook *(SRD 69)*

- Most widely used NIST data product
- Contains an extensive set of data for over 70,000 molecular species – *online since 1997 (!)*
  - Thermochemical and thermophysical properties
  - IR, UV/Vis, electronic and mass spectra
  - Ion and ion-cluster data

- Collects data from many NIST and non-NIST sources in one spot
- Used 24/7 worldwide - ~6,500 people a day
- 3-D structures can now be viewed online
- peter.linstrom@nist.gov



Chemistry WebBook Examples

State: $3d\ ^2E$

Energy (cm^{-1})	Med.	Transition	λ_{min} (nm)	λ_{max} (nm)	References
$T_o = 66536$	gas	$3d^2E''$-X	144	150	Herzberg and Shoosmith, 1956 Herzberg, 1961 DiGiuseppe, Hudgens, et al., 1982

Electronic spectra

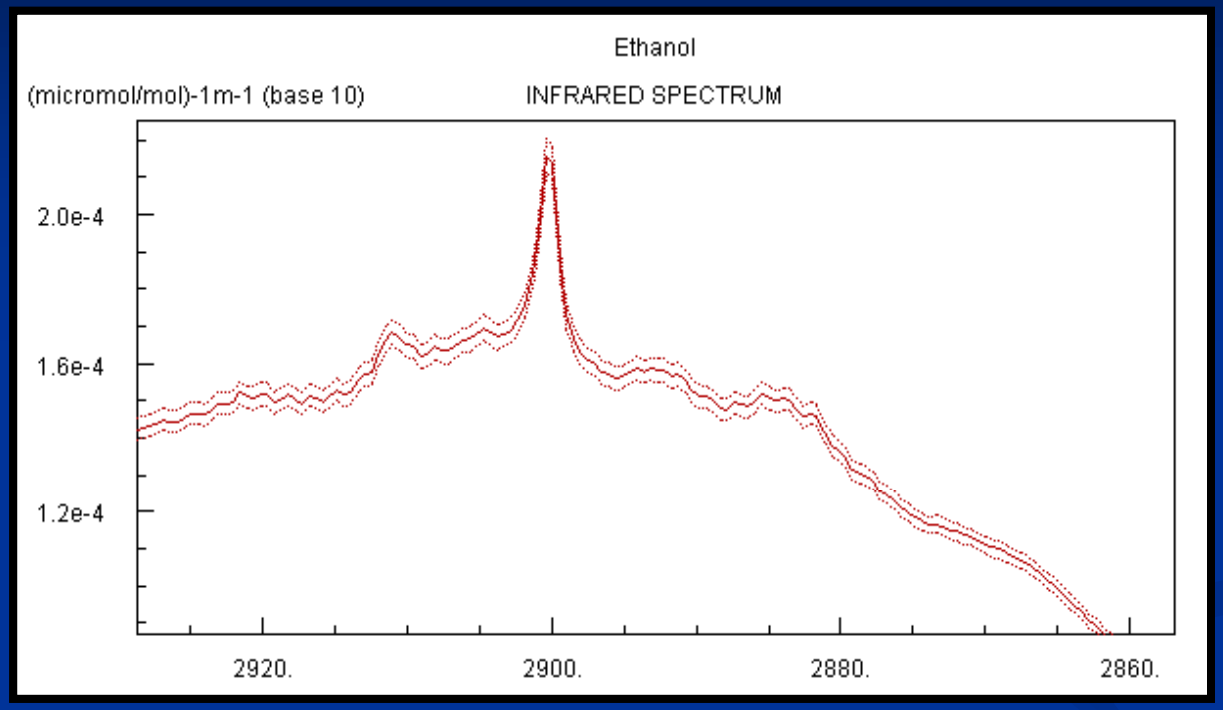
Thermo-chemical data

Gas phase thermochemistry data

Go To: Top, References, Notes / Error Report

Quantity	Value	Units	Method	Reference	Comment
$\Delta_f H°_{gas}$	145.69	kJ/mol	Review	Chase, 1998	Data last reviewed in June, 1969
$\Delta_f H°_{gas}$	147. ± 1.	kJ/mol	N/A	Tsang, 1996	
Quantity	**Value**	**Units**	**Method**	**Reference**	**Comment**
$S°_{gas,1\ bar}$	194.17	J/mol*K	Review	Chase, 1998	Data last reviewed in June, 1969

Chemistry WebBook Examples



Infrared spectra with uncertainty

Chemical (ion) reaction data

Appearance energy determinations

Ion	AE (eV)	Other Products	Method	Reference	Comment
$C_5H_{10}^+$	10.04 ± 0.05	H_2O	EI	Harnish, Holmes, et al., 1990	*LL*

Interatomic Potentials Repository

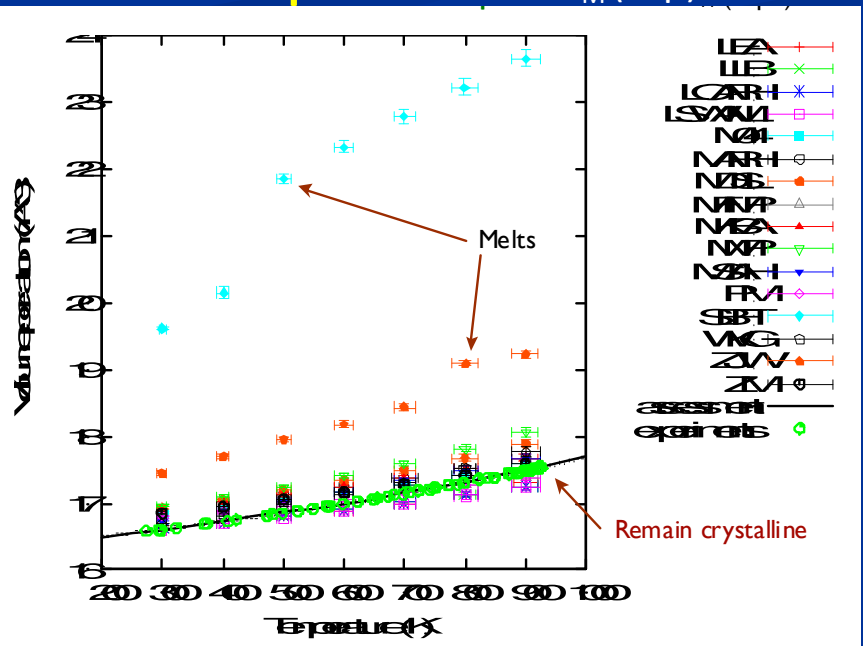
- Accurate interatomic potentials (forcefields) from known and trusted sources are essential in molecular simulation.
- If you can't trace your file or potential to the original source, you don't really know what you have. This calls results into question and is bad for both users and developers of potentials.
- Repository: http://www.ctcms.nist.gov/potentials/
- **100+ element and alloy interatomic potentials are available for download.**
- submitted or vetted by their authors and referenced
- files from other users or LAMMPS can be checked against documented versions
- Recent usage: ~5500 content pages per month to ~1000 IP addresses (not crawlers)
- Current and future work:
  - test results (with appropriate reference data) for interatomic potentials on the website
  - commentaries on the strengths and weaknesses of models and data
  - error assessment beyond standard deviations
  - more potentials, including non-metallic potentials
- **Contact: Chandler Becker**, cbecker@nist.gov

Available now:

Elements	Selected multi-component systems
Ag, Al, Au, Co, Cs, Cu, Fe, K, Li, Mg, Mo, Na, Nb, Ni, Pb, Pt, Rb, Ru, Si, Ta, Ti, V, W, Zr	Ag-Cu
	Al-Cu, Al-Fe, Al-H, Al-Mg, Al-Mn-Pd, Al-Ni, Al-Pb, Al-Si-Mg-Cu-Fe, Al-Ti
	C-H-O
	Cu-Ag, Cu-Al, Cu-Fe, Cu-Ni, Cu-Pb, Cu-Ta, Cu-Zr
	Fe-Al, Fe-C, Fe-Cu, Fe-Cu-Ni, Fe-Ni, Fe-P, Fe-V
	Mg-Al
	Ni-Al, Ni-Al-H, Ni-Cu, Ni-Fe, Ni-Zr
	UO2, (U,Pu,Np)O2

Al atomic volumes from EAM potentials

T_M (exp) = 933 K



Assessment: Eric Lass, et al., in preparation (2012)

CALPHAD File Repository

C.E. Campbell and U.R. Kattner, NIST
L.M. Bartolo, Kent State Univ.

- **Motivation:**
  - A CALPHAD assessment for a given system requires collecting all the available experimental and computational data, evaluating the data, and developing functional composition, temperature, and pressure descriptions. ***A file repository will improve efficiency and reproducibility of the method.***
- **Current progress:**
  - Established a workspace to test repository structure
  - Repository format tested with files from recently published CALPHAD assessments
  - Categories used to tag data include, but are not limited to:
    - Authors and source information
    - Systems (i.e. A-B)
    - Property class (thermodynamics, diffusion, molar volume, elastic properties)
    - Phases (gas, liquid, disordered and ordered solids)
    - Types of resources (functional description files, experimental data files, macros, scripts)

Future Work:

- Implement a more user-friendly search interface
- Recruit collaborators to test structure and input work
- Define standards for phase names

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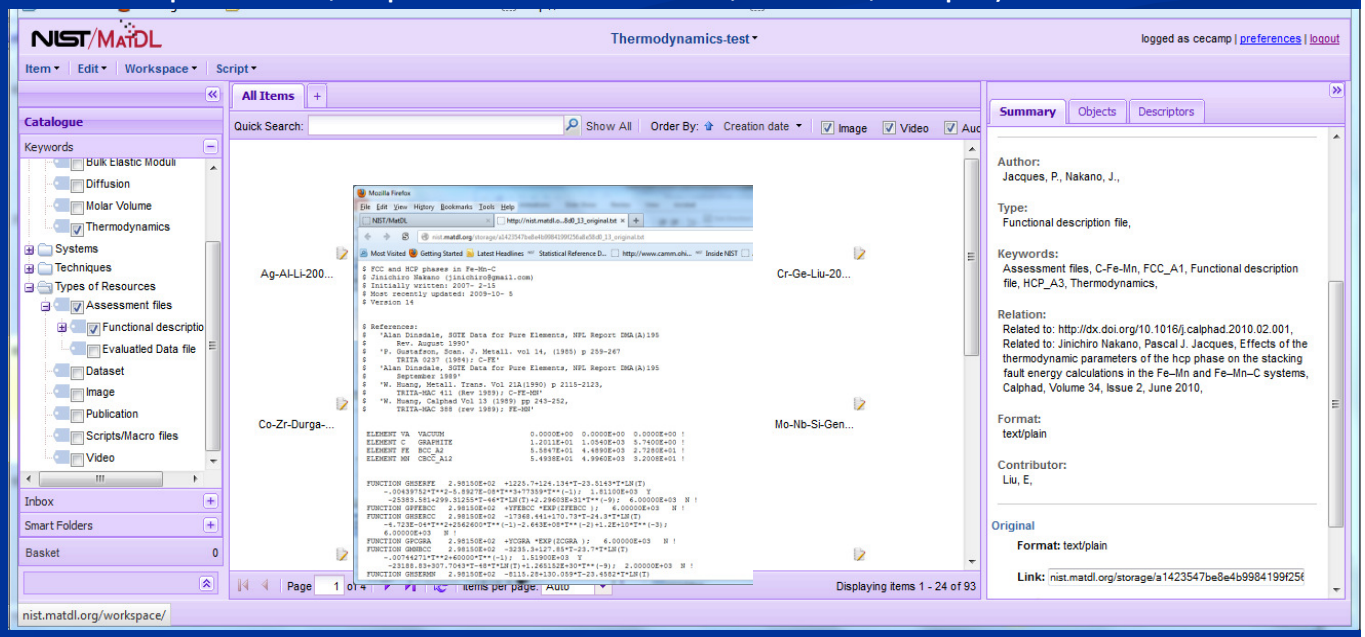

Similar workspace structures are being explored and developed for first-principles and experimental work.

Current Efforts Toward a General Data Repository

C.E. Campbell, U.R. Kattner, A.A. Dima, D. Foxvog

Initial focus is on phase-based data used by CALPHAD-based assessments.

- **Developing needed universal identifiers**
  - **Crystal Structure**
  - **Phase Names**
  - **Materials** (including processing history and composition)
- **Developing ontologies to describe materials data with initial emphasis on**
  - Phase equilibria
  - Thermochemistry
  - Diffusion
- **Investigating a variety of data-interchange and representation formats** (e.g. JSON, BSON, XML)
- **Developing tools to transform data for use in other modeling tools**
- **Constructing a Wiki to define terminology**

carelyn.campbell@nist.gov; ursula.kattner@nist.gov

NIST Standard Reference Simulation Website

http://go.usa.gov/rHYm

- **Objectives:** Provide well-documented results from molecular simulation (Monte Carlo, Molecular Dynamics) that can be treated like experimental standard reference data.

- **Examples:**
  - equations of state
  - phase coexistence conditions
  - transport properties

- **Intended Use:**
  - reference data for simulation users
  - data for algorithm validation
  - re-use of published data for original research

- **Maintainers:**

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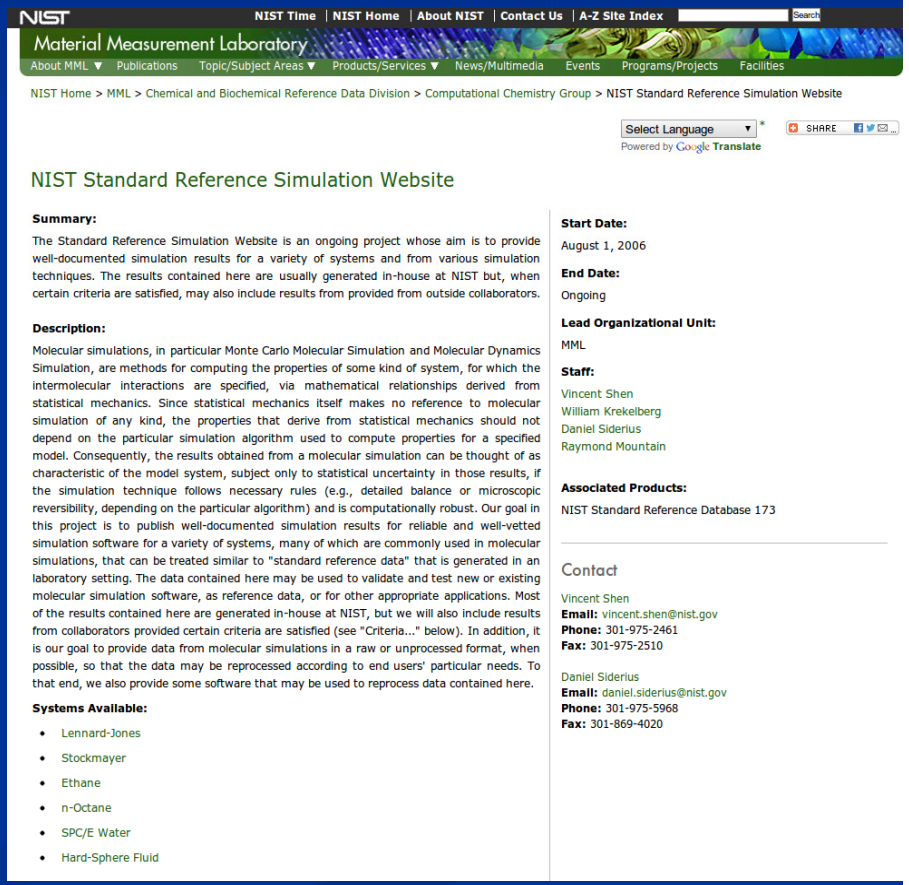
Daniel Siderius, daniel.siderius@nist.gov
William Krekelberg, william.krekelberg@nist.gov



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NIST Standard Reference Simulation Website

Summary:

The Standard Reference Simulation Website is an ongoing project whose aim is to provide well-documented simulation results for a variety of systems and from various simulation techniques. The results contained here are usually generated in-house at NIST but, when certain criteria are satisfied, may also include results from provided from outside collaborators.

Description:

Molecular simulations, in particular Monte Carlo Molecular Simulation and Molecular Dynamics Simulation, are methods for computing the properties of some kind of system, for which the intermolecular interactions are specified, via mathematical relationships derived from statistical mechanics. Since statistical mechanics itself makes no reference to molecular simulation of any kind, the properties that derive from statistical mechanics should not depend on the particular simulation algorithm used to compute properties for a specified model. Consequently, the results obtained from a molecular simulation can be thought of as characteristic of the model system, subject only to statistical uncertainty in those results, if the simulation technique follows necessary rules (e.g., detailed balance or microscopic reversibility, depending on the particular algorithm) and is computationally robust. Our goal in this project is to publish well-documented simulation results for reliable and well-vetted simulation software for a variety of systems, many of which are commonly used in molecular simulations, that can be treated similar to "standard reference data" that is generated in an laboratory setting. The data contained here may be used to validate and test new or existing molecular simulation software, as reference data, or for other appropriate applications. Most of the results contained here are generated in-house at NIST, but we will also include results from collaborators provided certain criteria are satisfied (see "Criteria..." below). In addition, it is our goal to provide data from molecular simulations in a raw or unprocessed format, when possible, so that the data may be reprocessed according to end users' particular needs. To that end, we also provide some software that may be used to reprocess data contained here.

Systems Available:

- Lennard-Jones
- Stockmayer
- Ethane
- n-Octane
- SPC/E Water
- Hard-Sphere Fluid

Start Date:
August 1, 2006

End Date:
Ongoing

Lead Organizational Unit:
MML

Staff:
Vincent Shen
William Krekelberg
Daniel Siderius
Raymond Mountain

Associated Products:
NIST Standard Reference Database 173

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National Institute of Standards and Technology
U.S. Department of Commerce

MATERIAL MEASUREMENT LABORATORY

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Courtesy of
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http://www.nist.gov/srd/nist31.cfm
SRD 84, Inorganic Crystal Structure Database
http://www.nist.gov/srd/nist84.cfm

Contents

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Available Party Favors

- Demo CDROMs – Phase Equil. Diagrams *(SRD 31)*
- Demo CDROMs – ICSD (Inorg. Crystal Structures) *(SRD 84)*
- CDROMs - Selected Practice Guides

- ***Also:*** laptop available running full versions of SRD 31 and SRD 84