

CODATA 2002

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**CREATING KNOWLEDGE FROM COMPUTED
DATA FOR THE DESIGN OF MATERIALS**

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Outline

- Using Scientific and Technical Data: the Reality
- The revolution in Computational Materials Science
- Illustrative Examples
 - Hydrogen storage
 - Microelectronics
 - Catalysis
- From Data to Knowledge, from Knowledge to Innovation

Industrial Research

REQUIREMENTS

SOLUTION

Analyze and Decide

Data

Organize data

Expand search space

Obtain new information
experiment and simulation

The Reality

REQUIREMENTS

SOLUTION

Analyze and Decide

Data

Optimize data

Expand search space

Obtain new information
experimentation

Humans strive for completeness, order, and symmetry



Scientific Progress



M. Planck



Louis de Broglie



E. Schrödinger



P. A. M. Dirac



D. Hartree



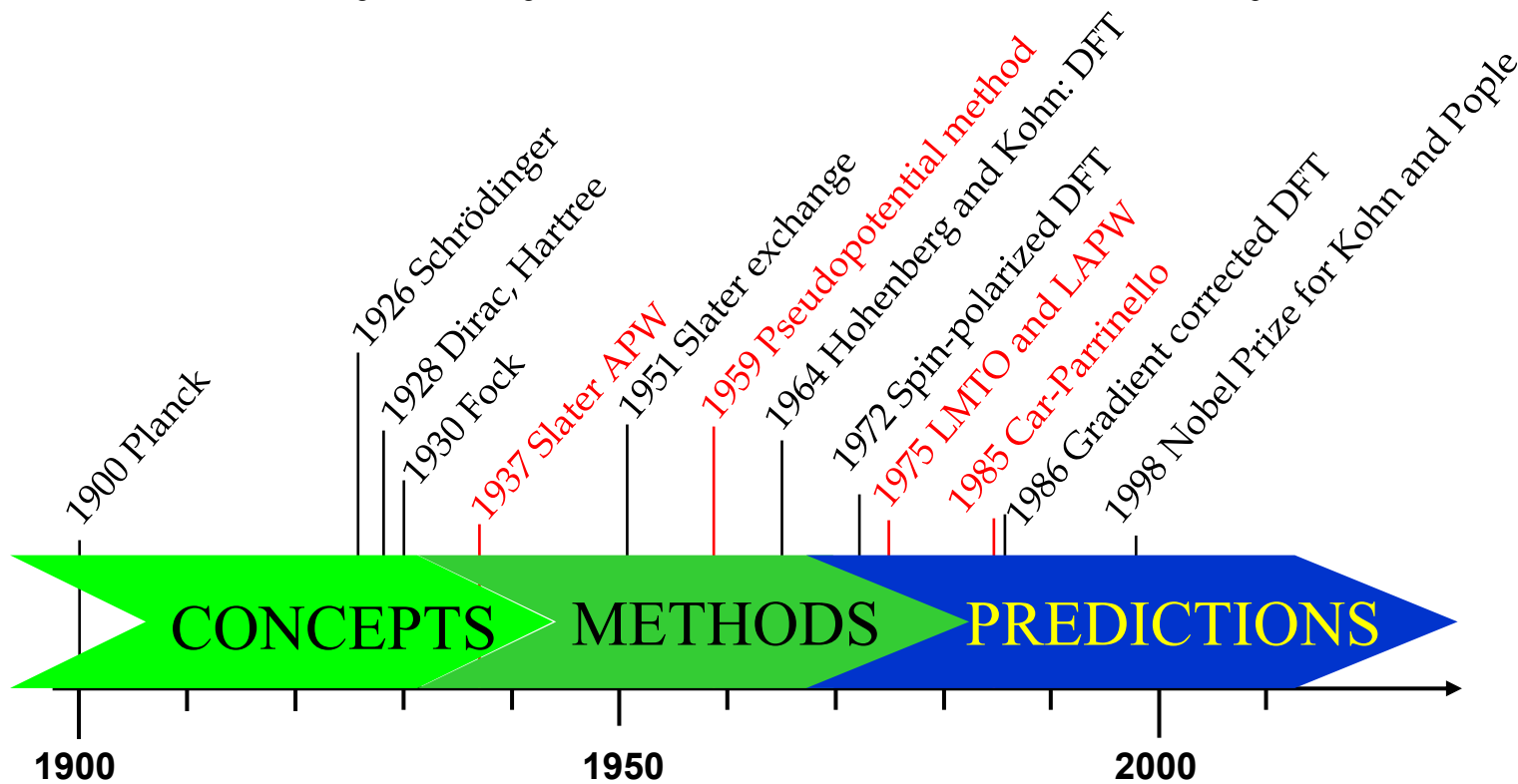
J. C. Slater



J. Pople



W. Kohn





Situation in 2002

- **A solid theoretical basis for computational materials science is in place:** Density Functional Theory (DFT)
- **The computational methodology has reached maturity in terms of generality, robustness, and speed:** VASP code
- **The tools are integrated and easy to use:** MedeA
- **Computations have become a reliable source of data:** computations augment experimental databases
- **Computational science continues to benefit from the dramatic progress in computer technology:** Moore's law continues to hold



Data from Computations

Elastic Constants of AlN

(GPa)	Expt ¹	Expt ²	Calculated
C_{11}	345	411	375
C_{12}	125	149	130
C_{13}	120	99	100
C_{33}	395	389	347
C_{44}	118	125	113
C_{66}	110	131	122
B	202	212	195

1. K.Tsubouchi, N. Mikoshiba, IEEE Trans. Sonics Ultrason. **SU-32**, 634 (1985)
2. L.E. McNeil, M. Grimsditch, R.H. French, J. Am. Ceram. Soc. **76**, 1132 (1993)



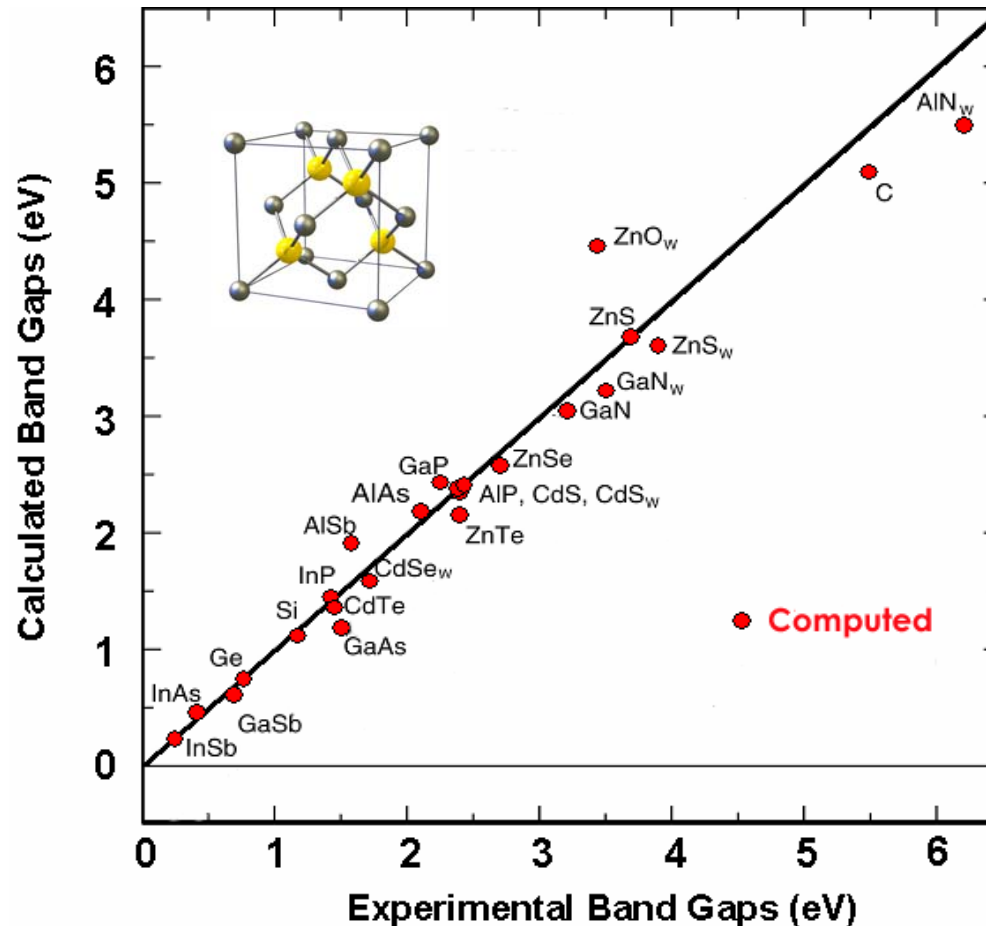
Example: Non-Compressible Materials

Bulk modulus (Gpa)

	Experiment ¹	Calculated
Carbon (diamond)	443	443.5
Osmium	462	457.6

1. Hyunhae Cynn, Lawrence Livermore Natl. Lab., Chemistry Autumn 2002 (ACS)

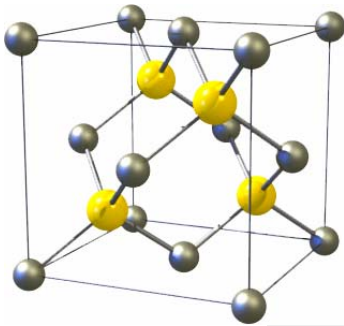
Bandgaps in Semiconductors



C. B. Geller, W. Wolf, S. Picozzi, A. Continenza, R. Asahi, W. Mannstadt, A. J. Freeman and E. Wimmer, *Appl. Phys. Lett.* **79**, 368 (2001)

Example:

Thermophotovoltaic Materials



InAs

The $\Gamma-L$ and $\Gamma-X$ separations (cf. Table I) show an overall better performance of sX compared with LDA. A remarkable case is the $\Gamma-L$ separation in InAs. The most often reported experimental value is 0.74 eV,¹⁵ whereas sX gives 1.21 eV. Recent measurements, by using improved techniques, resulted in a revised value of 1.10 ± 0.05 eV.¹⁷

A systematic investigation of effective masses reveals a similar picture, namely, that sX improves the overall agreement with experiment. In particular, the performance of sX in predicting m_c^Γ is rather remarkable (cf. Table II). Never-

Geller et al., Appl. Phys. Lett. **79**, 368 (2001)



A Fundamental Change

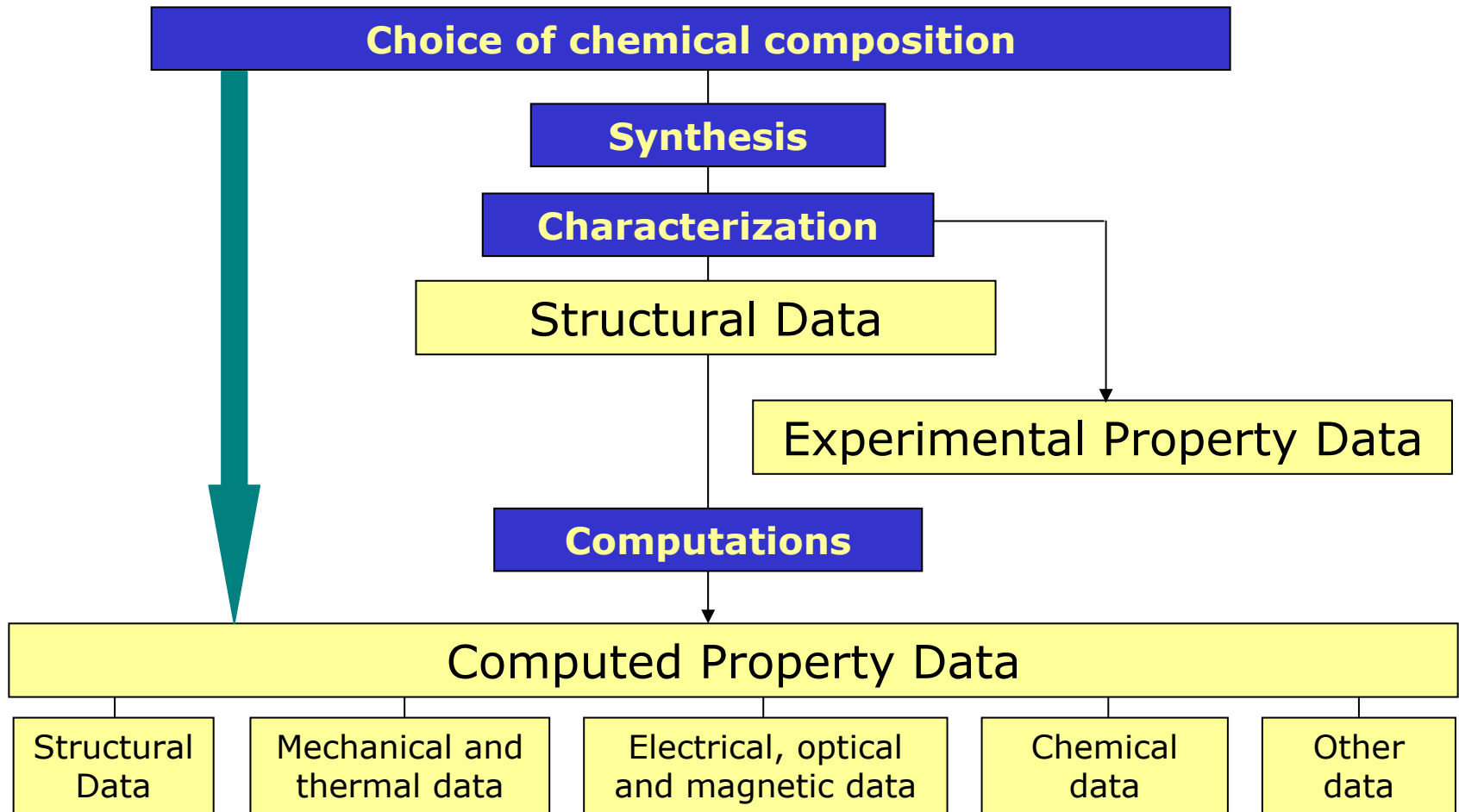
20th Century

If experiment and calculation disagree: re-do calculation

21st Century

**If experiment and calculation disagree: re-do experiment
or trust the calculation**

Data Creation





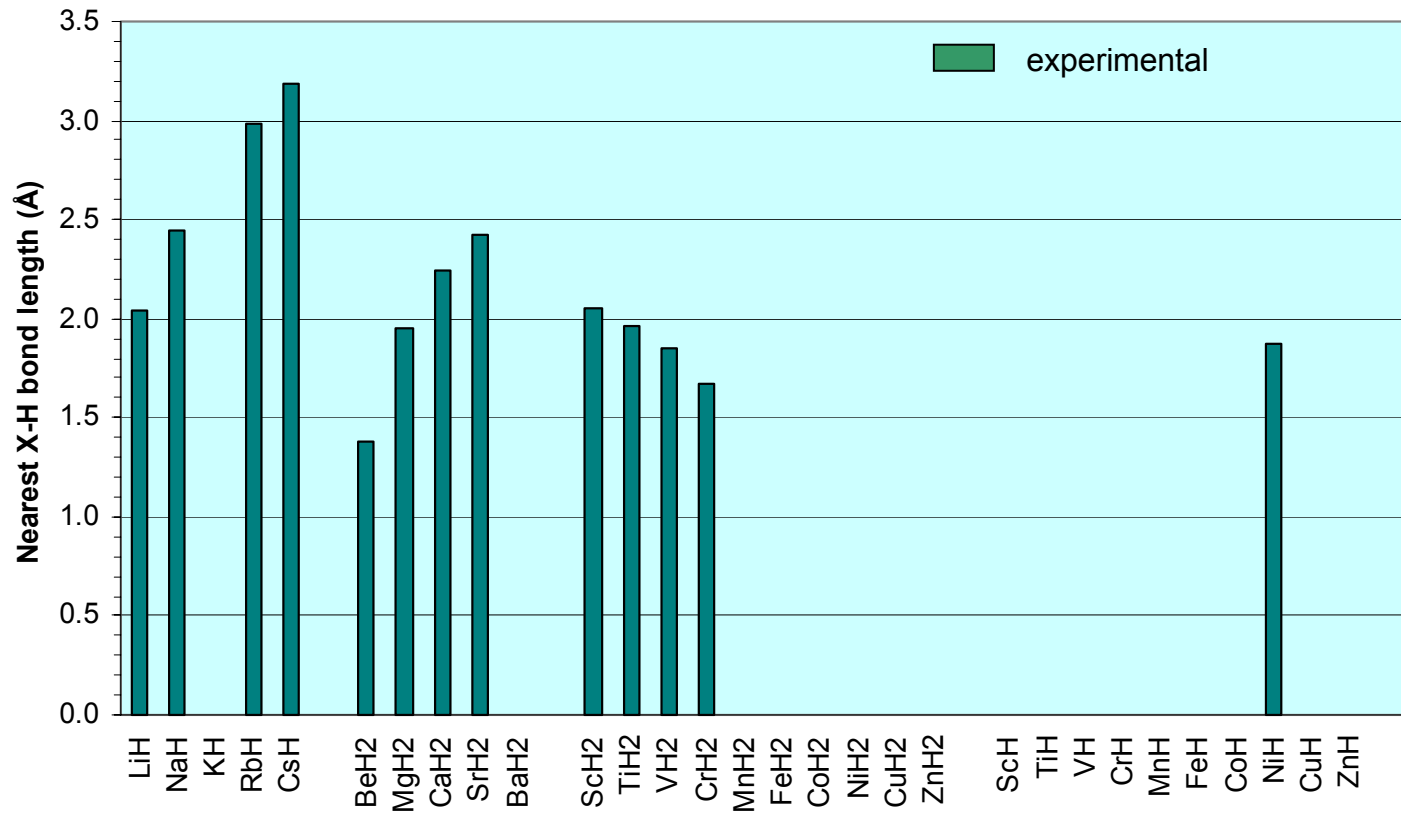
From Data to Knowledge



Examples

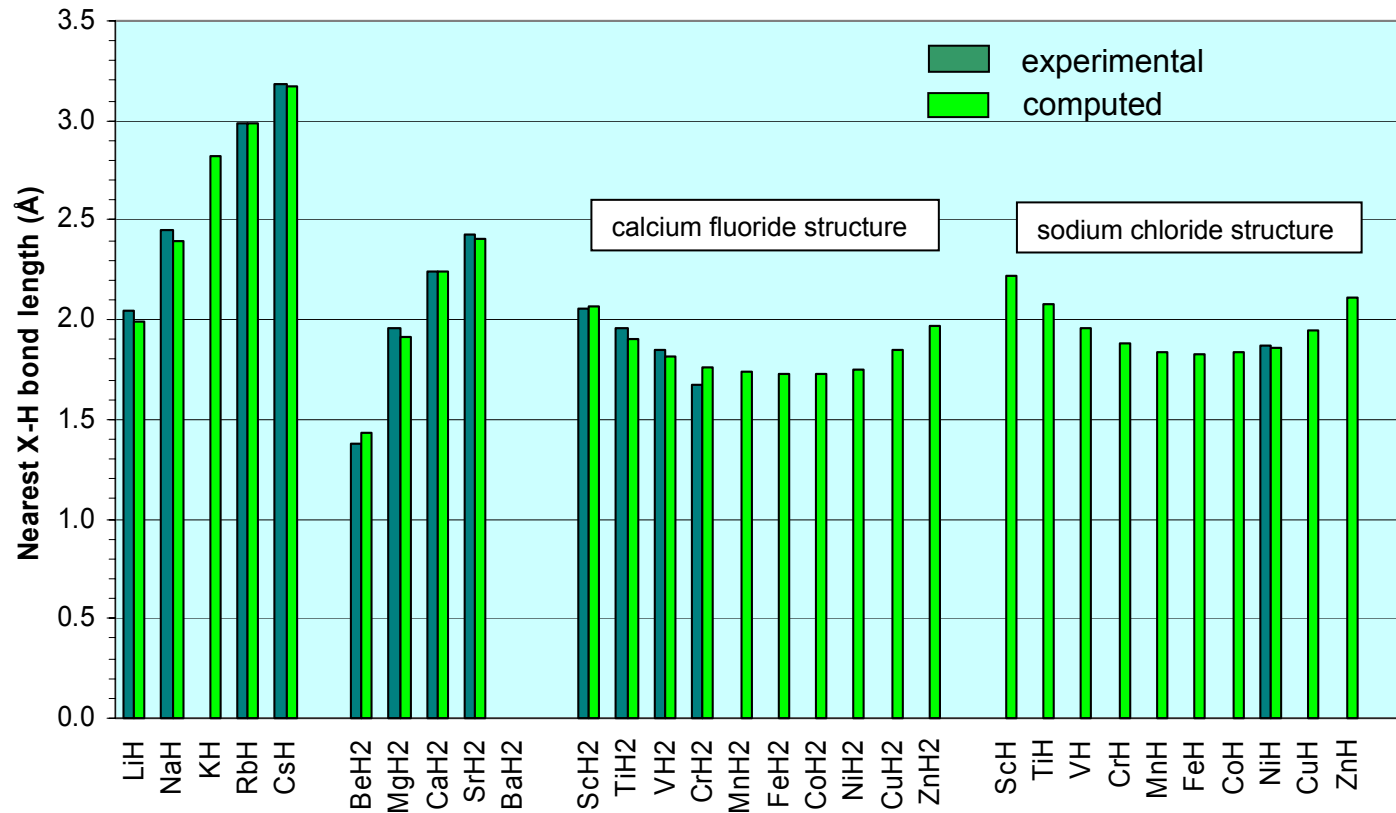
- **Hydrogen storage** -
structural and thermodynamic properties
- **Heterogeneous catalysis** -
chemical bond strength

Metal Hydrides



Metal Hydrides

Data and trends



Heterogeneous Catalysis

Where should
one search?

Metal sulfide Activity [1]

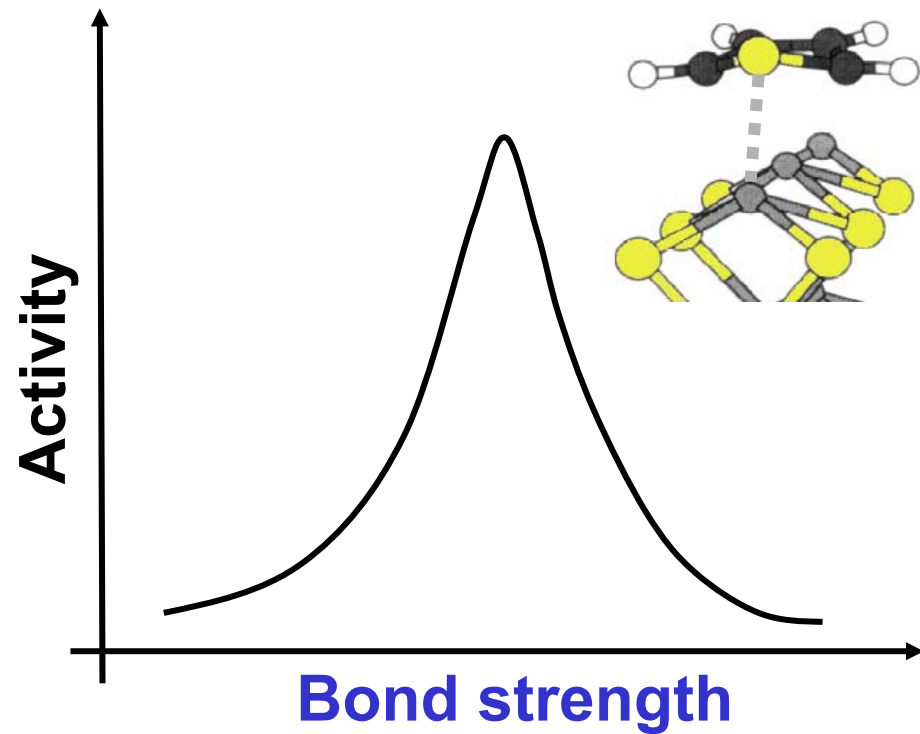
RuS ₂	379.50
OsS ₂	216.30
IrS ₂	171.80
Rh ₂ S ₃	106.10
ReS ₂	39.40
PtS	16.00
PdS	12.50
MoS ₂	8.00
Cr ₂ S ₃ ^a	4.80
WS ₂	3.20
NbS ₂	1.70
Ni ₃ S ₂	1.50
Co ₉ S ₈	1.40
VS ^a	1.10
FeS	1.10
TaS ₂	1.10
MnS ^a	0.60

[1] Pecoraro and Chinelli, J. Catal. **67**, 430 (1981)

Principle of Sabatier

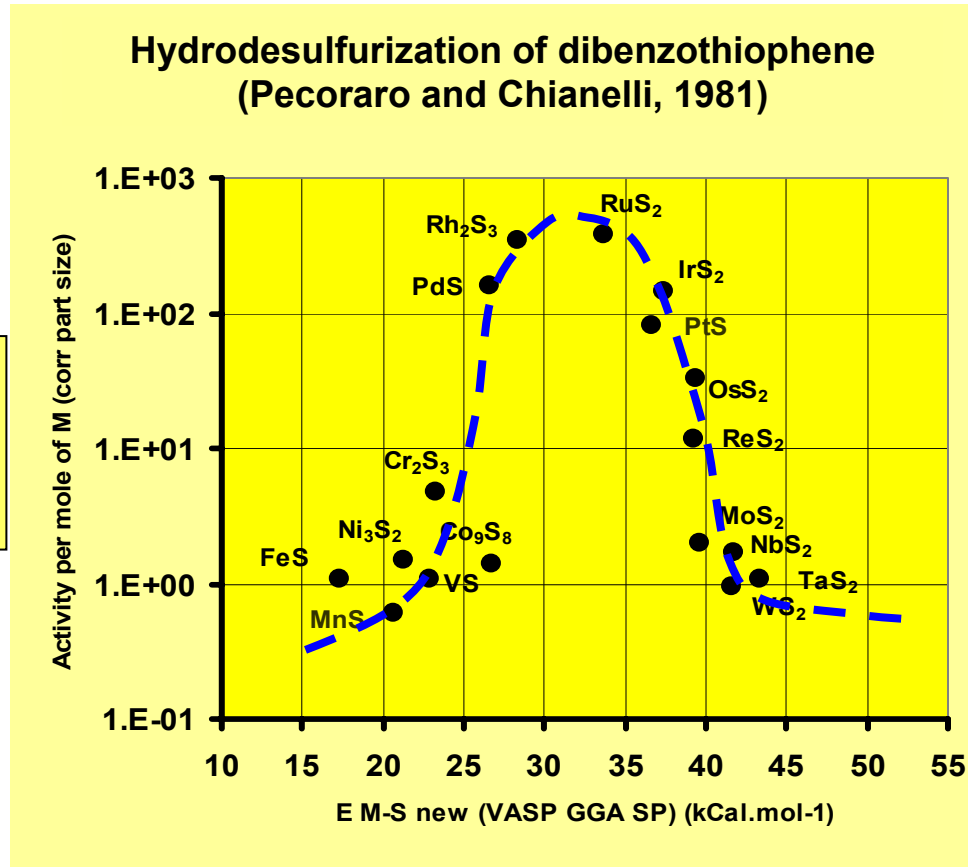


Paul Sabatier
1854 - 1941



P. Sabatier, *Berichte der Deutschen Chem. Gesellschaft* **44**, 1984 (1911)

Bond Strength as Descriptor



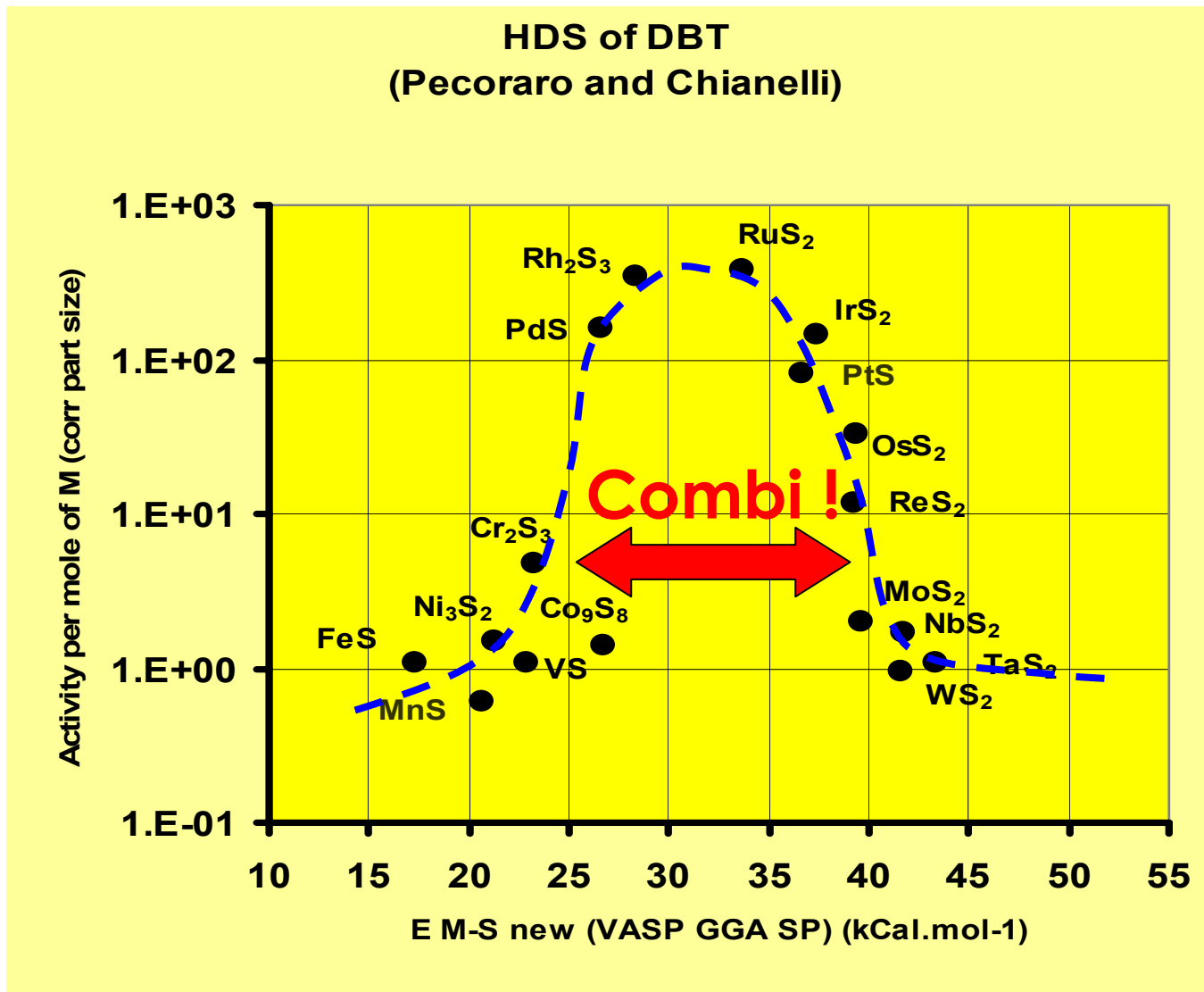
Activity data
from
experiment

Crystal structures
from ICSD
database

Bond strengths from VASP computations

H. Toulhoat, P. Raybaud, S. Kasztelan, G. Kresse and J. Hafner, *Catalysis Today* **50**, 629 (1999)

Synergy Effect

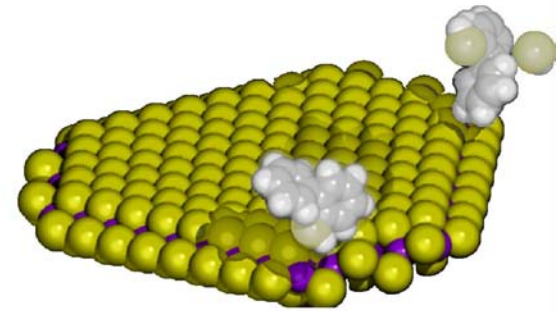


Combination of Experimental and Computed Data Enable Innovation

Metal sulfide Activity [1]

RuS ₂	379.50
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Ni ₃ S ₂	1.50
Co ₉ S ₈	1.40
VS ^a	1.10
FeS	1.10
TaS ₂	1.10
MnS ^a	0.60

Search
here!



Co promoted MoS₂ nanoparticles supported on alumina are used industrially

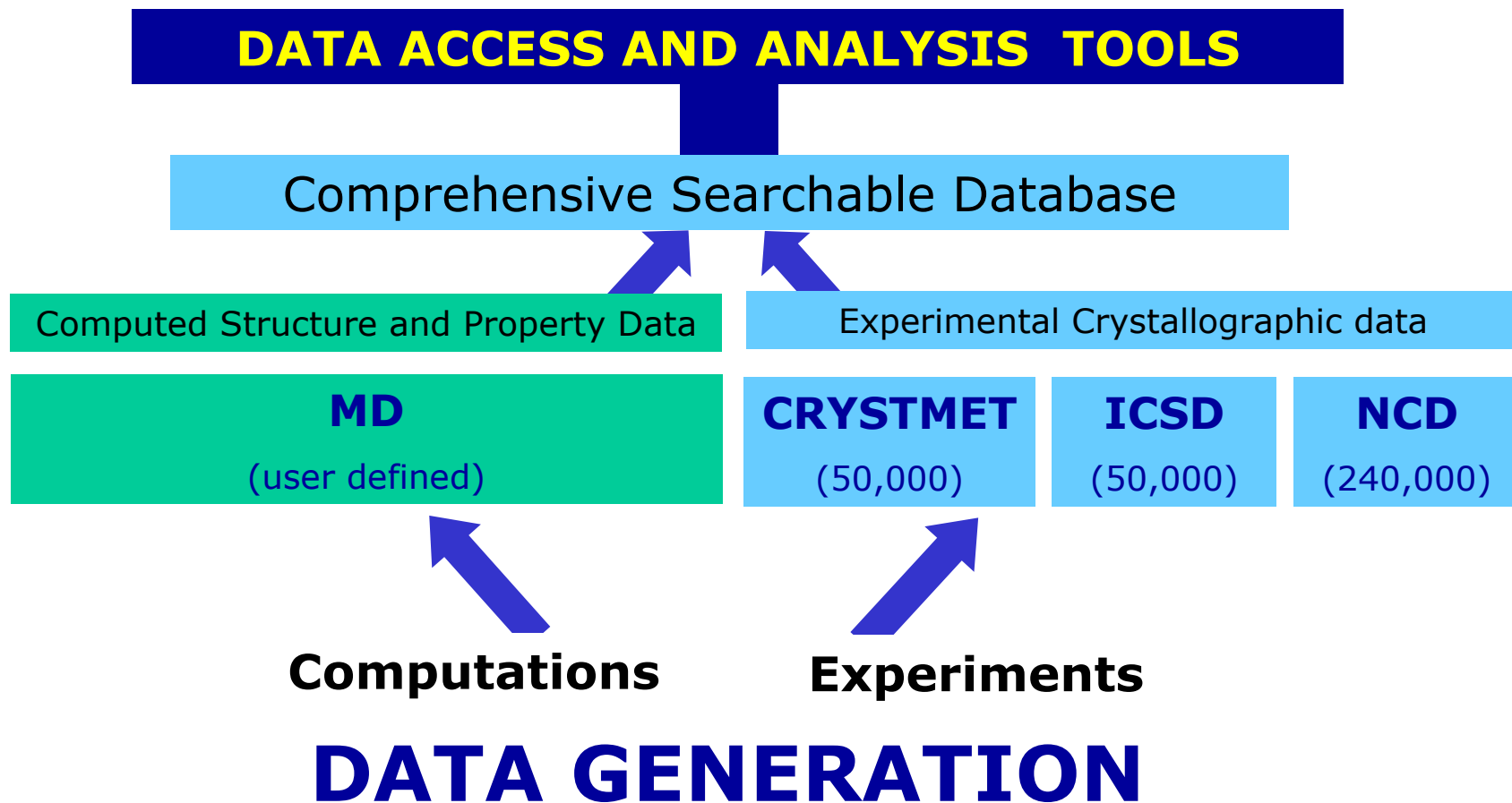
Figure from H. Schweiger et al.



Storage, Retrieval, Integrity

- Store computed data together with computational approach
- “Active database” – Retrieval of data can mean on-the-fly computation
- Standardization of computational procedures is the basis for integrity

MedeA: an Integrated Technology Platform



MedeA- an Integrated Technology Platform for Experimental and Computed Data

Materials Design: InfoMaticA -- Search

ID	completeness	space group name H-M	sum	structural	name systematic	length a
CRYSTMET.20074	Complete	Fm-3m	CTi			4.3284001
CRYSTMET.22882	Complete	Fm-3m	CTi			4.3270001
CRYSTMET.27805	Complete	Fm-3m	CTi			4.3280001
CRYSTMET.27864	Complete	Fm-3m	CTi			4.323
CRYSTMET.34897	Complete	Fm-3m	CTi			4.3260002
CRYSTMET.35038	Complete	Fm-3m	CTi			4.348
CRYSTMET.36278	Complete	Fm-3m	CTi			4.329
CRYSTMET.36323	Complete	Fm-3m	CTi			4.3291998
CRYSTMET.37912	Complete	Fm-3m	CTi			4.3379998
CRYSTMET.38541	Complete	Fm-3m	CTi			4.3249998
CRYSTMET.62979	Complete	Fm-3m	CTi			4.3499999
CRYSTMET.63032	Complete	Fm-3m	CTi			4.3299999
CRYSTMET.83951	None Available	Fd3m	CTi			8.6339998
ICSD.1546	Complete	FM3-M	TiC	TiC	Titanium carbide [1/1]	4.3280001
ICSD.26952	Complete	F23	TiC	TiC	Titanium carbide	4.5999999
MD.18	Complete	Fm-3m	CTi		CTi	4.3332853
MD.727	Complete	Fm-3m	CTi		CTi	4.3291998
NCD_Inorganic.037662	Unknown	Fm3m	C Fe0 Ti	Ti(C, Fe, Ti)	Titanium carbide [1^1]	4.321
NCD_Inorganic.037663	Unknown	Fm3m	C Ti	TiC	Titanium carbide [1^1]	4.3276

Search Criteria Detailed Information Coordinates Geometry Coordination Powder pattern

Require that Formula is TiC

Require that --Add new criterion--

Run search Clear

Displaying 25 of 25 hits

Atom: Ti/2 (Ti) Fractionals: 0.50000 0.00000 0.00000 Cartesians: 2.16460 0.00000 0.00000

Single search of
CRYSTMET, ICSD,
NCD and MD
(computed) database

Perspective

