CODATA 2002

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CREATING KNOWLEDGE FROM COMPUTED DATA FOR THE DESIGN OF MATERIALS

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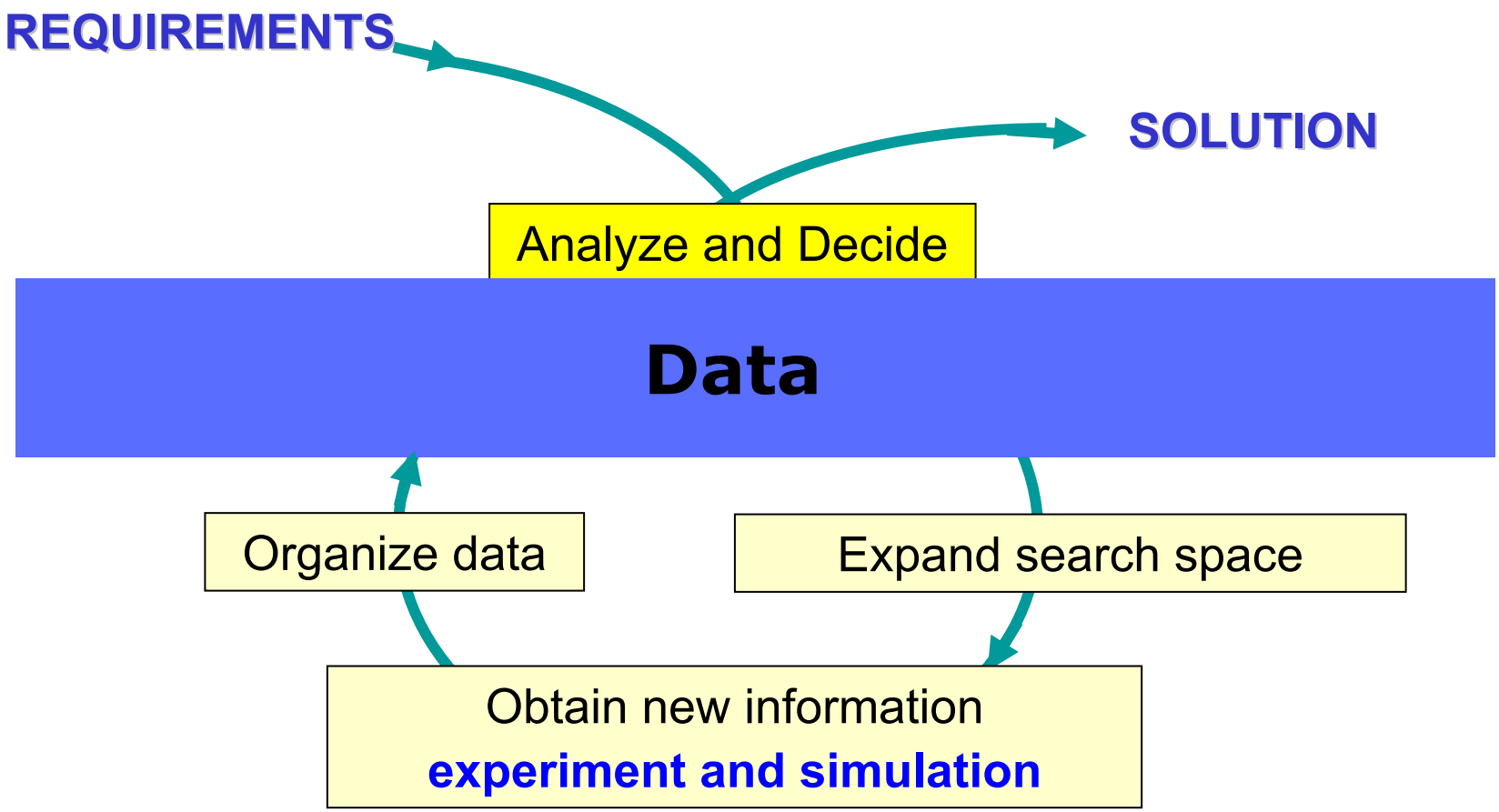
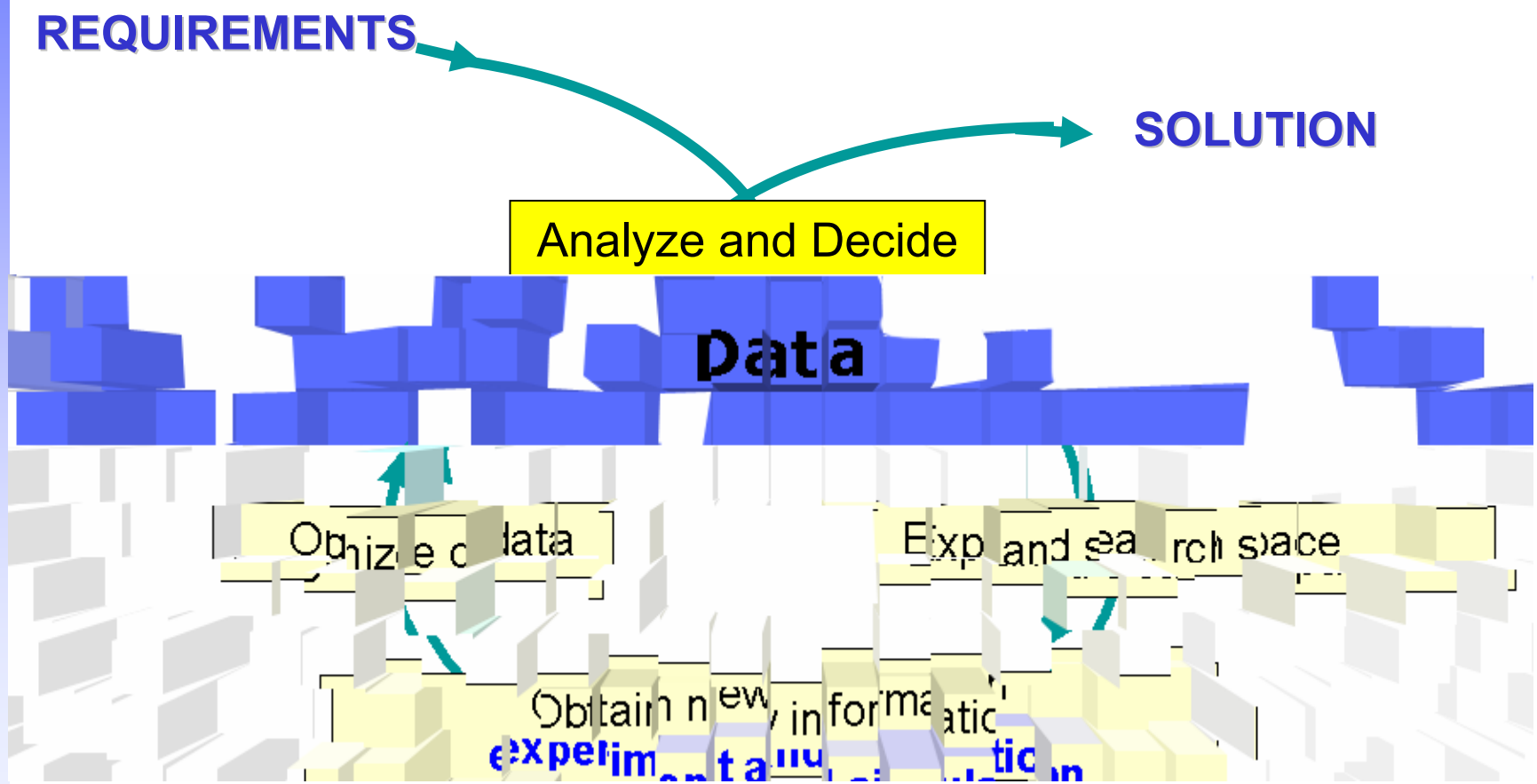
Outline

- 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



The Reality



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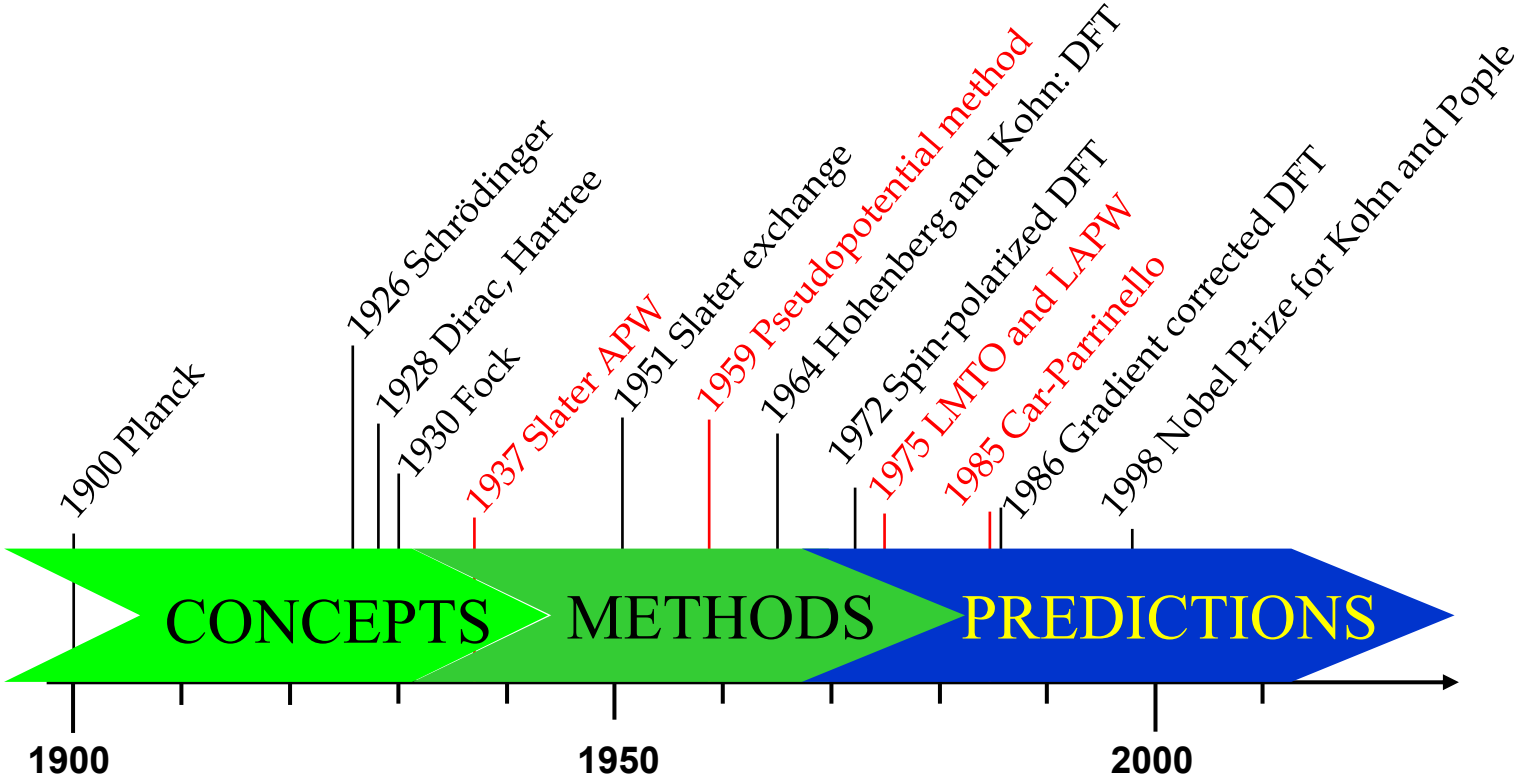
Humans strive for completeness, order, and symmetry

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 theorical 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)

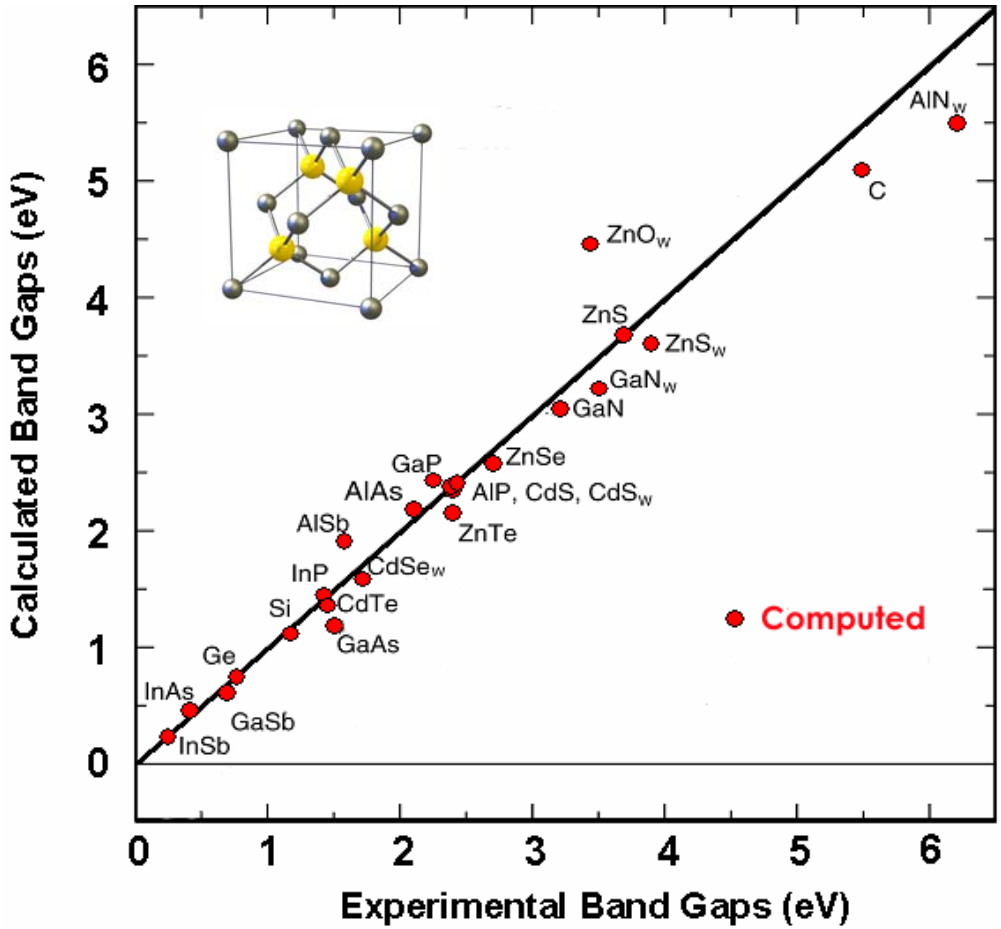
Example: Non-Compressible Materials

Bulk modulus (Gpa)

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

1. Hyunchae 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)

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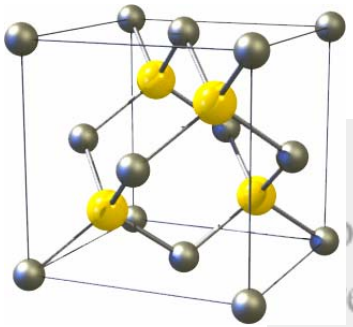
Example: Thermophotovoltaic Materials



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

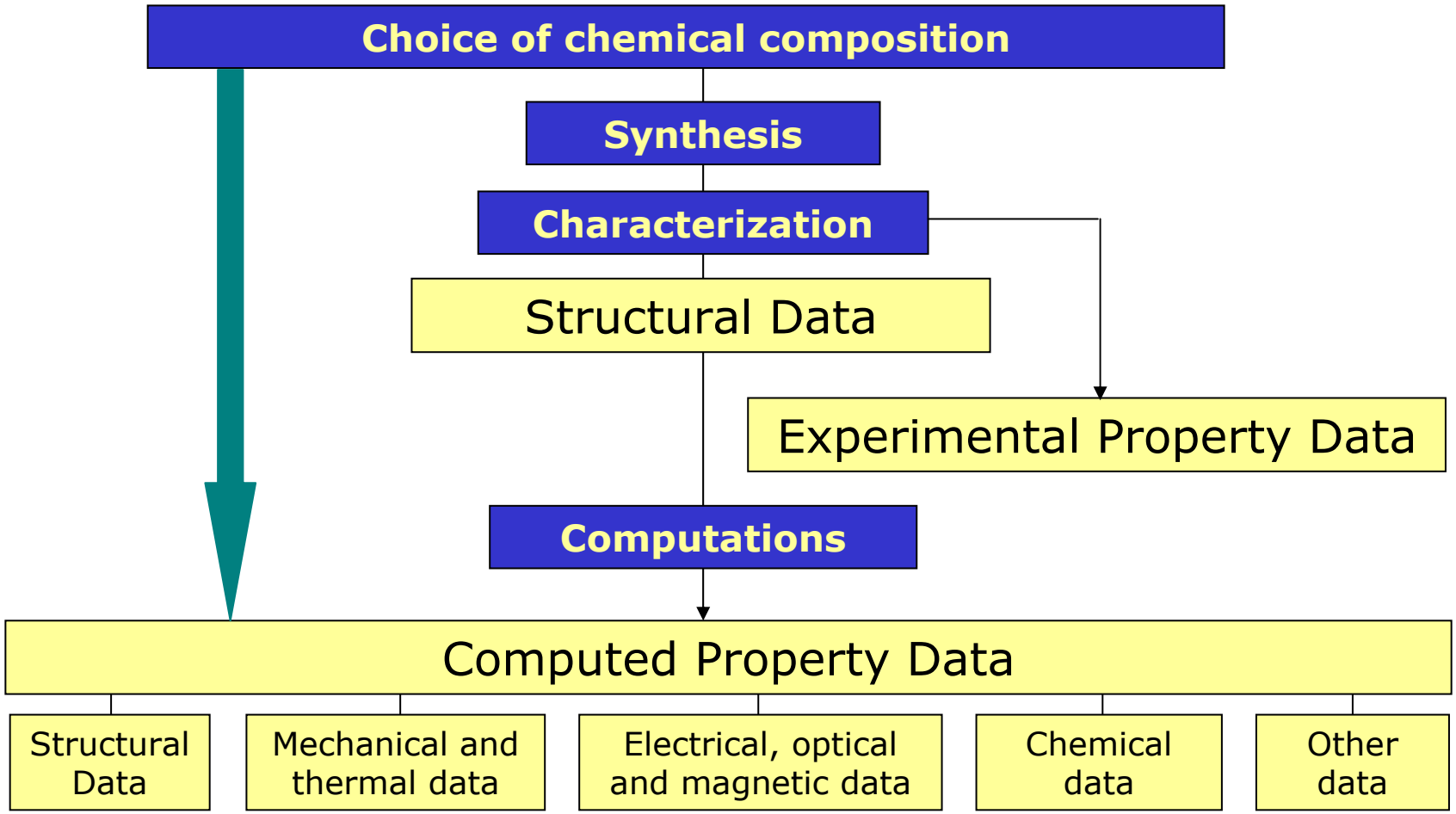
20th Century

If experiment and calculation disagree: re-do calculation

21st Century

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

Data Creation



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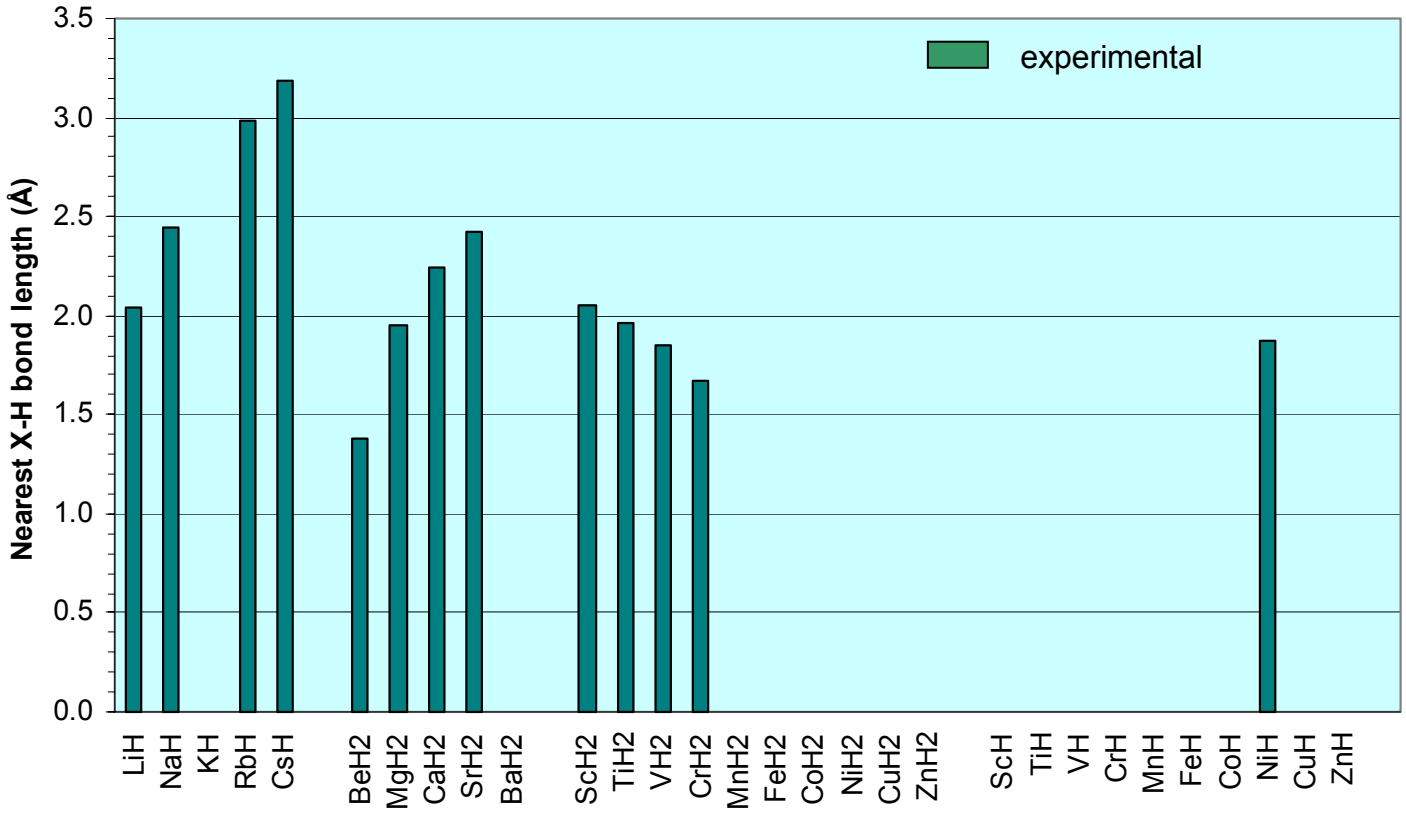
From Data to Knowledge

Examples

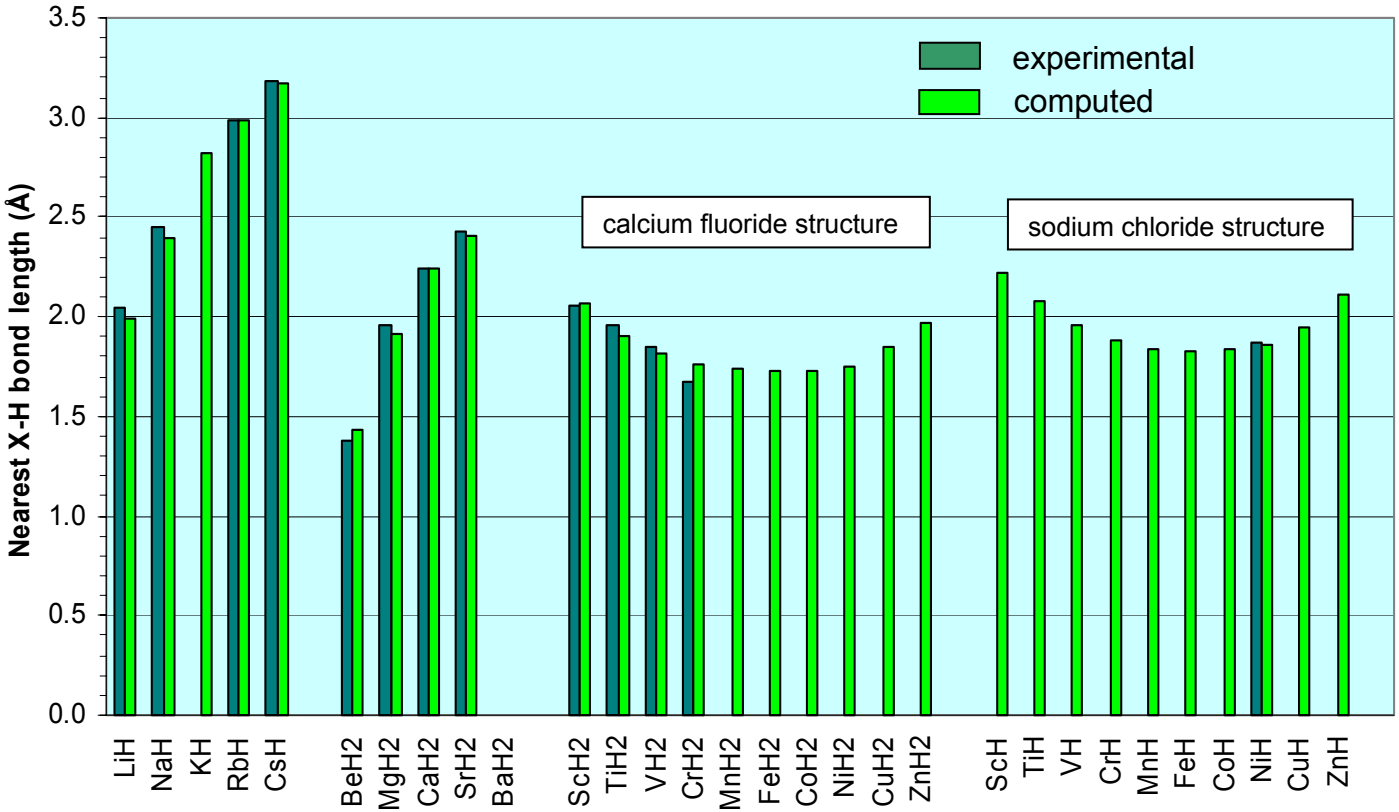
- **Hydrogen storage -**
  structural and thermodynamic properties
- **Heterogeneous catalysis -**
  chemical bond strength

Metal Hydrides



Metal Hydrides

Data and trends



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Heterogeneous Catalysis

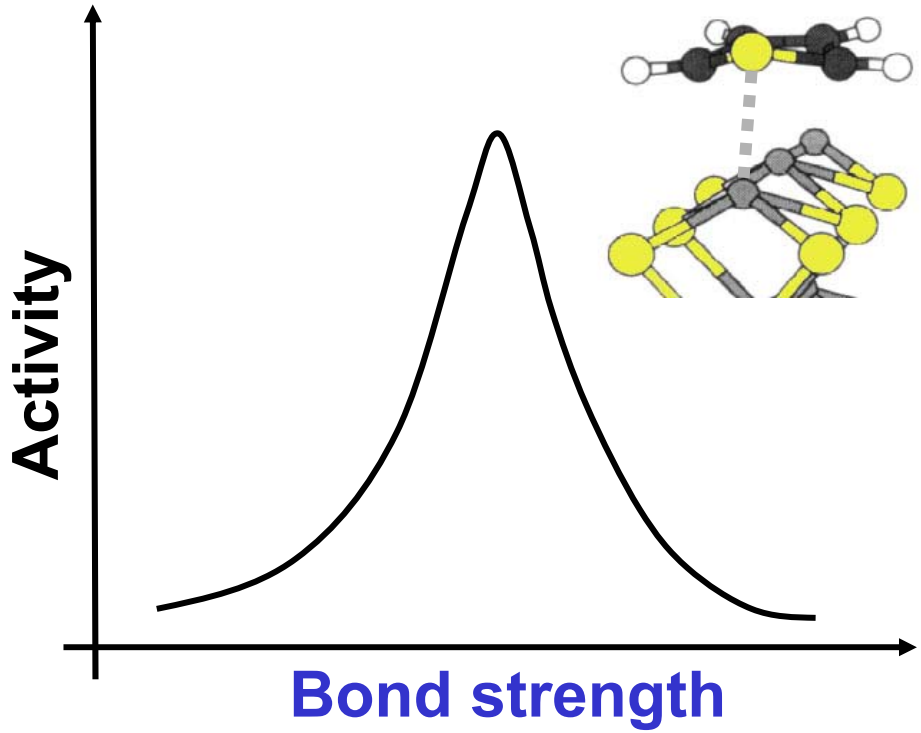
Metal sulfide	Activity [1]
RuS_2	379.50
OsS_2	216.30
IrS_2	171.80
Rh_2S_3	106.10
ReS_2	39.40
PtS	16.00
PdS	12.50
MoS_2	8.00
Cr_2S_3[a]	4.80
WS_2	3.20
NbS_2	1.70
Ni_3S_2	1.50
Co_9S_8	1.40
VS[a]	1.10
FeS	1.10
TaS_2	1.10
MnS[a]	0.60

Where should one search?

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

Principle of Sabatier

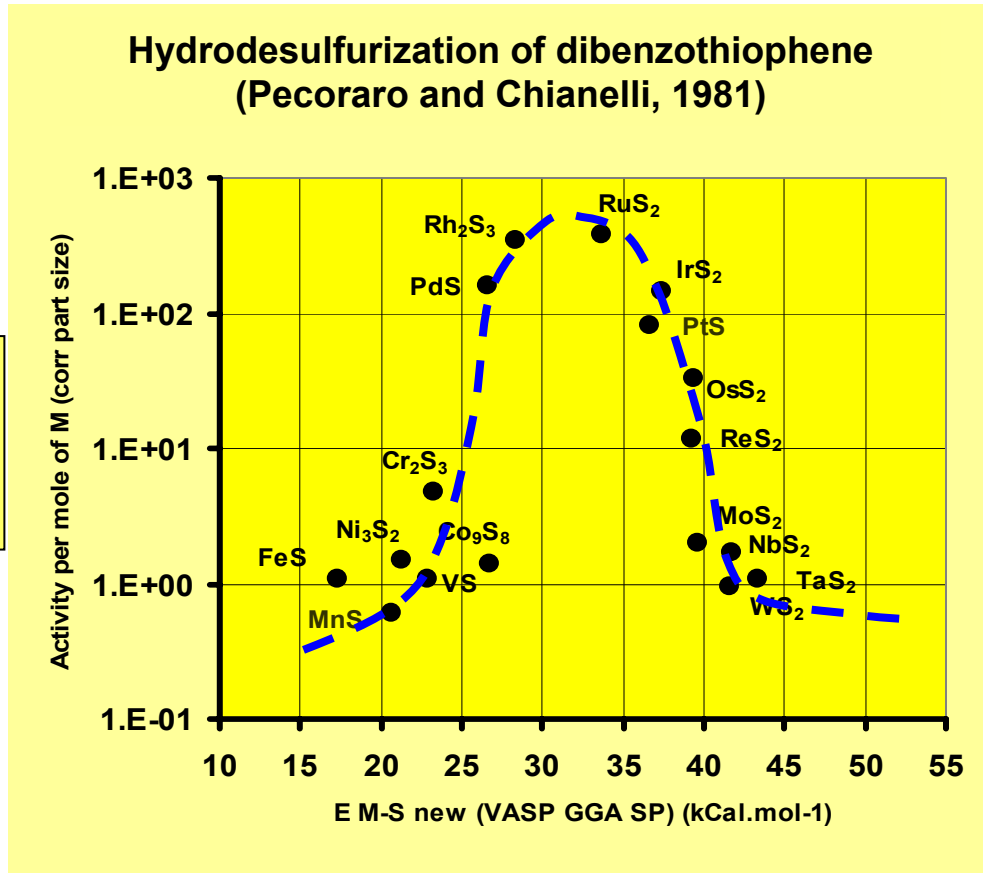
Paul Sabatier
1854 - 1941



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)

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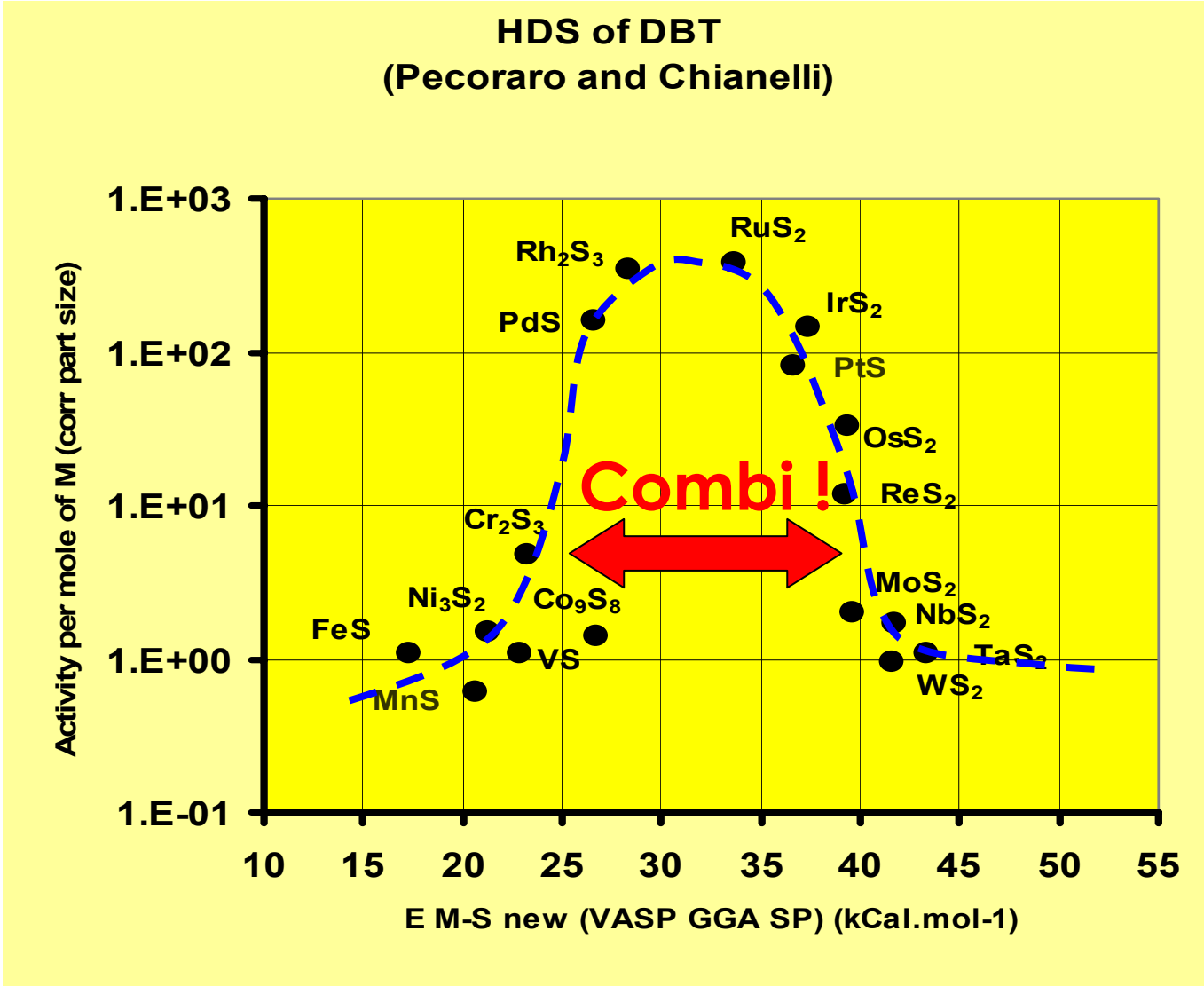
Synergy Effect



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Combination of Experimental and Computed Data Enable Innovation

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RuS_2	379.50
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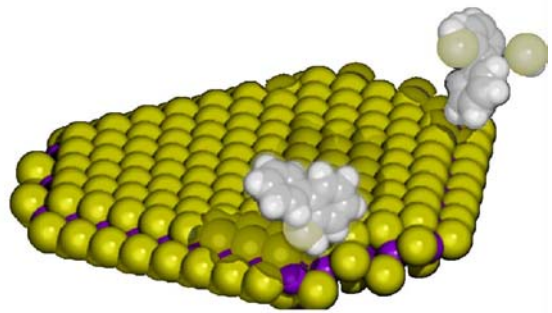
Ni_3S_2	1.50
Co_9S_8	1.40
VS[a]	1.10
FeS	1.10
TaS_2	1.10
MnS[a]	0.60

Search here!



Co promoted MoS_2 nanoparticles supported on alumina are used industrially

Figure from H. Schweiger et al.

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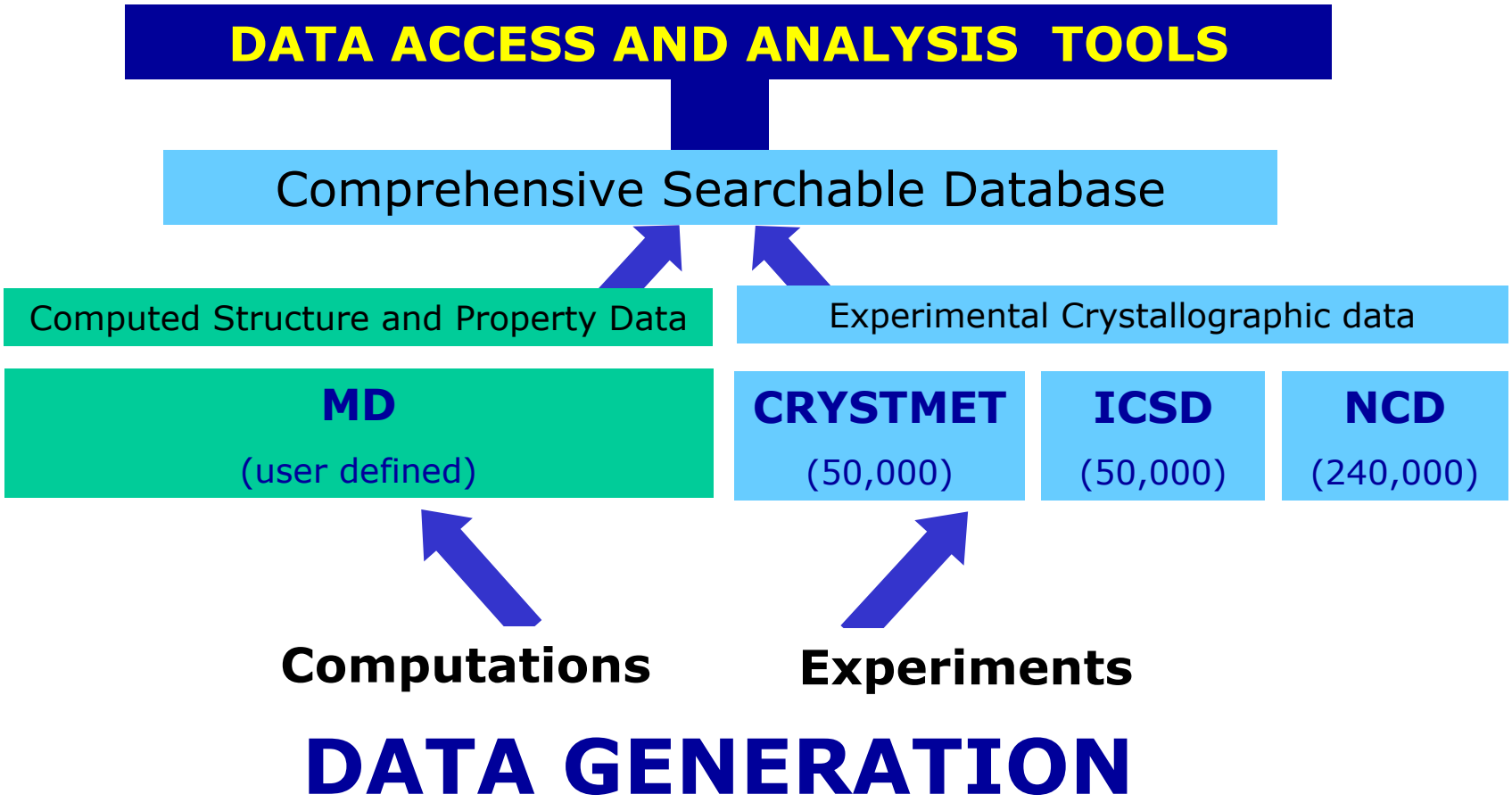
Storage, Retrieval, Integrity

- 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



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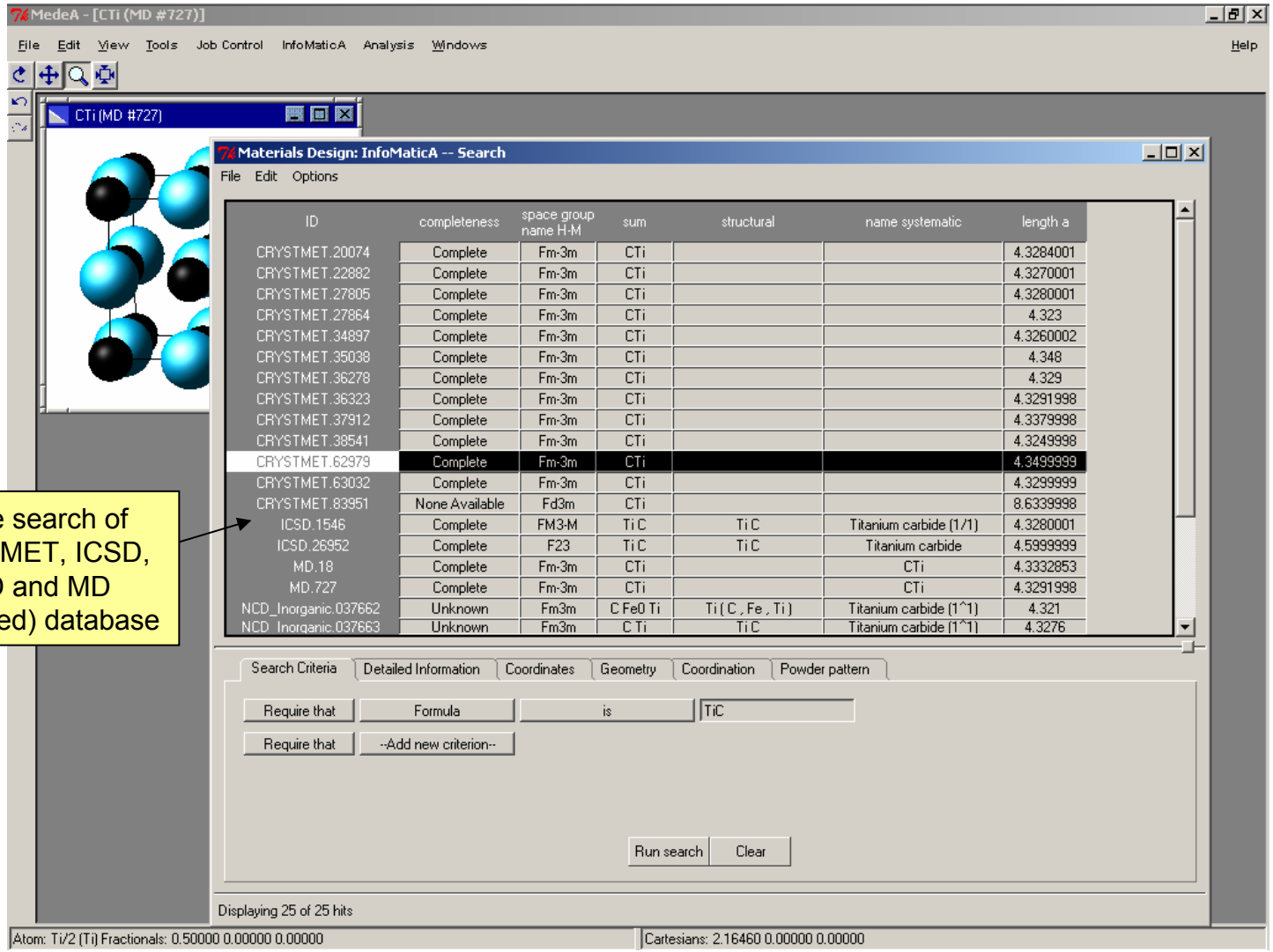
MedeA- an Integrated Technology Platform for Experimental and Computed Data



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

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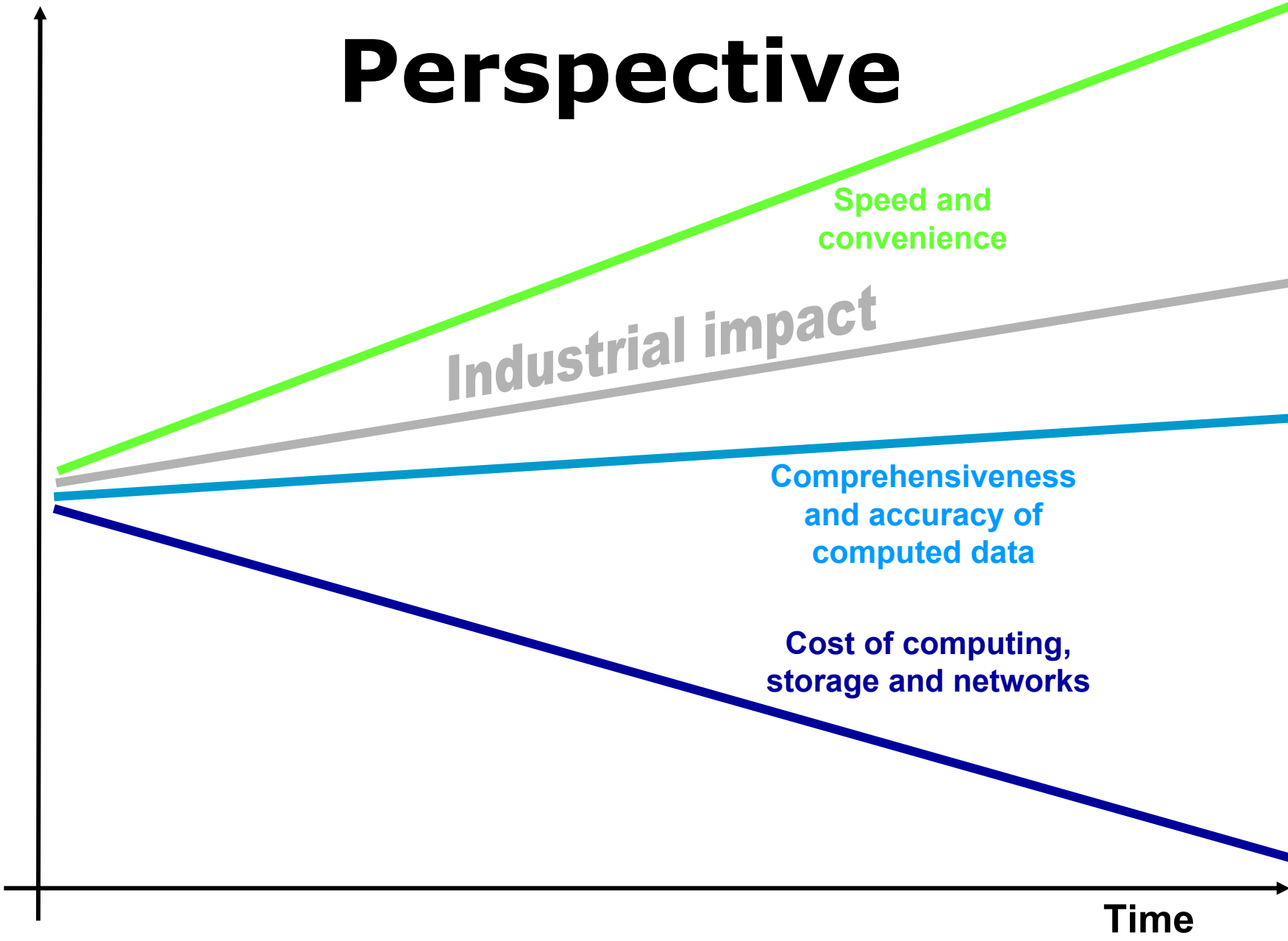
Perspective



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