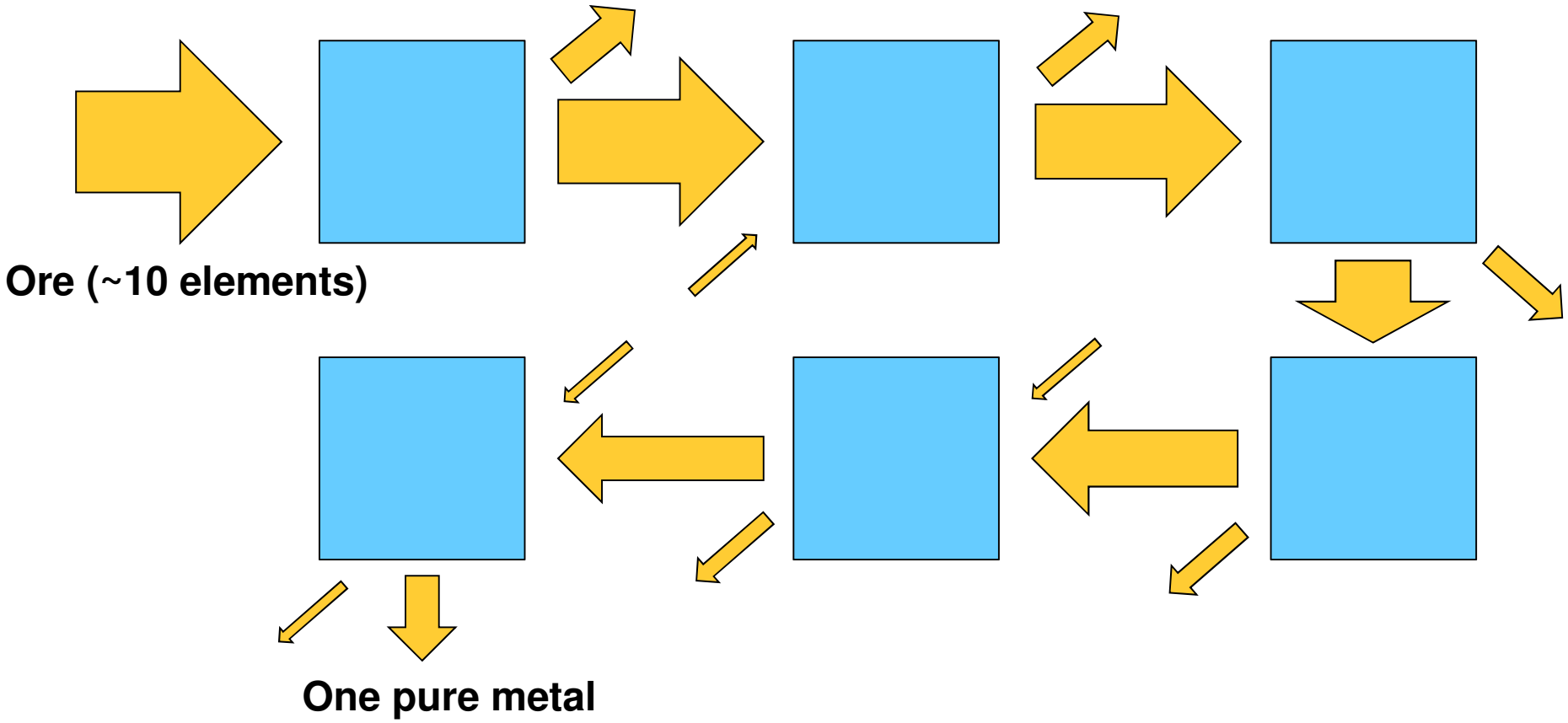
Scanning chemical compound space for radically new processing solutions: De-bismuthizing lead

Moritz to Baben

GTT-Technologies, Herzogenrath, Germany

The art of metallurgical refining



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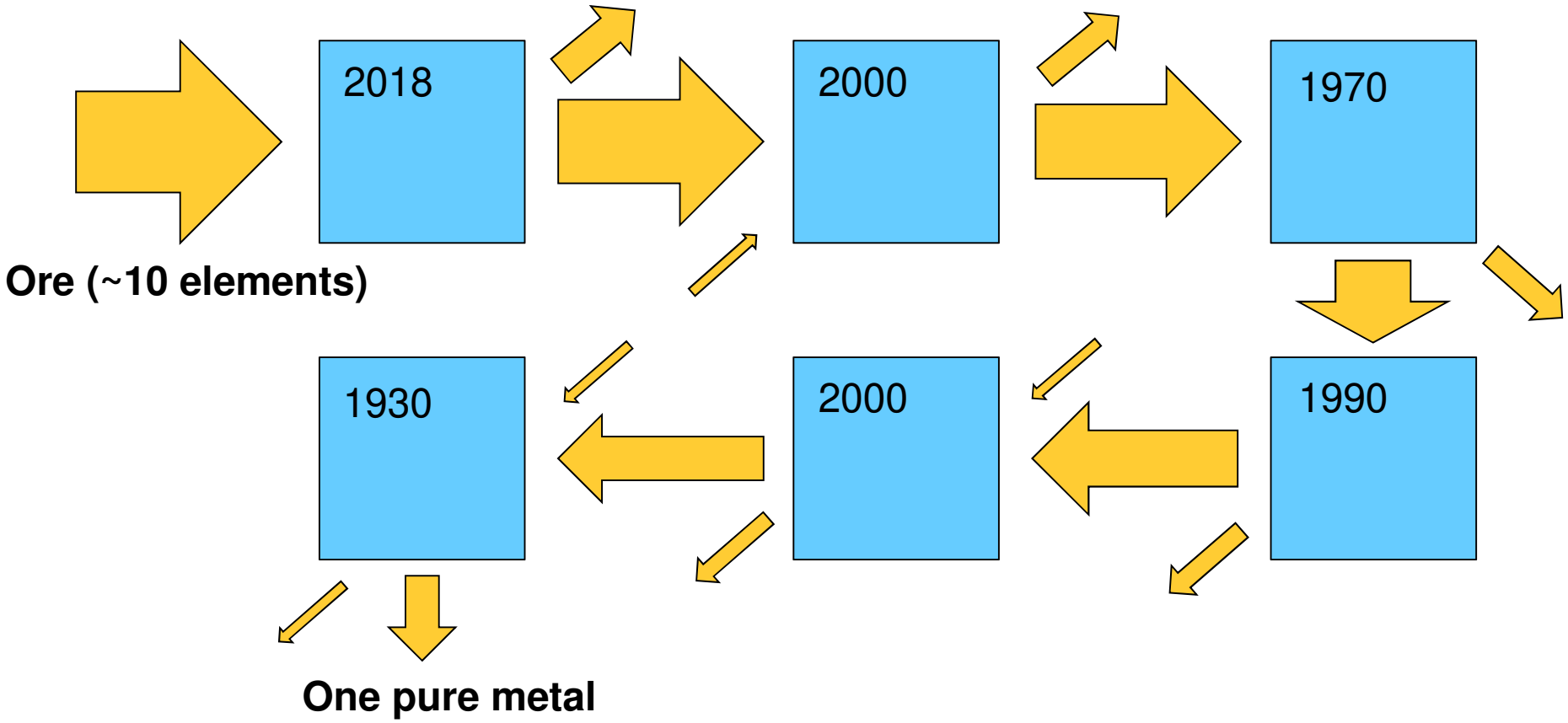

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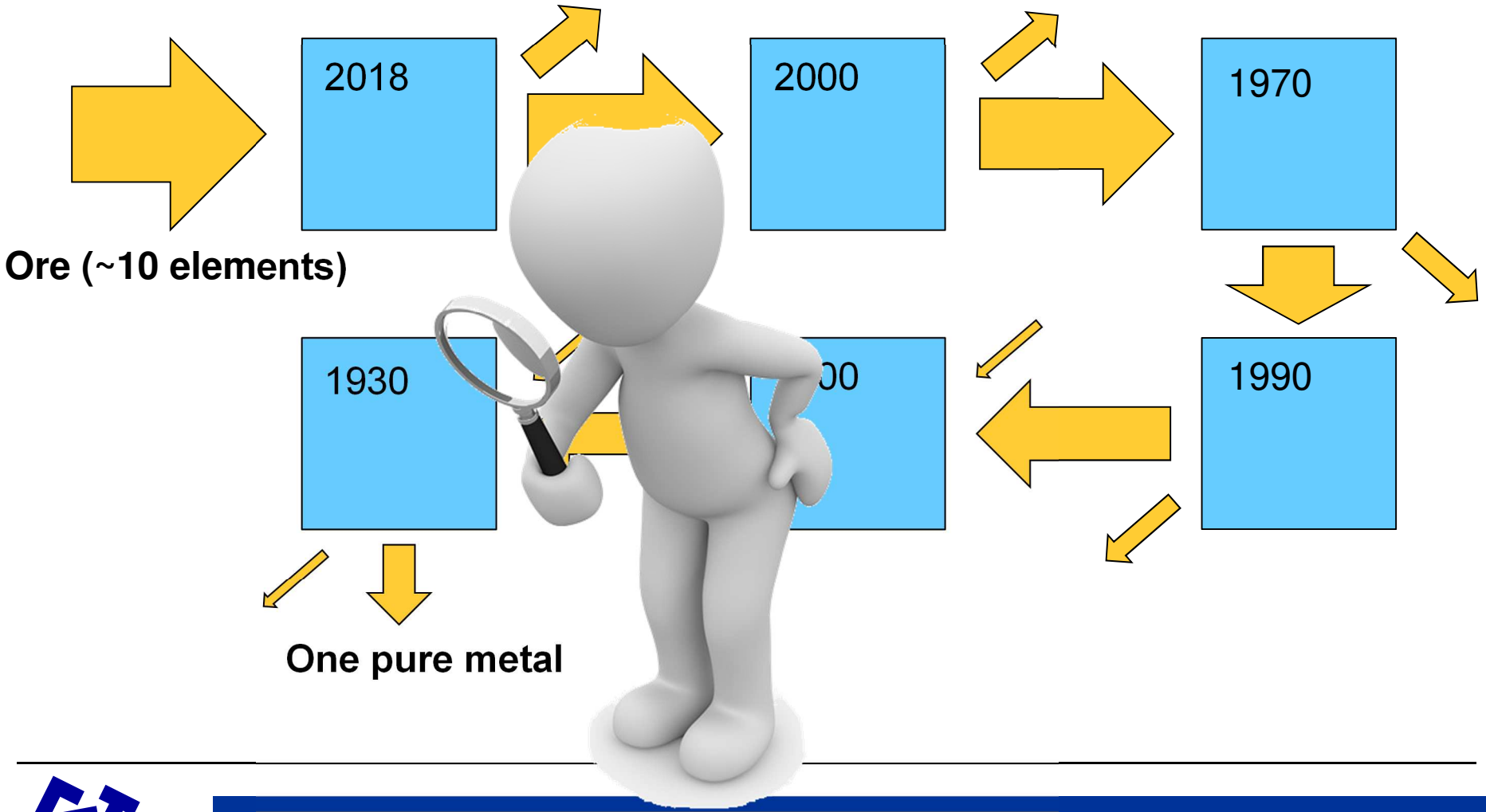

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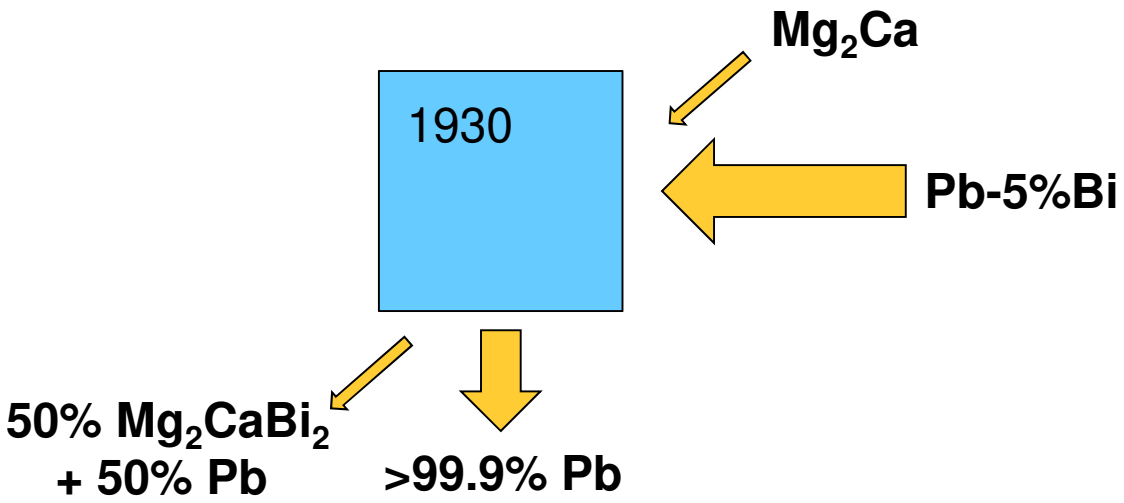
De-bismuthizing after Kroll-Betterton

Developed in the 1930s
Expensive and time-consuming - but it works!



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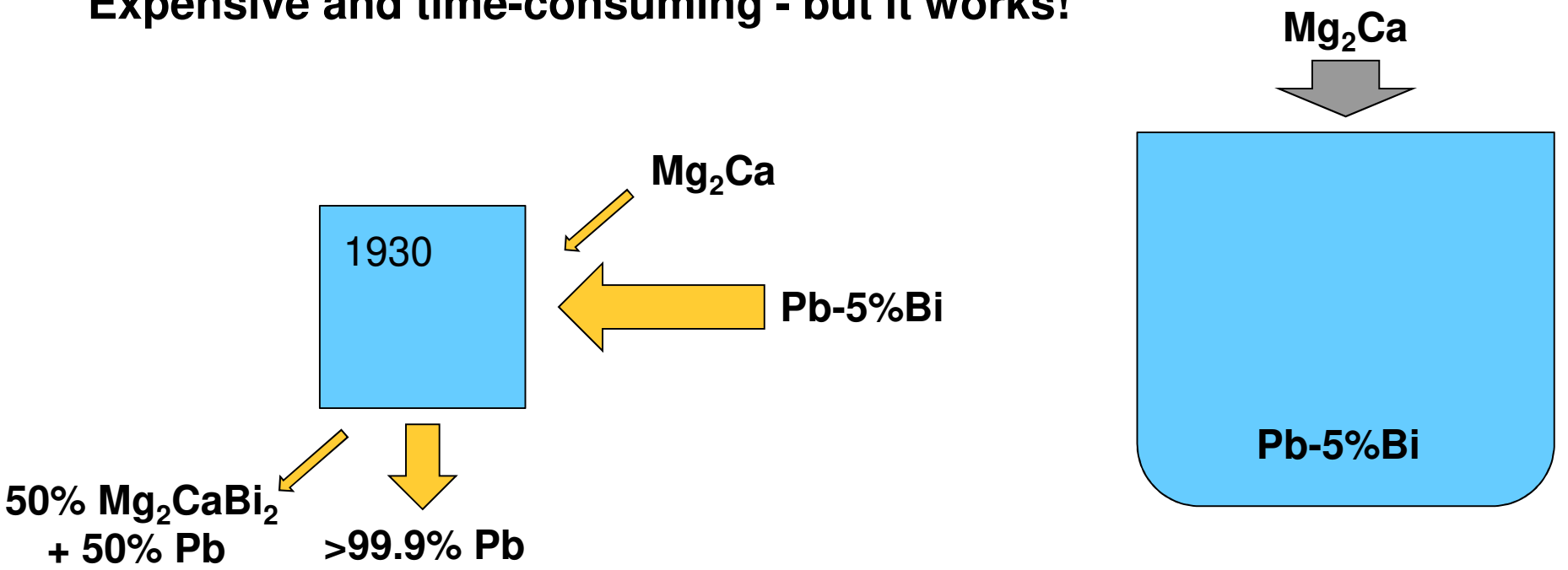

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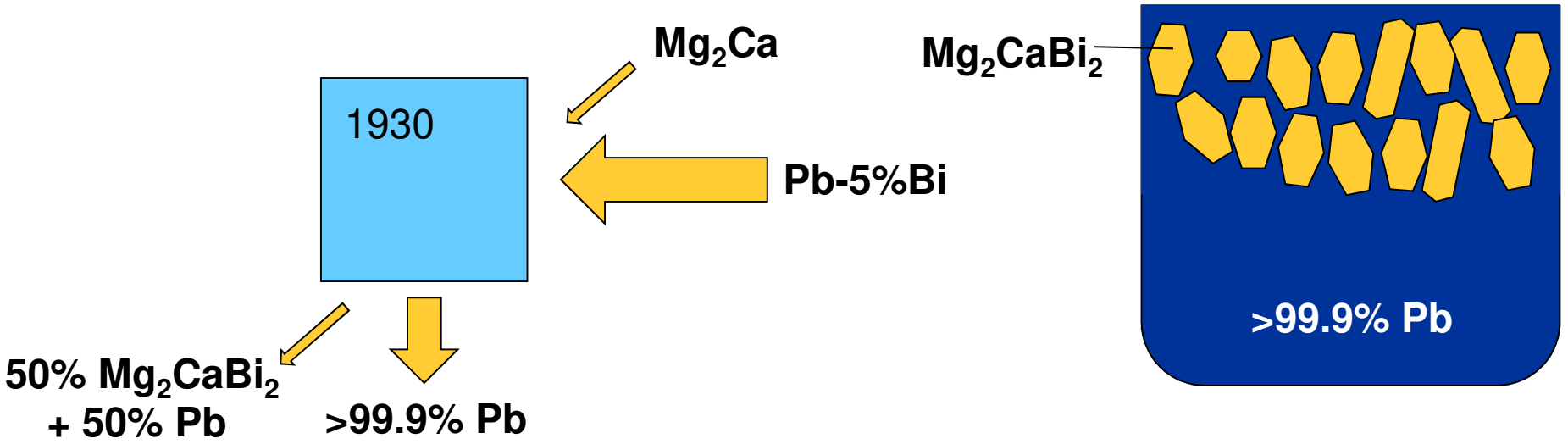

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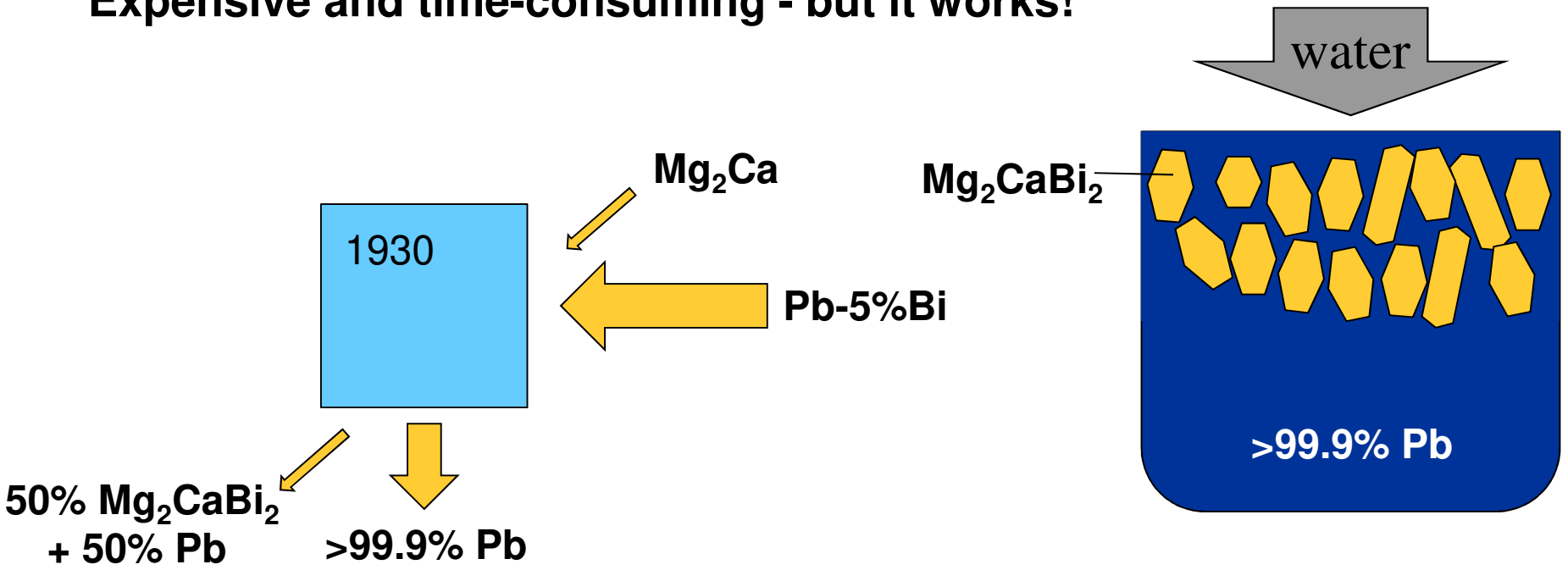

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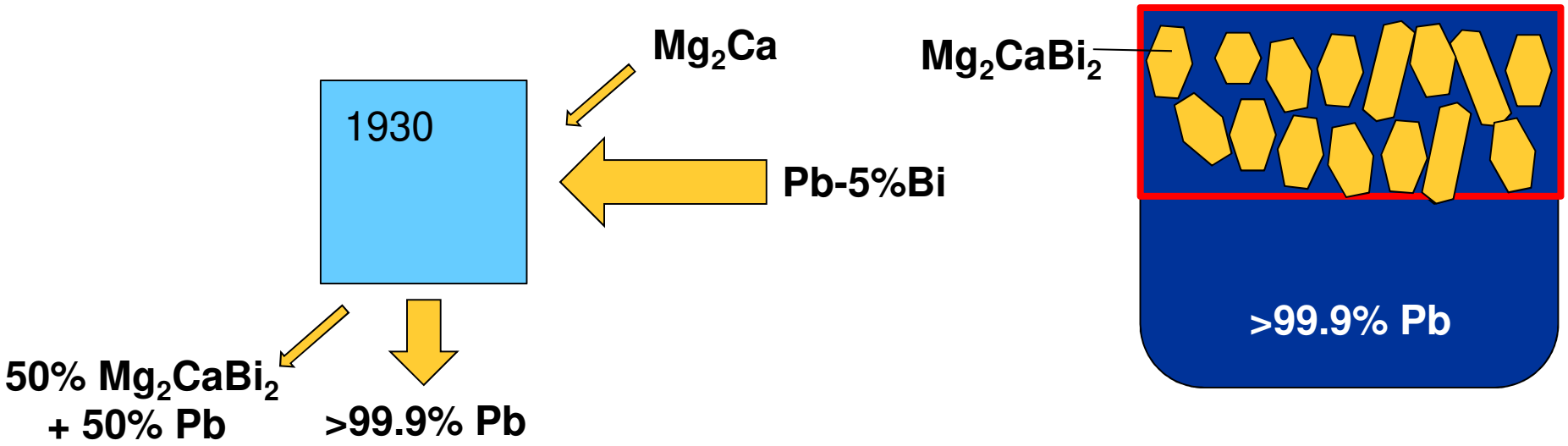

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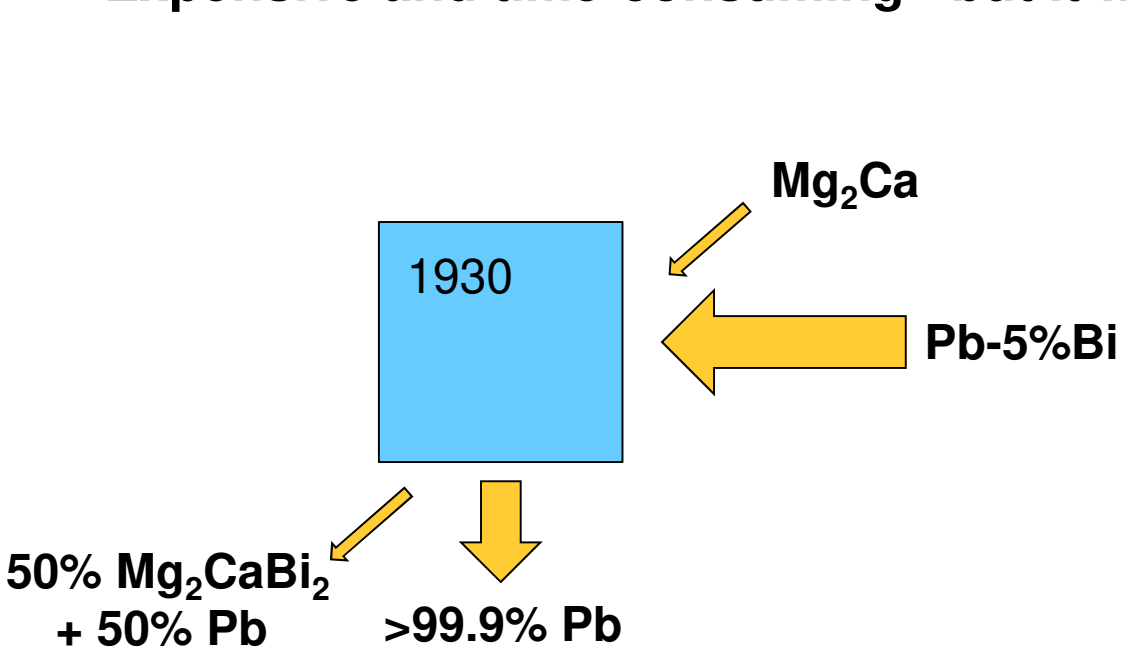

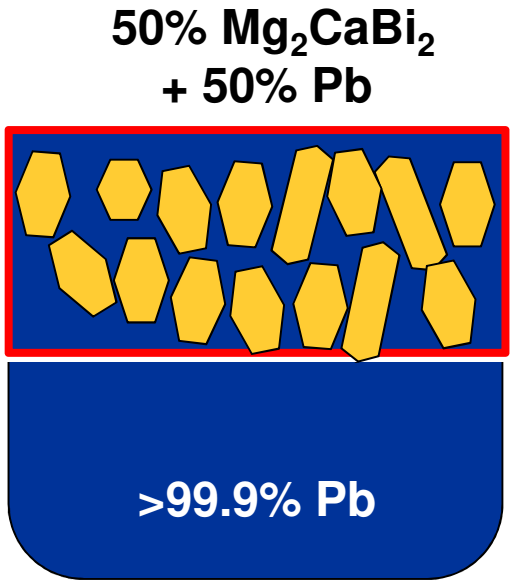

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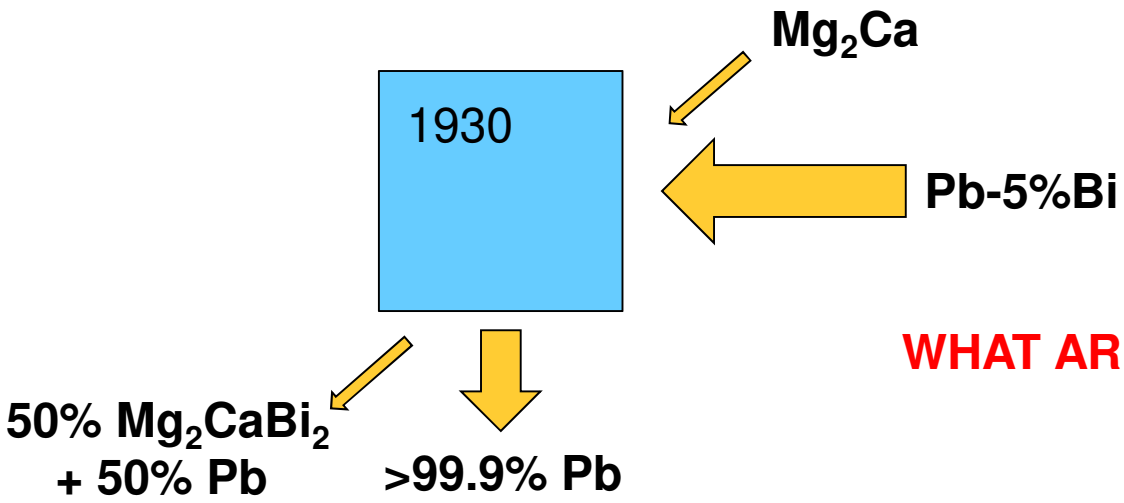

WHAT ARE THE ALTERNATIVES?

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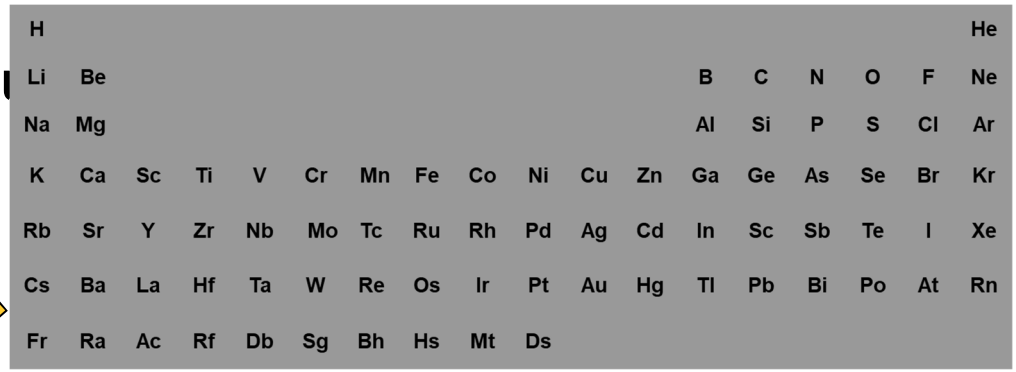


1930

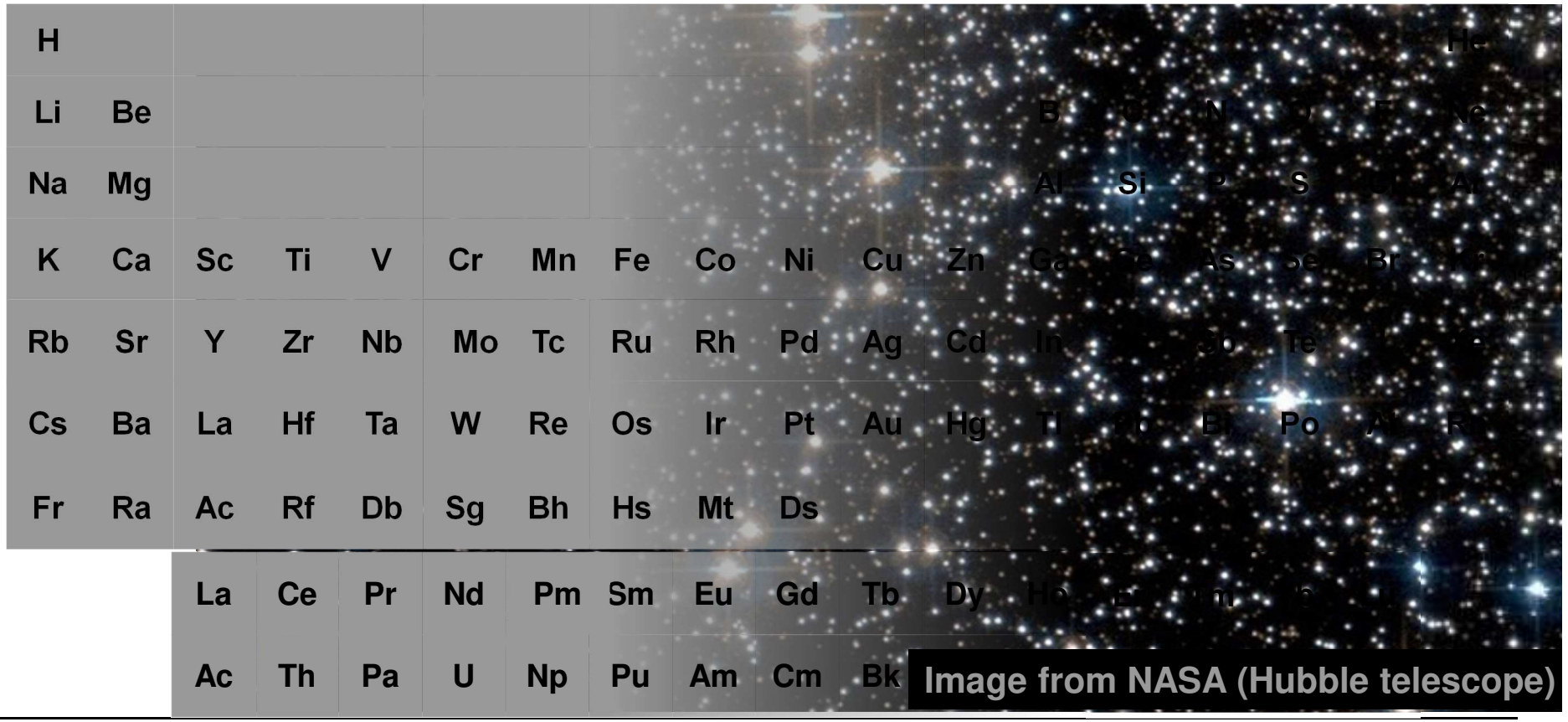
Pb-5%Bi

50% Mg_2CaBi_2 + 50% Pb

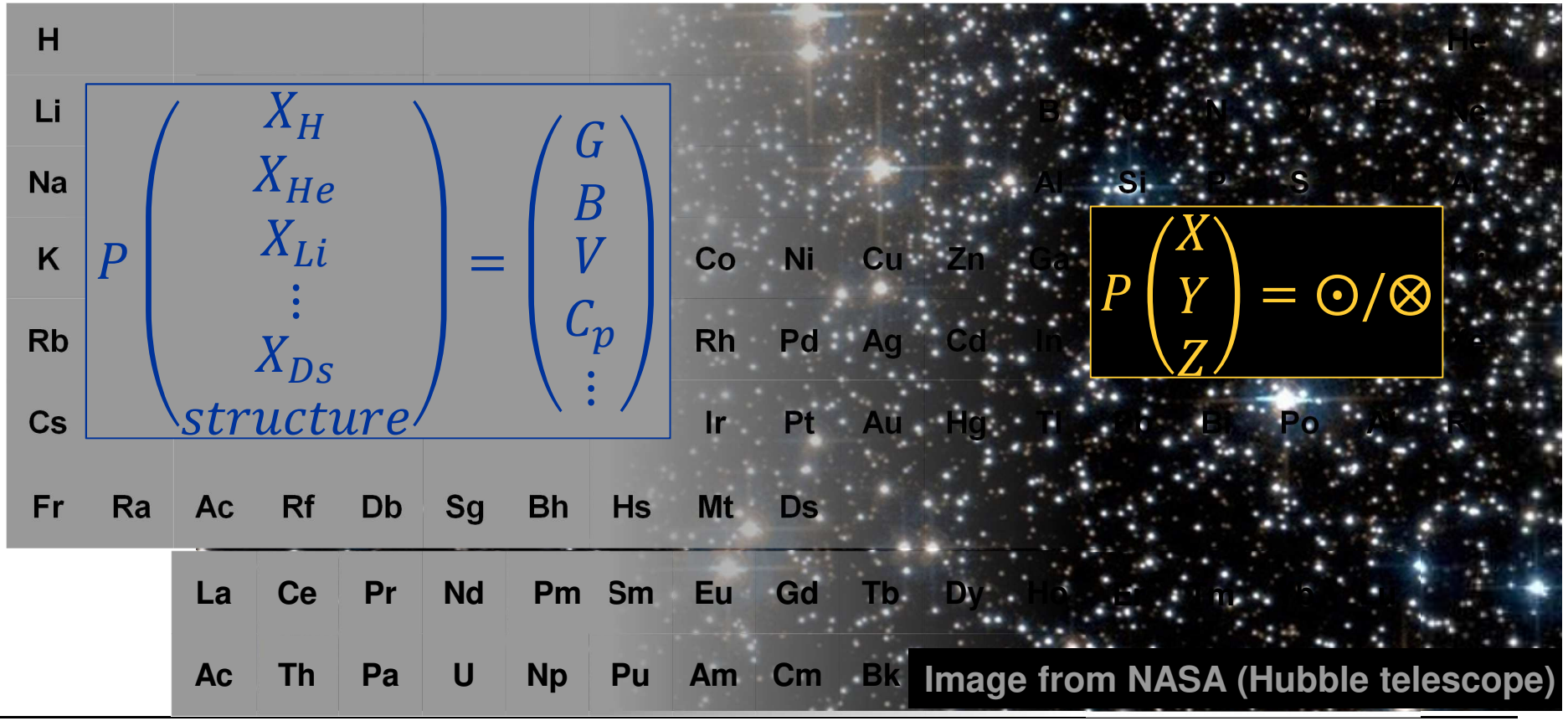
>99.9% Pb

WHAT ARE THE ALTERNATIVES?
~ 70 possible elements
~ 2500 possible binary combinations

Chemical Compound Space

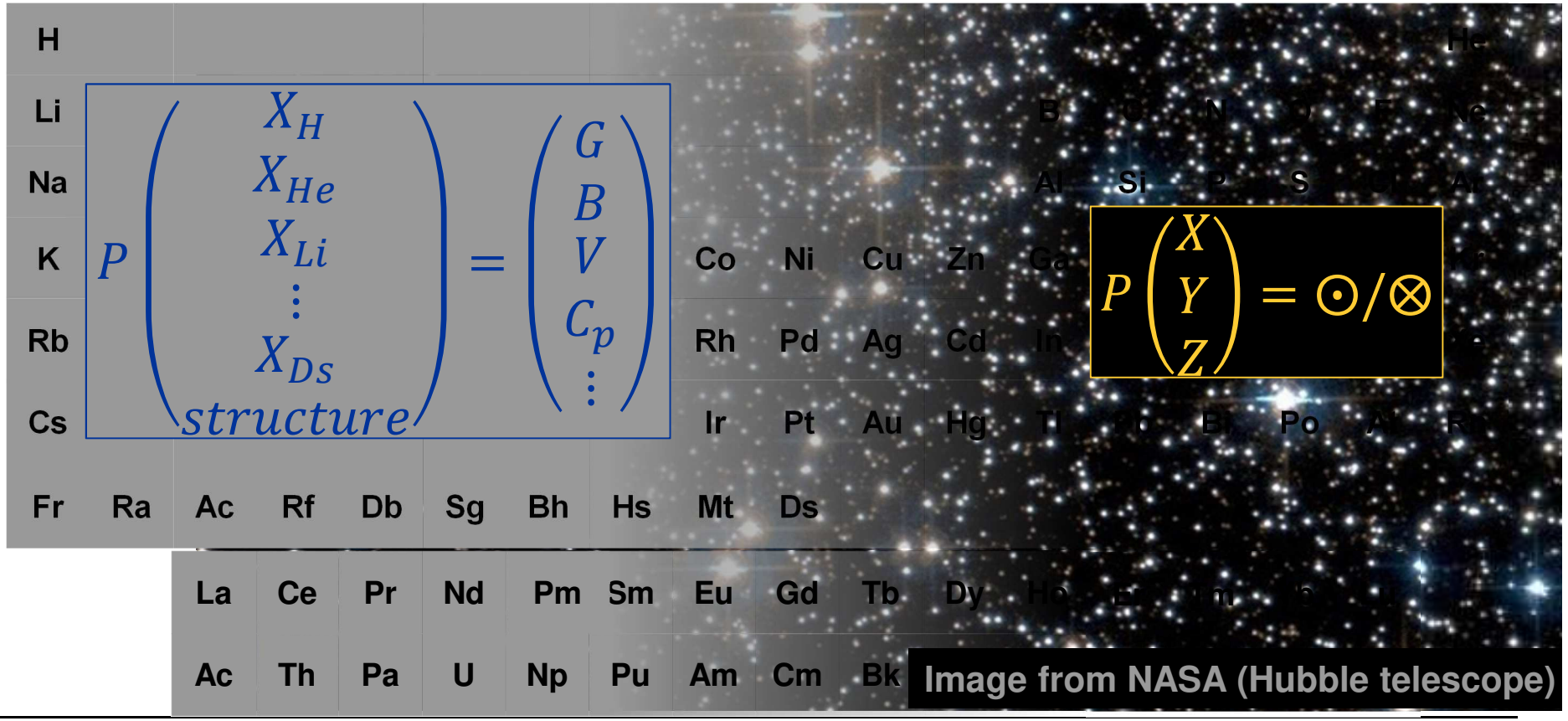


Chemical Compound Space



Chemical Compound Space

How do you navigate?



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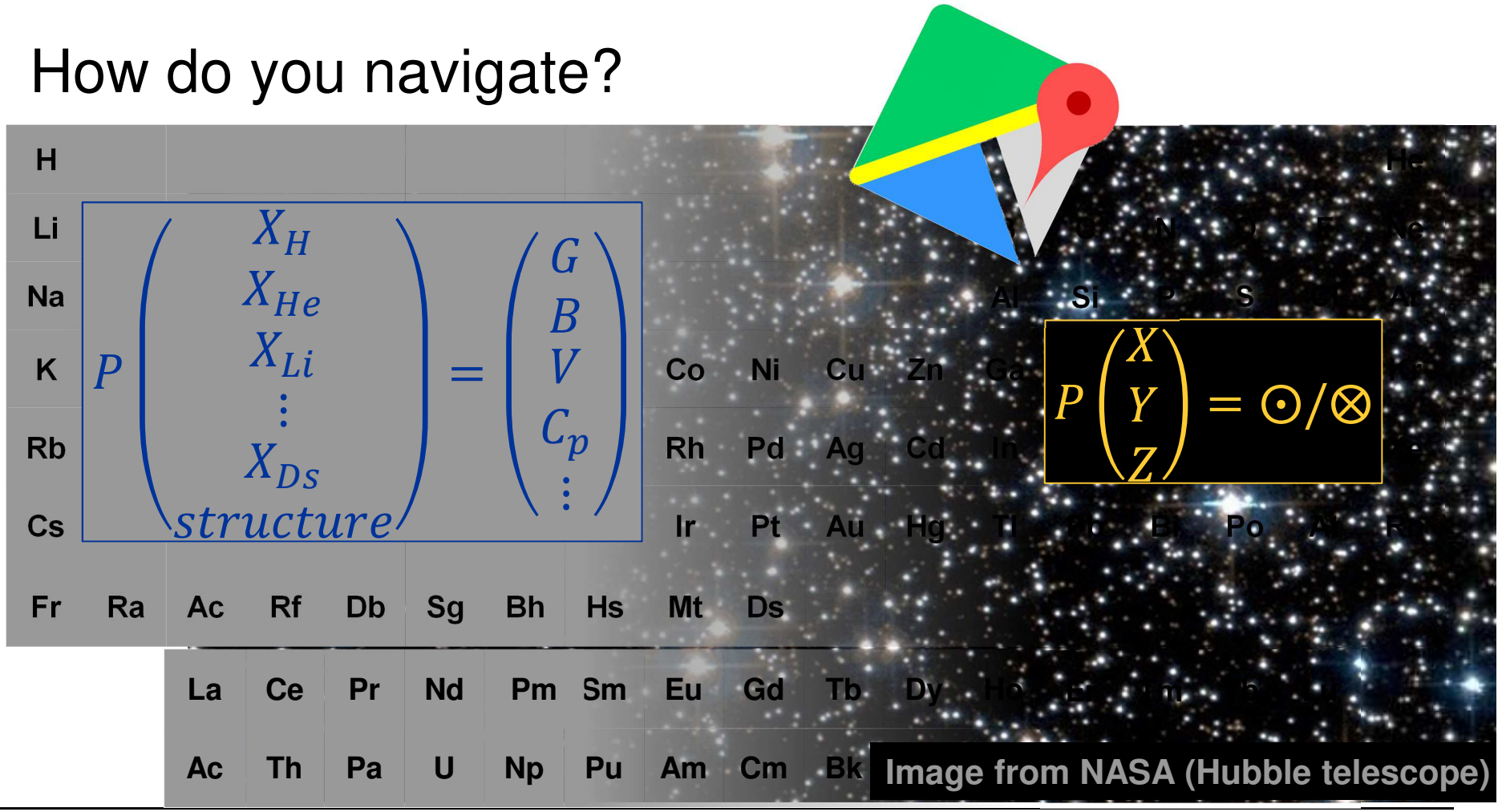
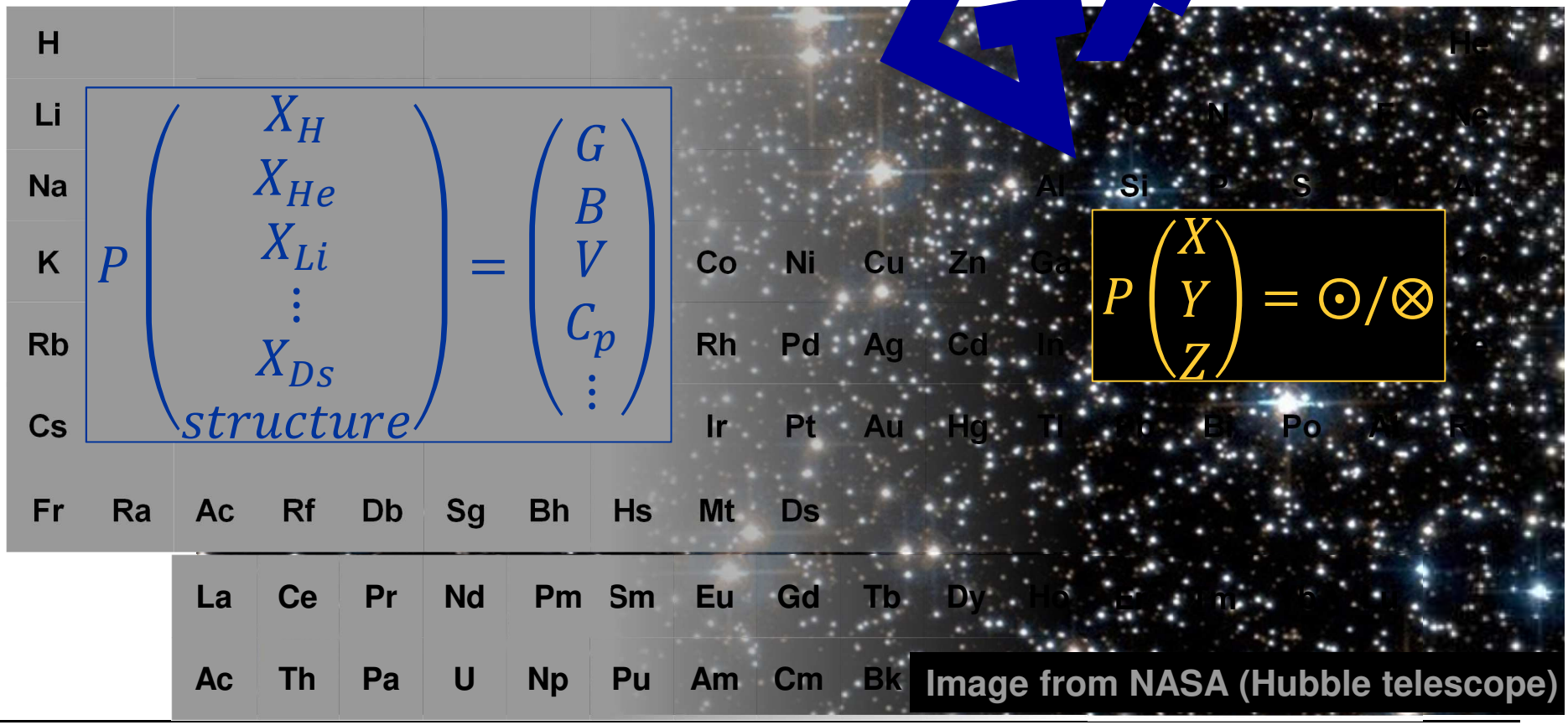


Chemical Compound Space

How do you navigate?



Chemical Compound Space

	CalPhaD
Number of phases	4868 (FactPS) 3768 (SGTE PS) 317 (SGTE Solutions)
T-ranges	298 K - 5000 K
Solution phases	solid liquid aqueous gas
origin	Experiments (Assessments since 1970s)

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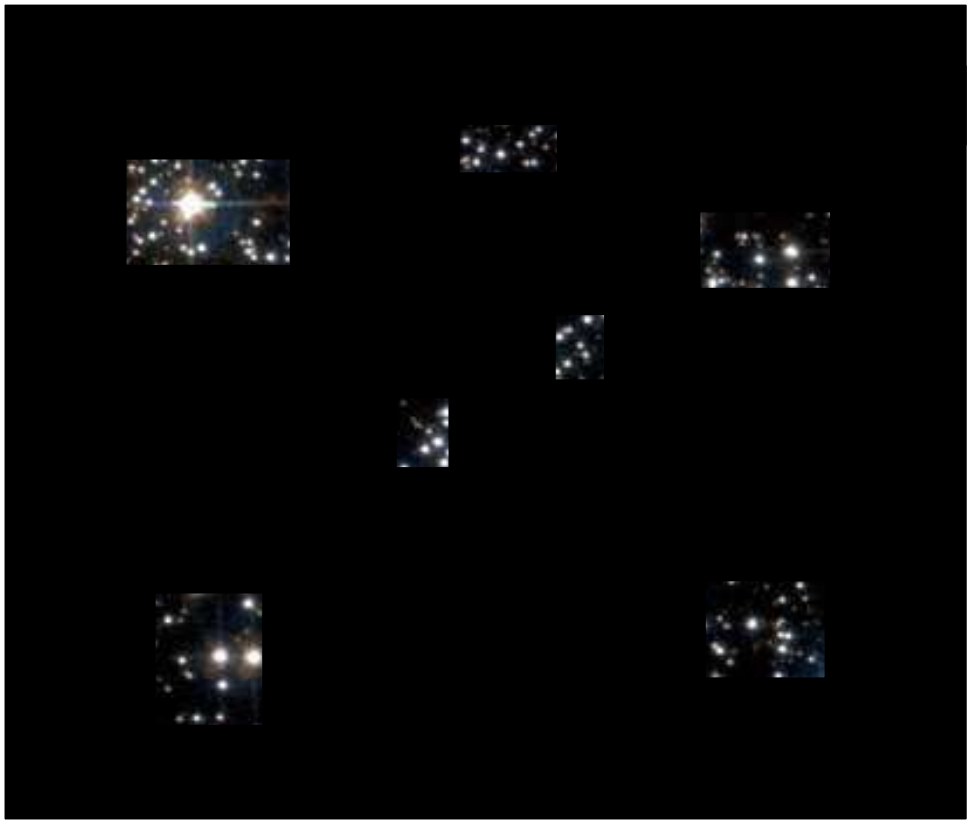


Chemical Compound Space

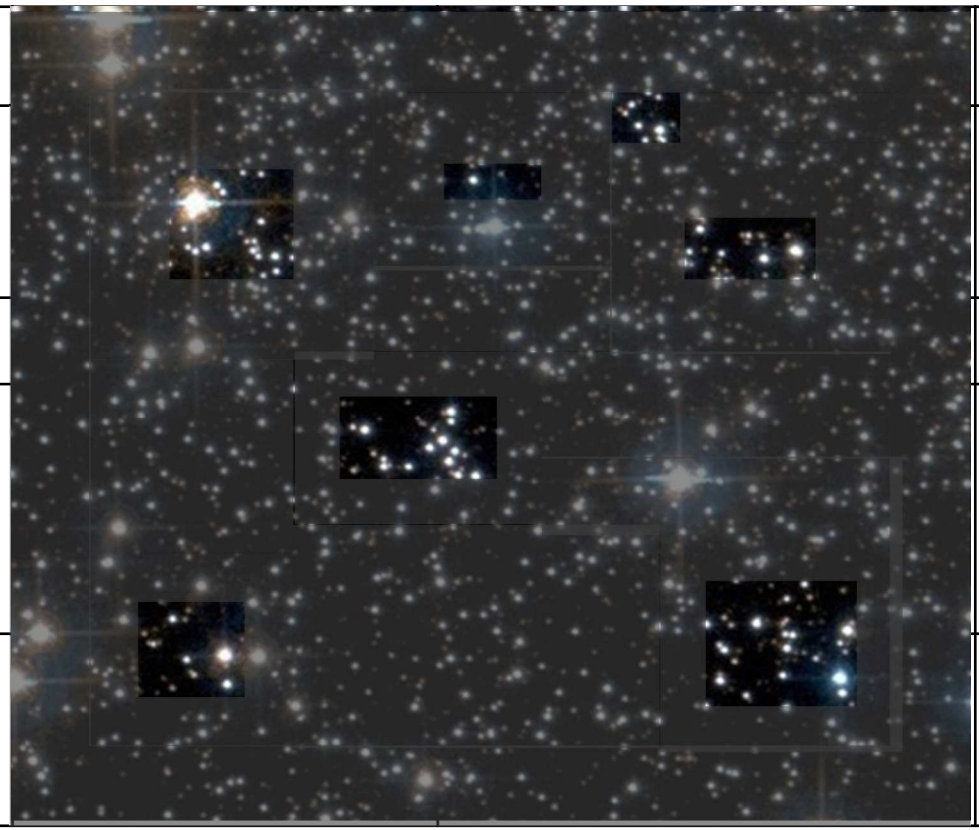
	CalPhaD	Ab initio
Number of phases	4868 (FactPS) 3768 (SGTE PS) 317 (SGTE Solutions)	67‘000 (materialsproject) 470‘000 (oqmd) 1‘680‘000 (aflowlib)
T-ranges	298 K - 5000 K	0 K
Solution phases	solid liquid aqueous gas	---
origin	Experiments (Assessments since 1970s)	Materials Genome Initiative (since 2011)

Chemical Compound Space

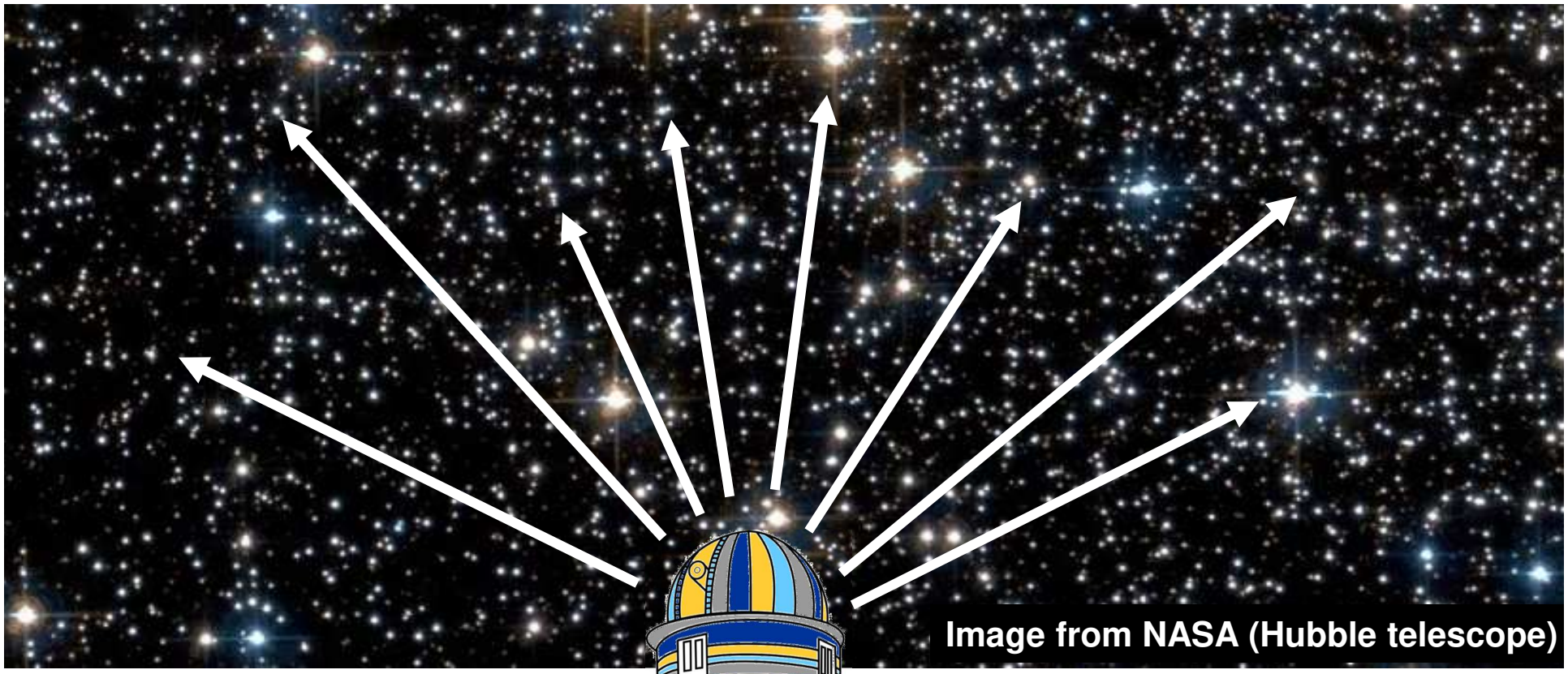
	CalPhaD	Ab initio	aiMP 1.0
Number of phases	4868 (FactPS) 3768 (SGTE PS) 317 (SGTE Solutions)	67‘000 (materialsproject) 470‘000 (oqmd) 1‘680‘000 (aflowlib)	67‘000
T-ranges	298 K - 5000 K	0 K	298 - 5000 K
Solution phases	solid liquid aqueous gas	---	--- (soon: solid)
origin	Experiments (Assessments since 1970s)	Materials Genome Initiative (since 2011)	materialsproject.org + extrapolation

Chemical Compound Space

New database

		aiMP 1.0
Number of phases		67‘000
T-ranges		298 - 5000 K
Solution phases		--- (soon: solid)
origin		materialsproject.org + extrapolation

Materials Informatics



From *ab initio* to CalPhaD

$$G(T) = H(T) - TS(T)$$

$$H(T) = H^{0K} + \int_{0K}^{T} C_P(T)dT$$

⇨ H^{0K}, $C_p(T)$

→ DFT!

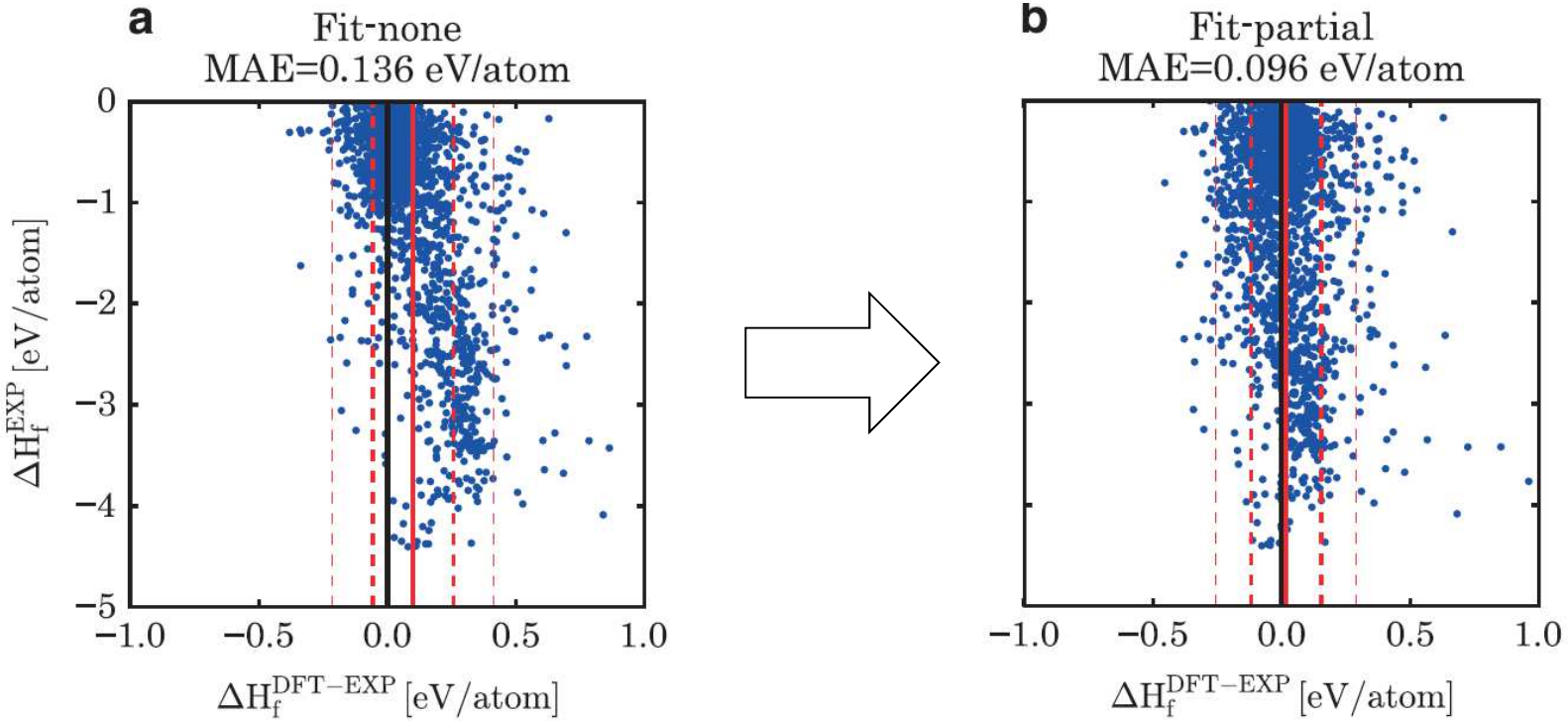
$$S(T) = S^{0K} + \int_{0K}^{T} \frac{C_P(T)}{T} dT$$

⇨ S^{0K}, $C_p(T)$

= 0 (3rd law)

Accuracy of *ab initio* enthalpies

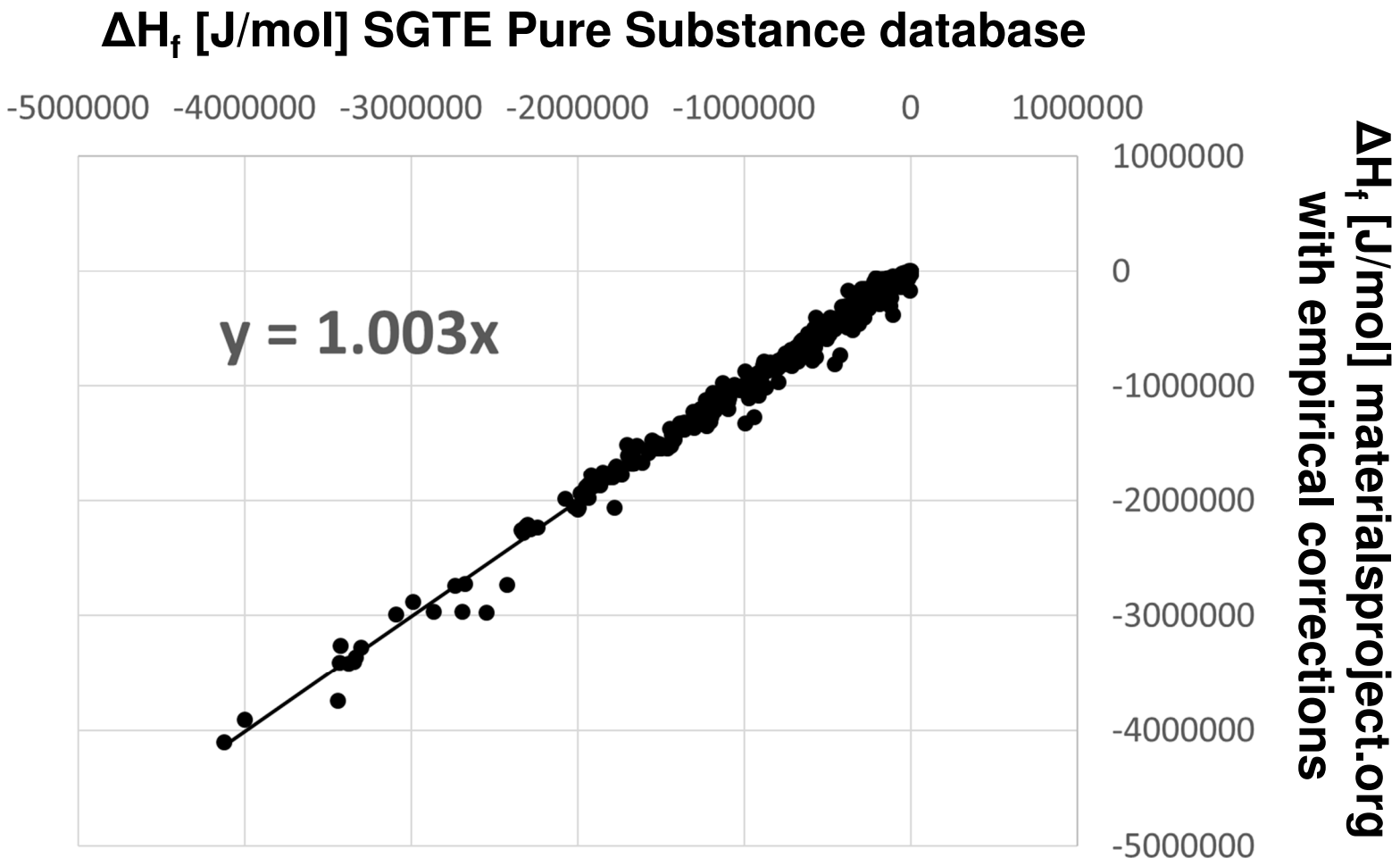
For some elements (e.g. O) the most stable state changes between 0K and 298K. → Correct H^{298K} for all oxides etc. [3]



[1] S. Kirklin et al., npj Computational Materials 1 (2015) 15010.

oqmd.org

Accuracy of *ab initio* enthalpies



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= 0 (3rd law)

From *ab initio* to CalPhaD

$$G(T) = H(T) - TS(T)$$ 298 K < T < 5000 K

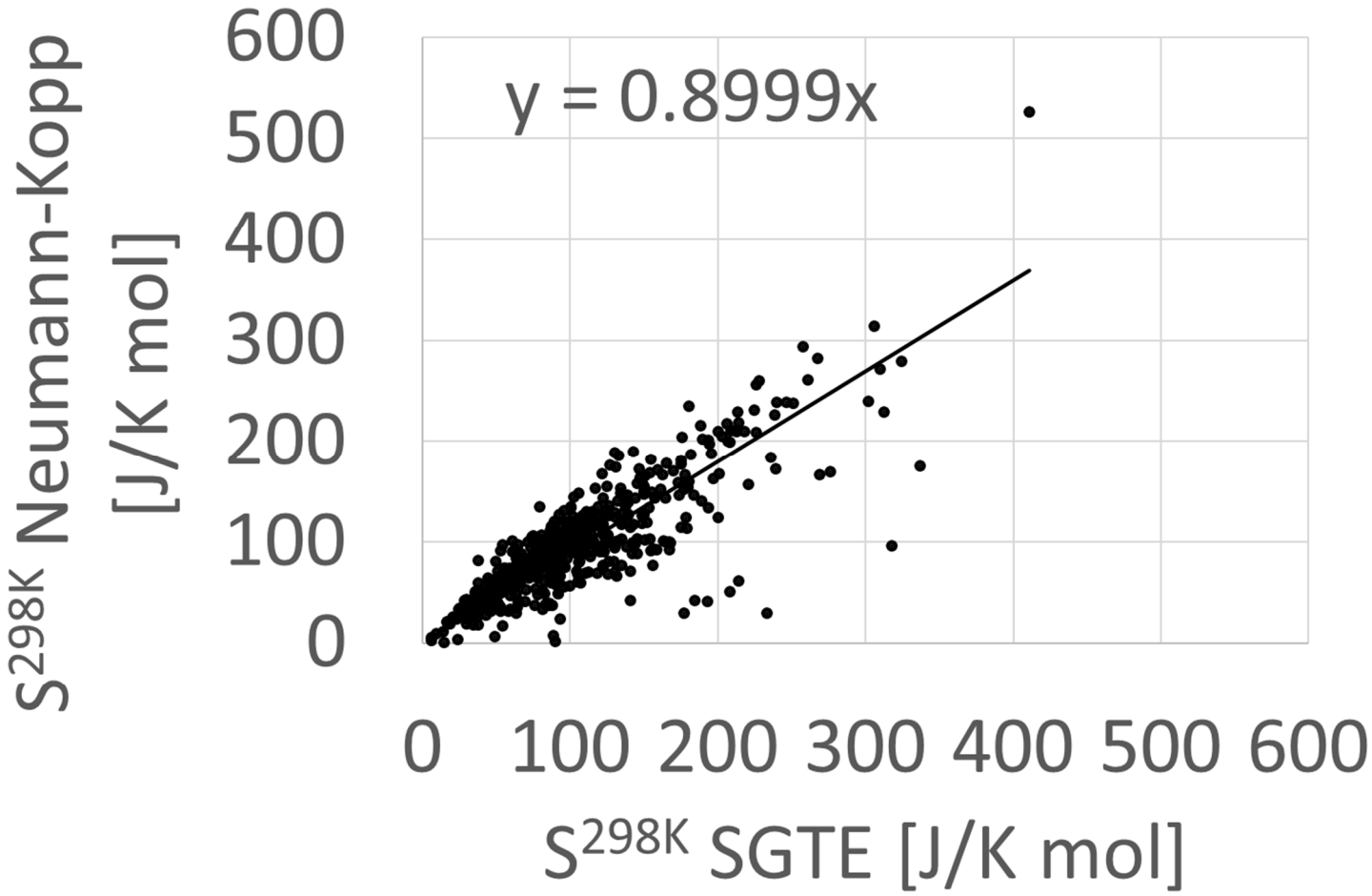
$$H(T) = H^{298K} + \int_{298K}^{T} C_P(T)dT$$ ⇨ H^{298K}, $C_p(T)$

→ DFT!

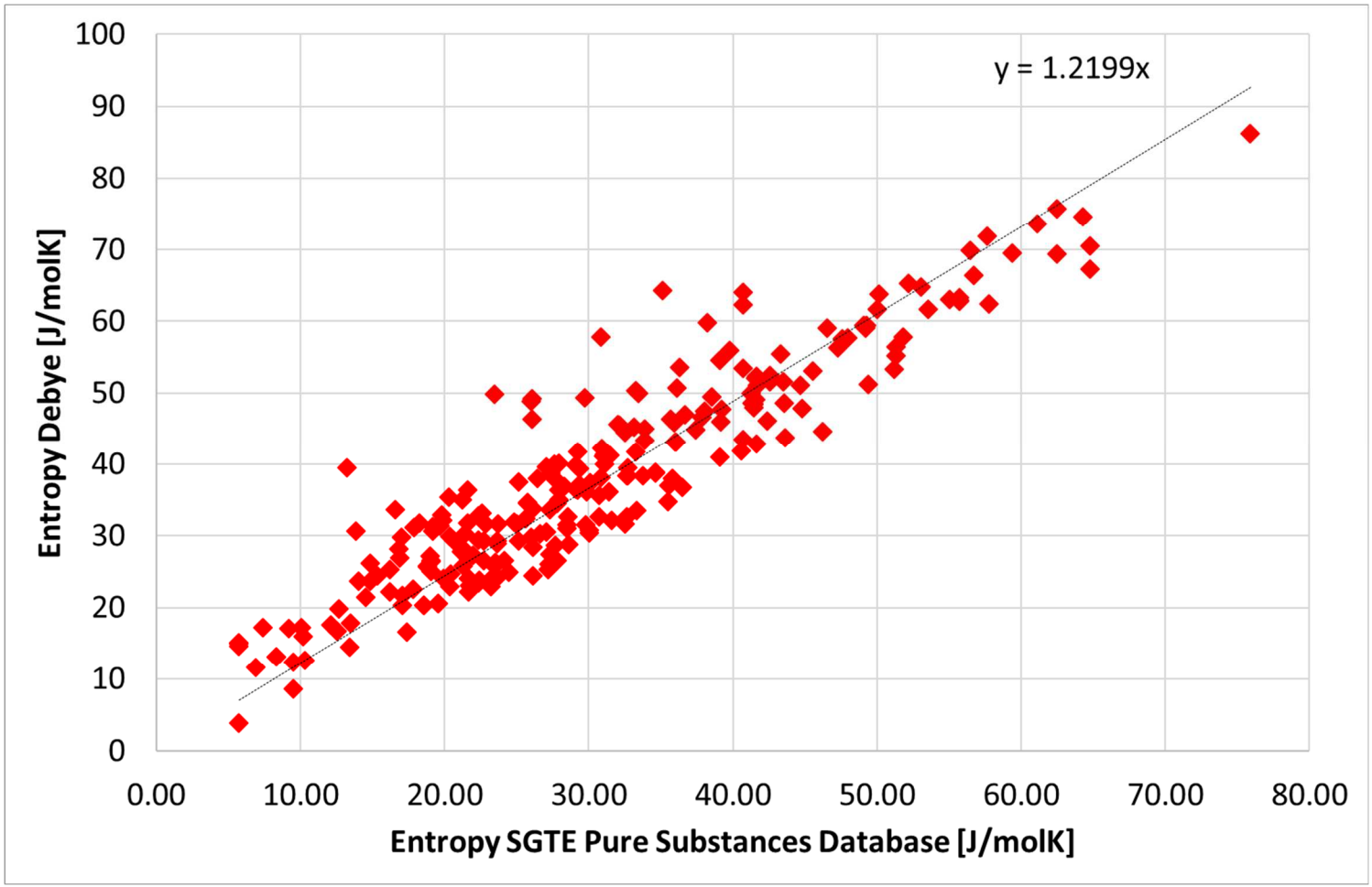
$$S(T) = S^{298K} + \int_{298K}^{T} \frac{C_P(T)}{T} dT$$ ⇨ S^{298K}, $C_p(T)$

~~= 0 (3rd law)~~

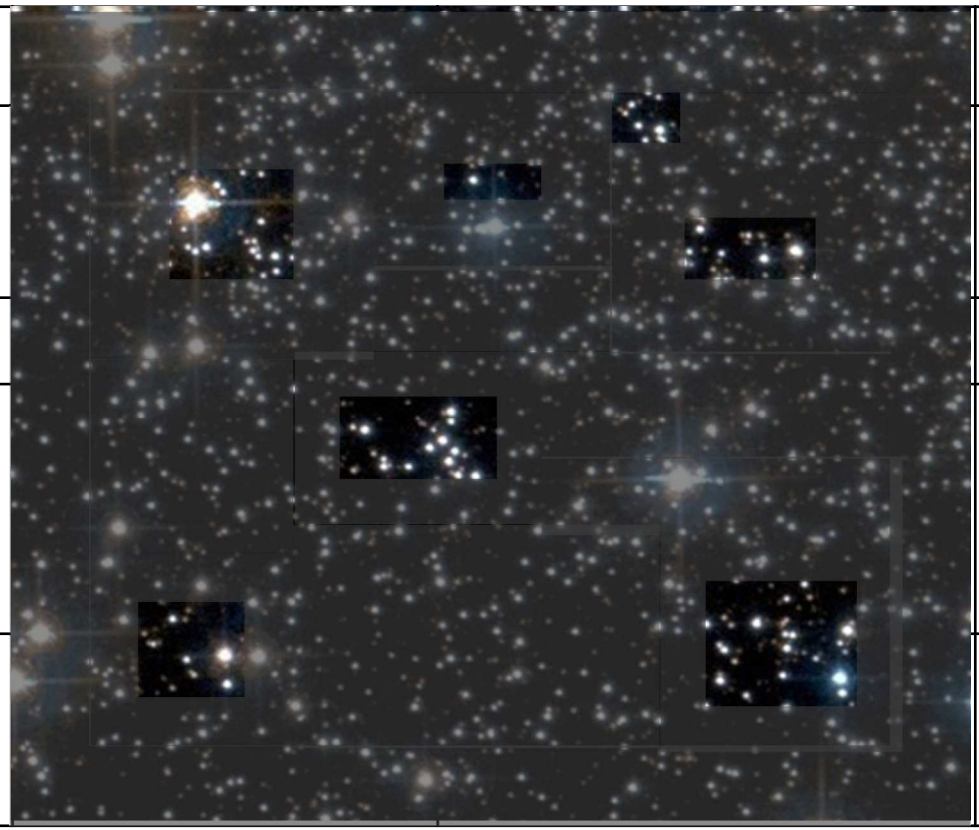
Neumann-Kopp for S^{298K}



Alternative: S^{298K} from Debye model



Chemical Compound Space

		**aiMP 1.0**
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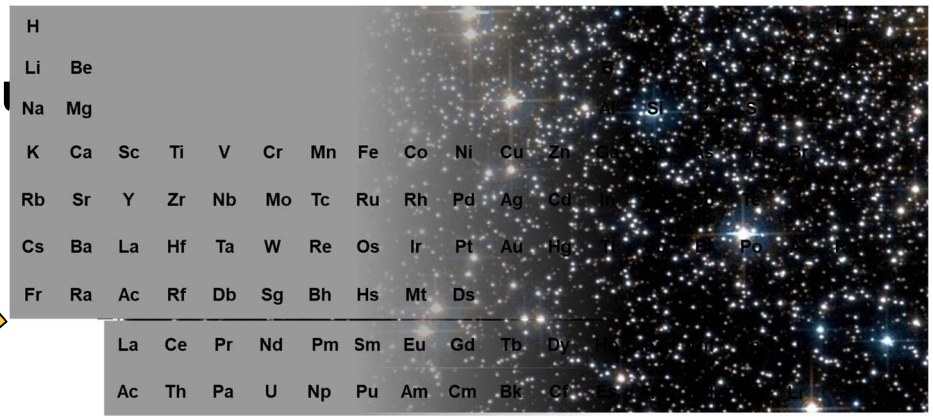

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WHAT ARE THE ALTERNATIVES?
~ 70 possible elements
~ 2500 possible binary combinations

Rational Process and Materials Design

MATERIALS INFORMATICS:
Test ALL ~2500 combinations Pb-Bi-X-Y

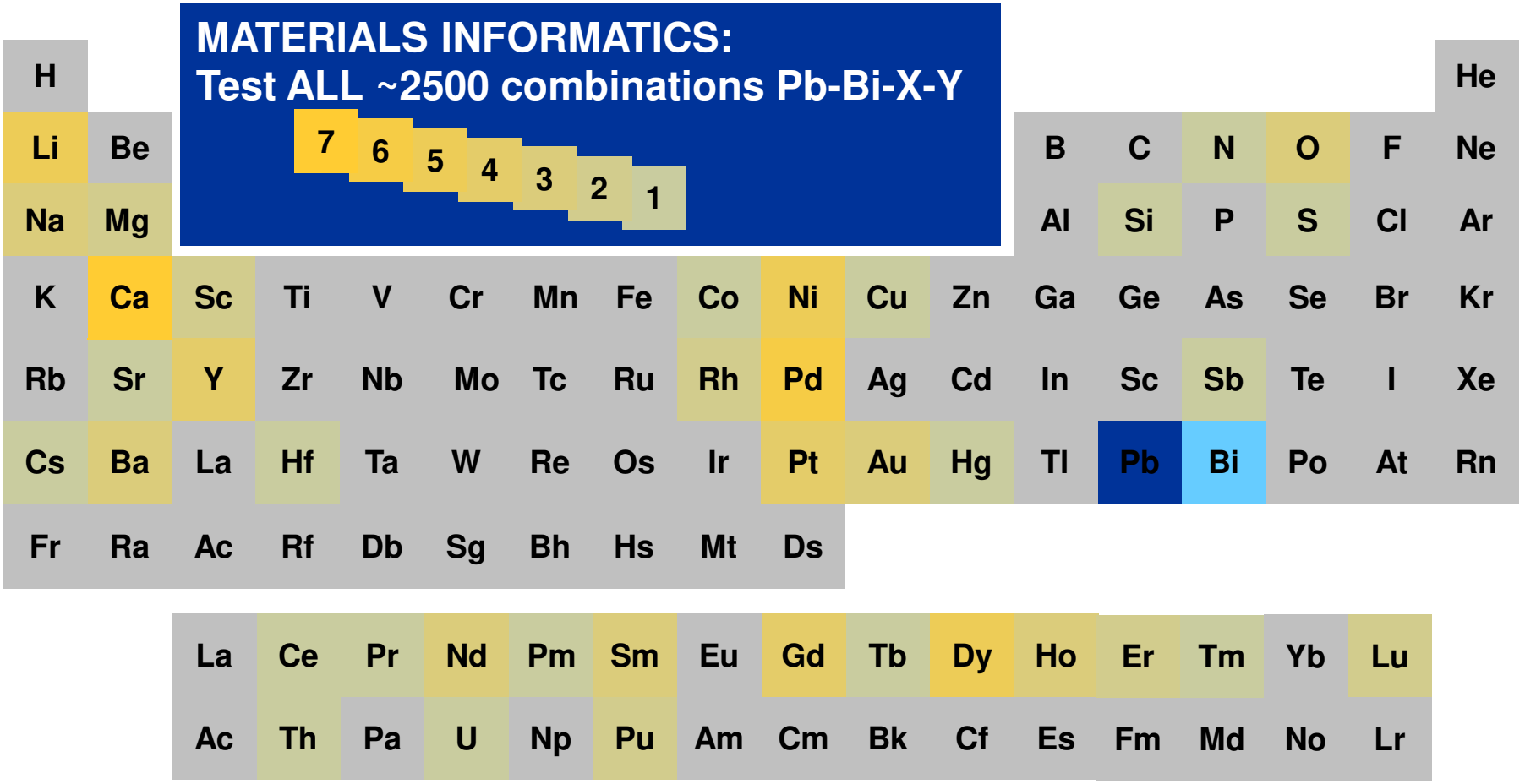
aiMP1.0 + SGTE Solutions + 50 lines of simple macro code in

→ 53 systems Pb-Bi-X-Y as good as Pb-Bi-Ca-Mg

H																He
Li	Be															Ne
Na	Mg															Ar
K	Ca															Kr
Rb	Sr															Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds							

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Rational Process and Materials Design



Conclusions

- aiMP is a CalPhaD compatible database integrated in FactSage based on
  - materialsproject.org
  - Empirical corrections to *ab initio* calculated enthalpy of formation
  - Empirical models for C_p and $S^{298K\#}$
- aiMP can be used for quickly scanning chemical compound space for radically different processing solutions

Thank you for your attention!