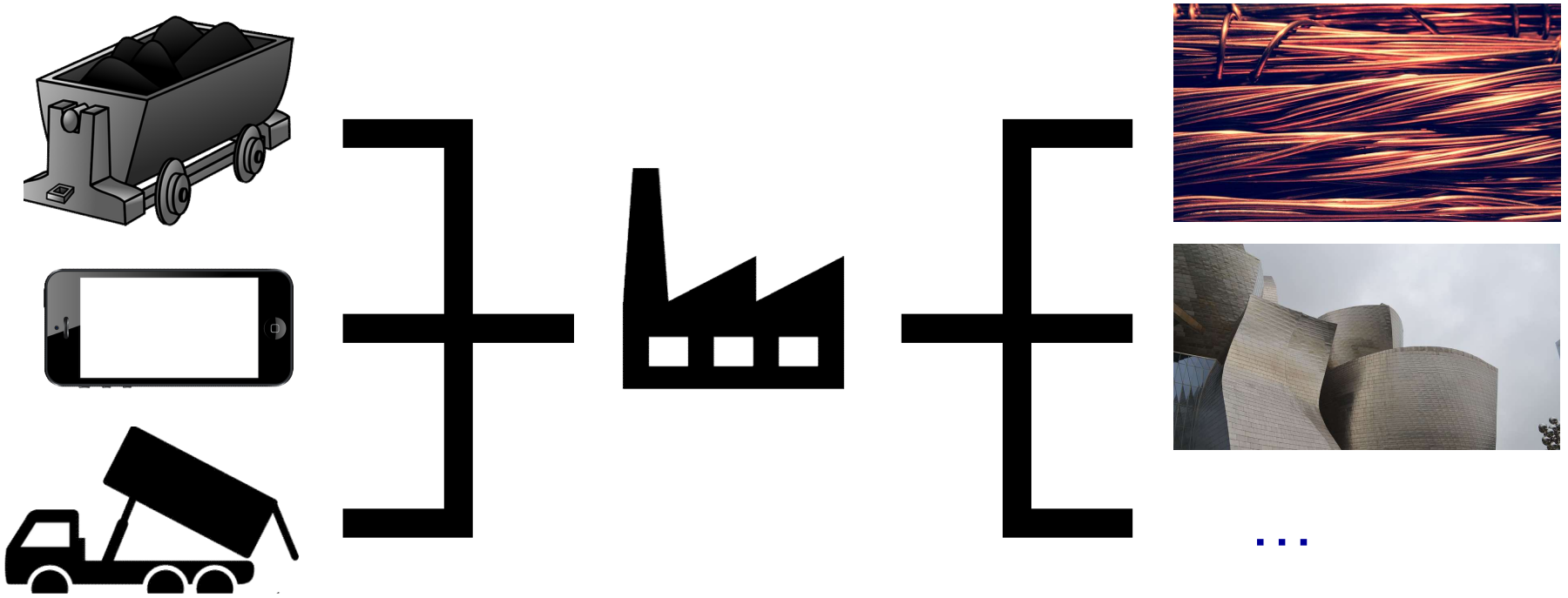
The aiMP database

M. to Baben[1], F. Tang[1], C. Aras[1], C. Kattuputhur[1], K. Hack[1]

[1] GTT-Technologies

What is metallurgy about?



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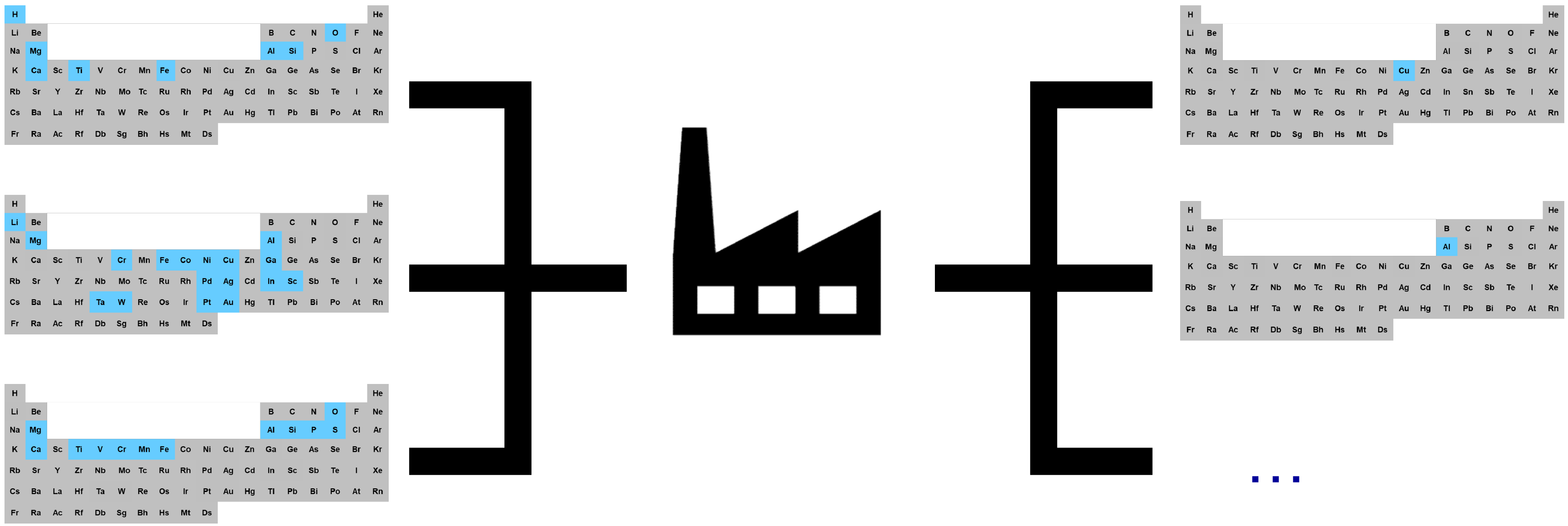
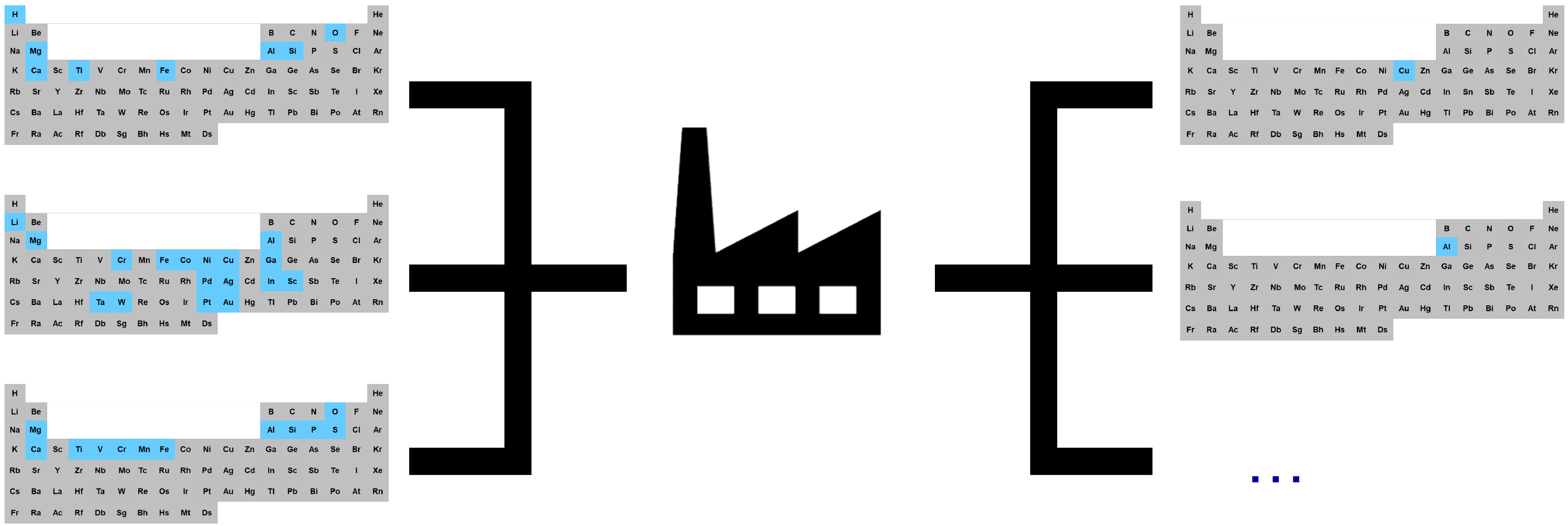


What is metallurgy about?

Navigation in chemical compound space!



Moritz to Baben

What is metallurgy about?

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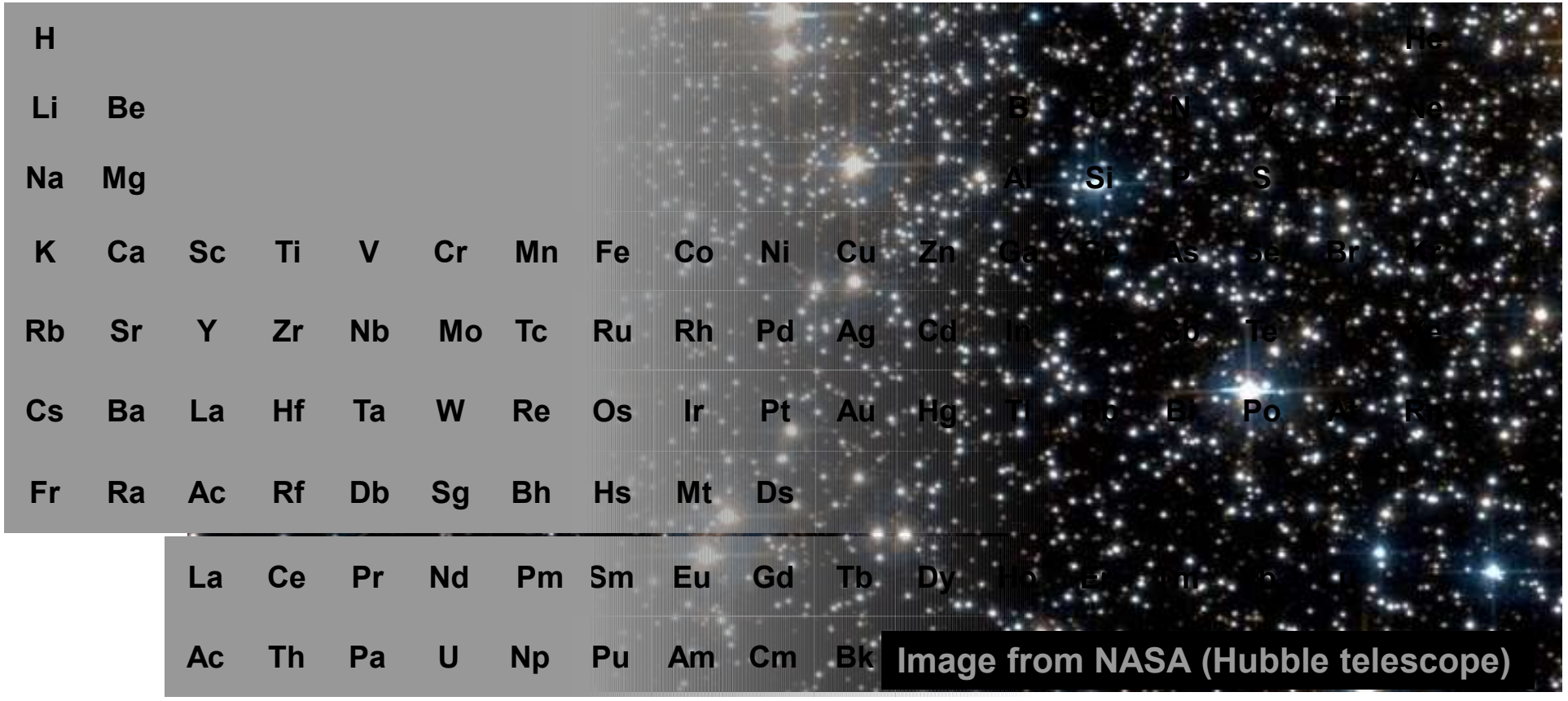

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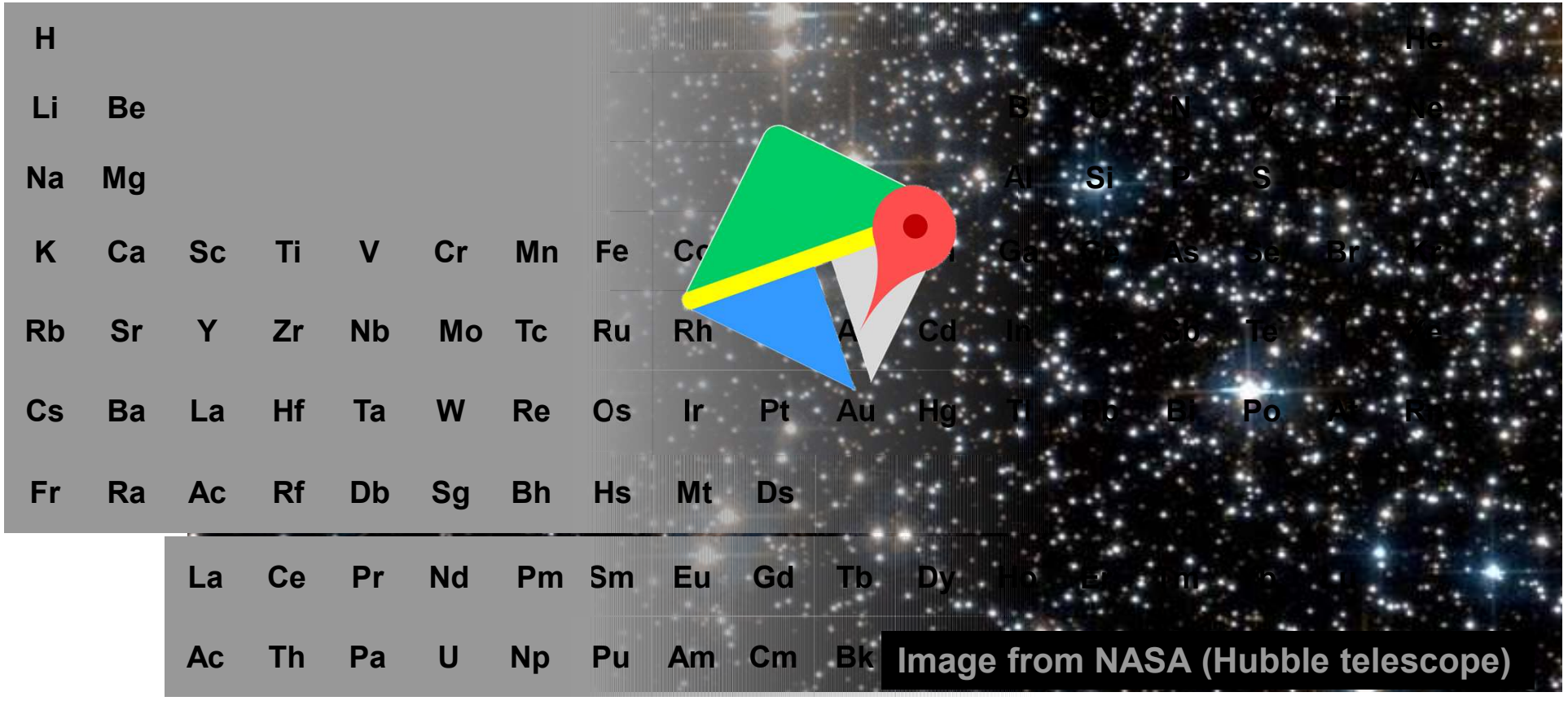

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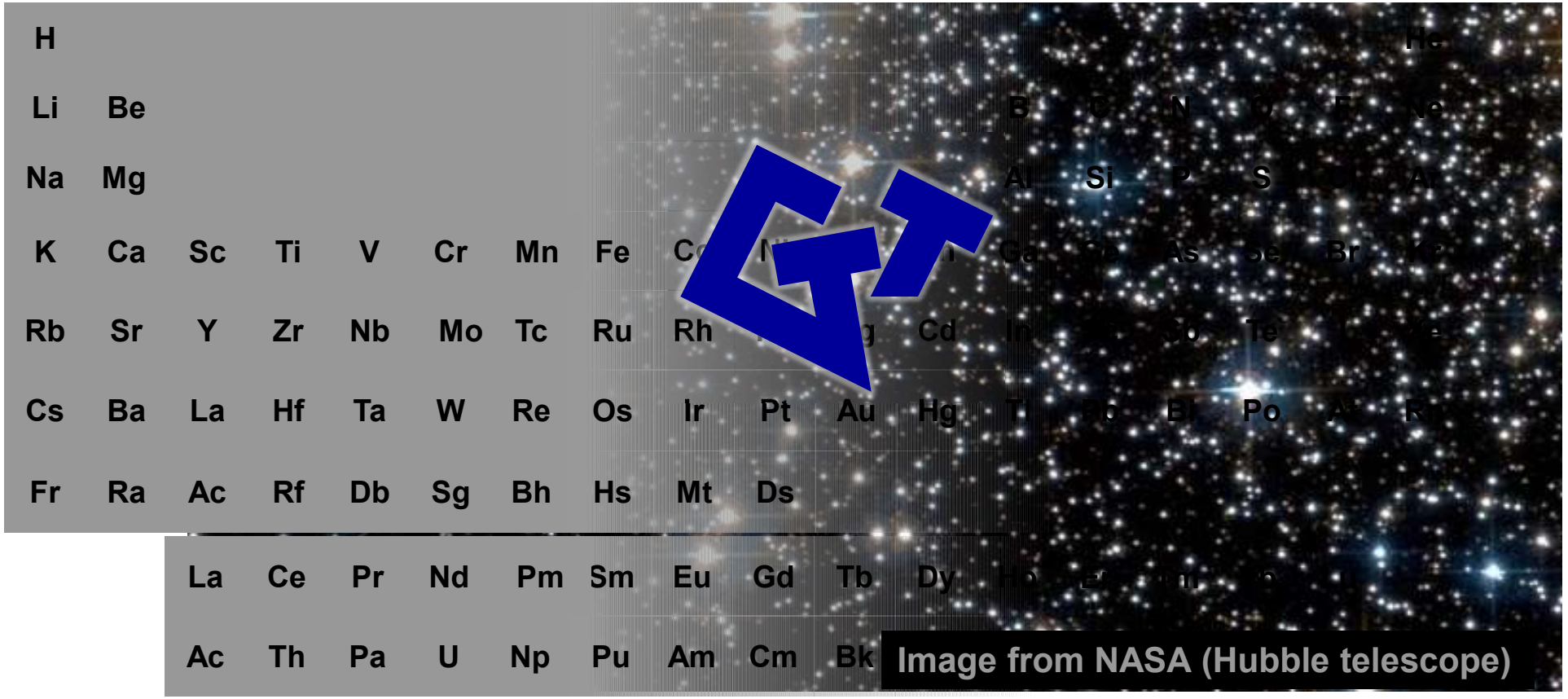
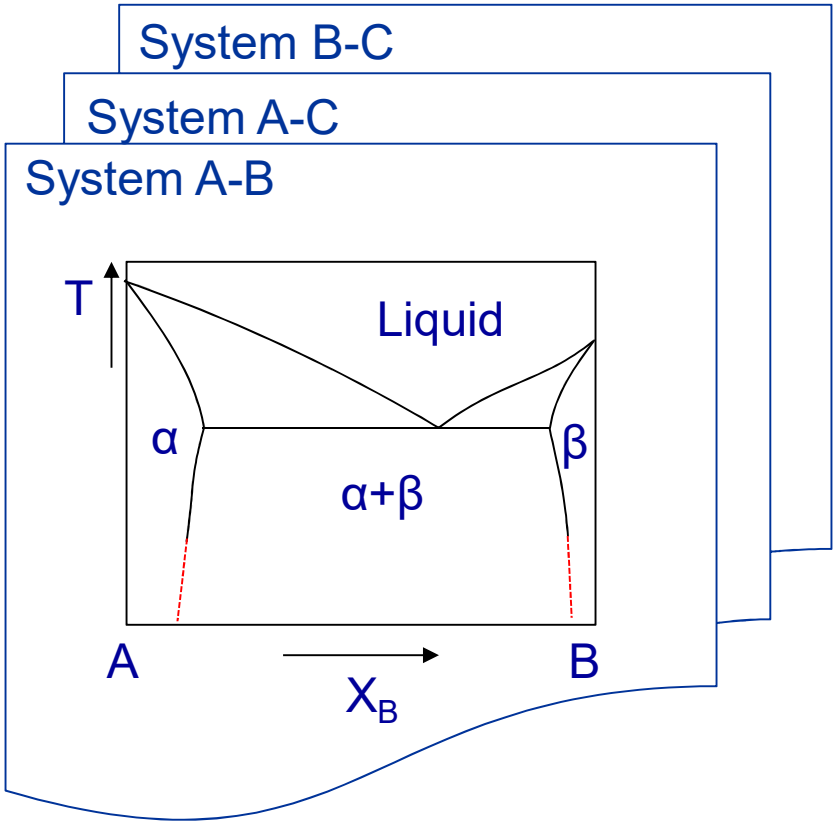
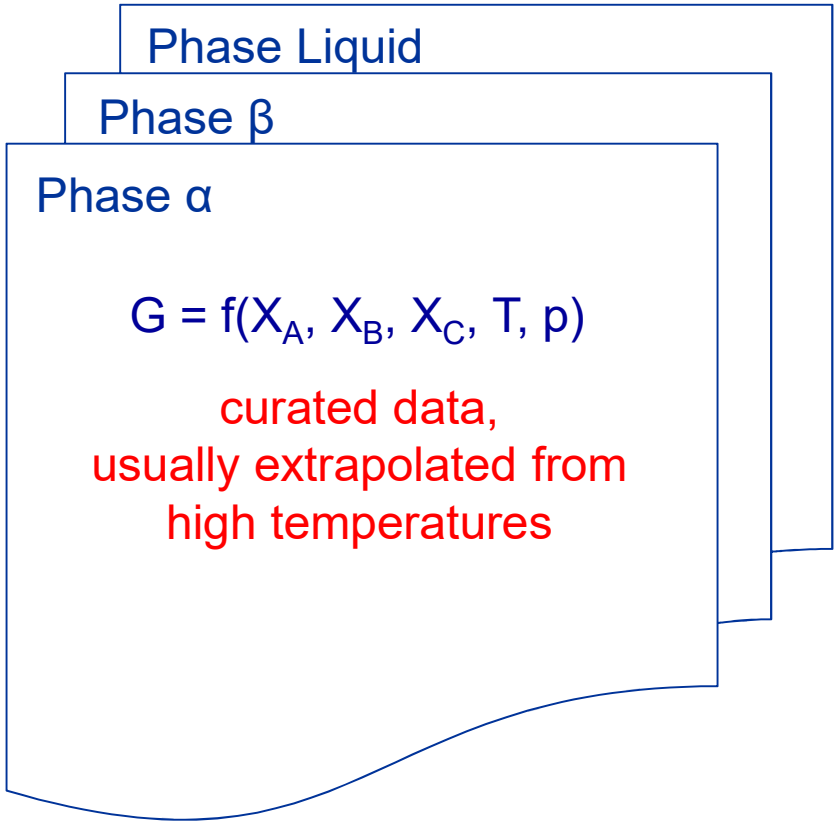


What is the CalPhaD (Calculation of Phase Diagrams) method?





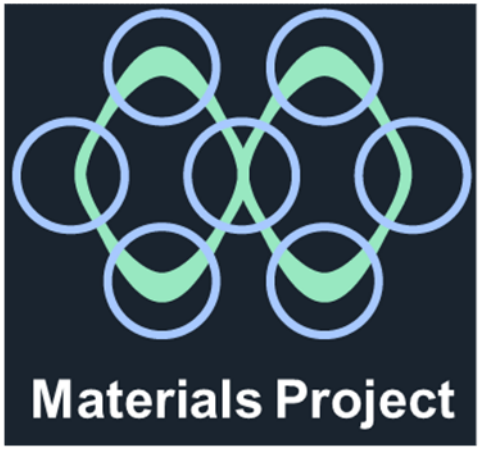
Phase diagram database ⟺ **Gibbs energy database**

Thermodynamic data

- Large updates in FactSage7.3:
  Copper and Lead databases are ~doubled in scope
- Largest databases available:
  FactPS: 6912 compounds
  SGTE Solutions: 319 solutions, 1166 compounds

Thermodynamic data

- aiMP2.3 (ab initio materialsproject.org):
  - 120‘539 compounds (was 67‘000 in aiMP1.0, end of 2017)
  - ΔH_f^{0K} from materialsproject.org
  - semi-empirical corrections for ΔH_f^{298K}
  - empirical models for C_p
  - machine learning for S^{298K}
  - Ideal FCC and BCC solution phases



Why aiMP?

Navigation in chemical compound space!

Content of FSlead database

H																He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	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

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Cs	Ba	La	Hf									Bi	Po	At	Rn		
Fr	Ra	Ac	Rf														
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Why aiMP?

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Content of FSlead database

Excellent to get around in Aachen, but useless if you want to go to Cologne…

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Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	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
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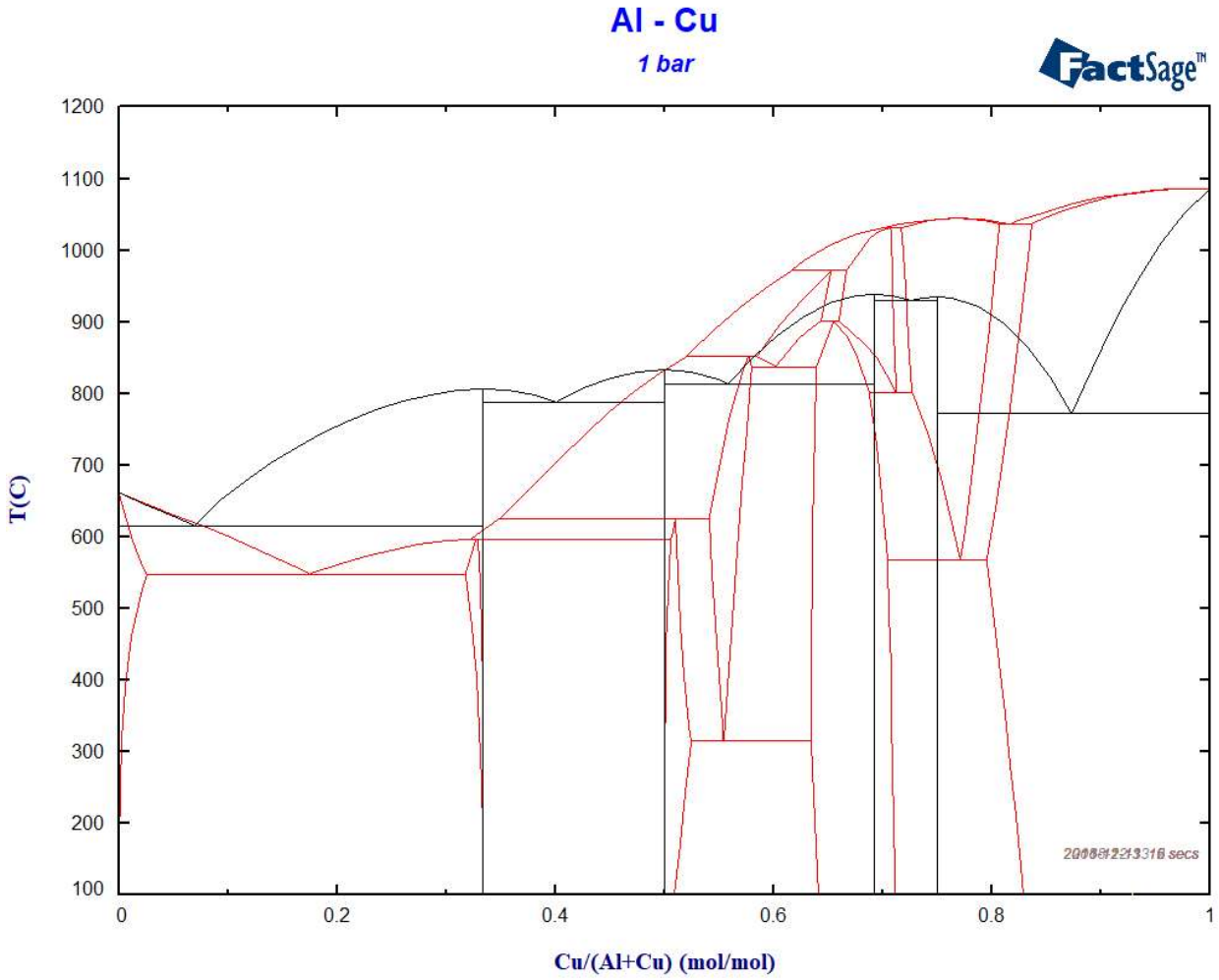
Rb	Sr	Y											Te	I	Xe		
Cs	Ba	La											Po	At	Rn		
Fr																	
		Ac											No	Lr			

Not made for details, but you now have a chance to get to Cologne!

Accuracy of aiMP (black) vs. SGTE (red)



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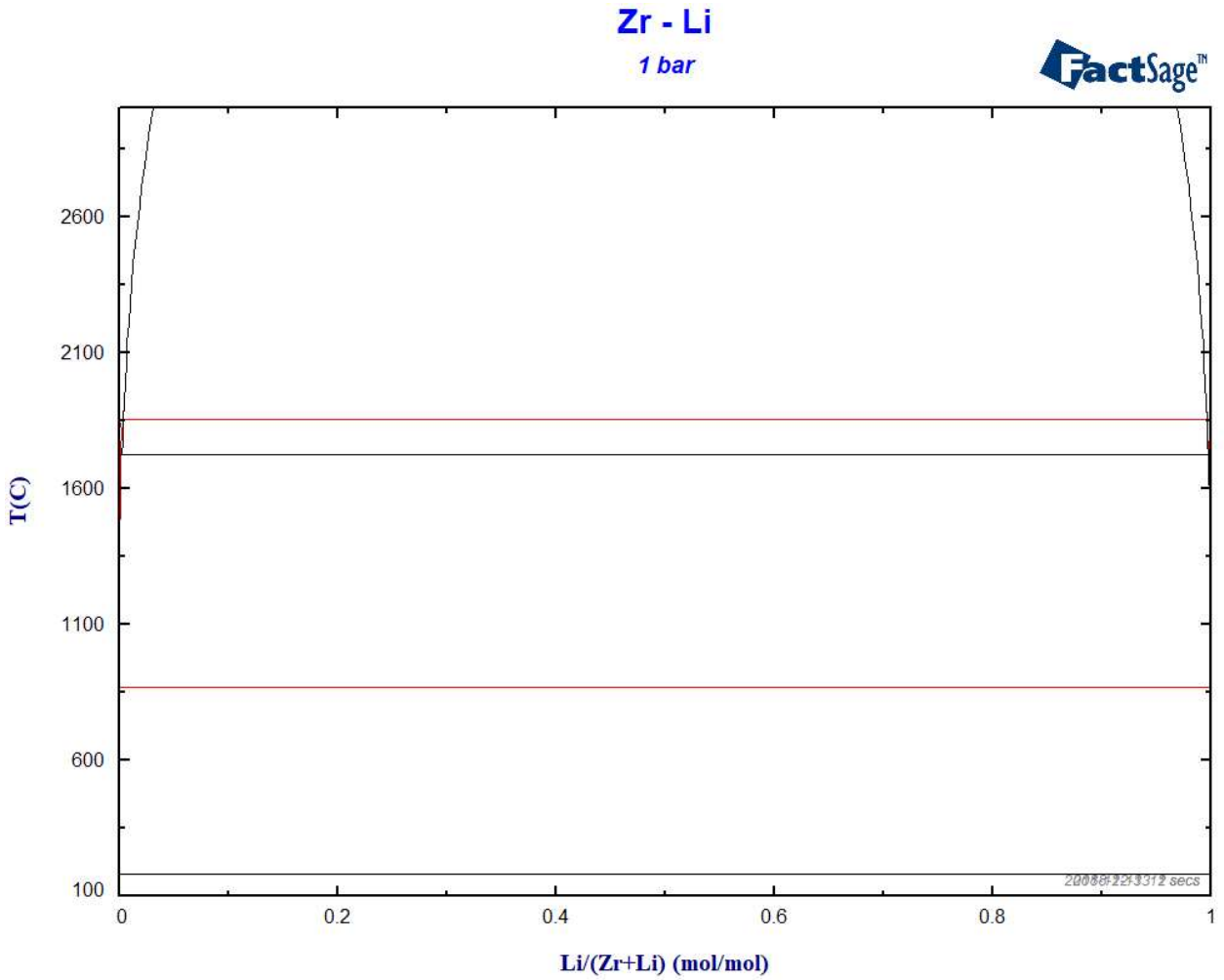

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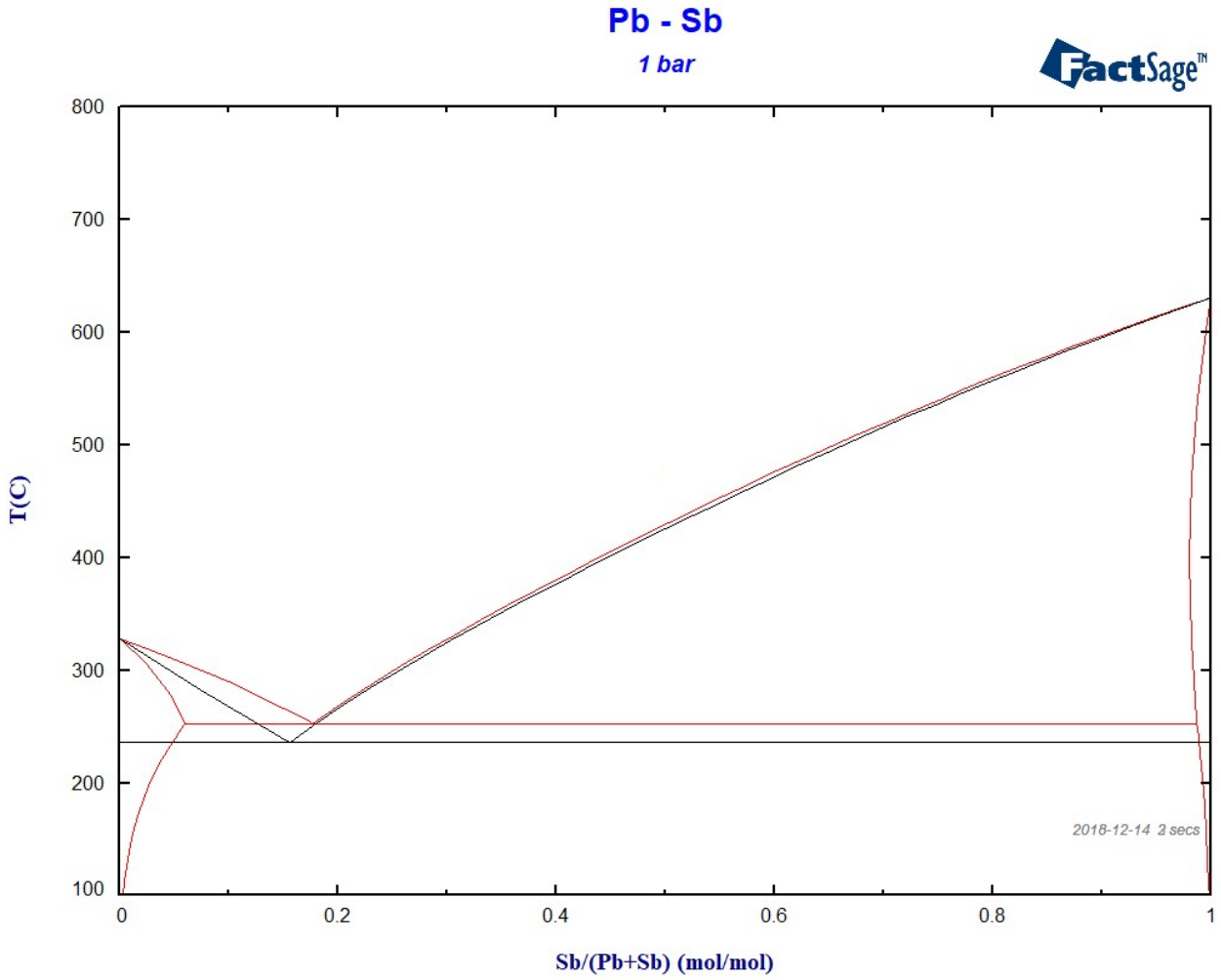

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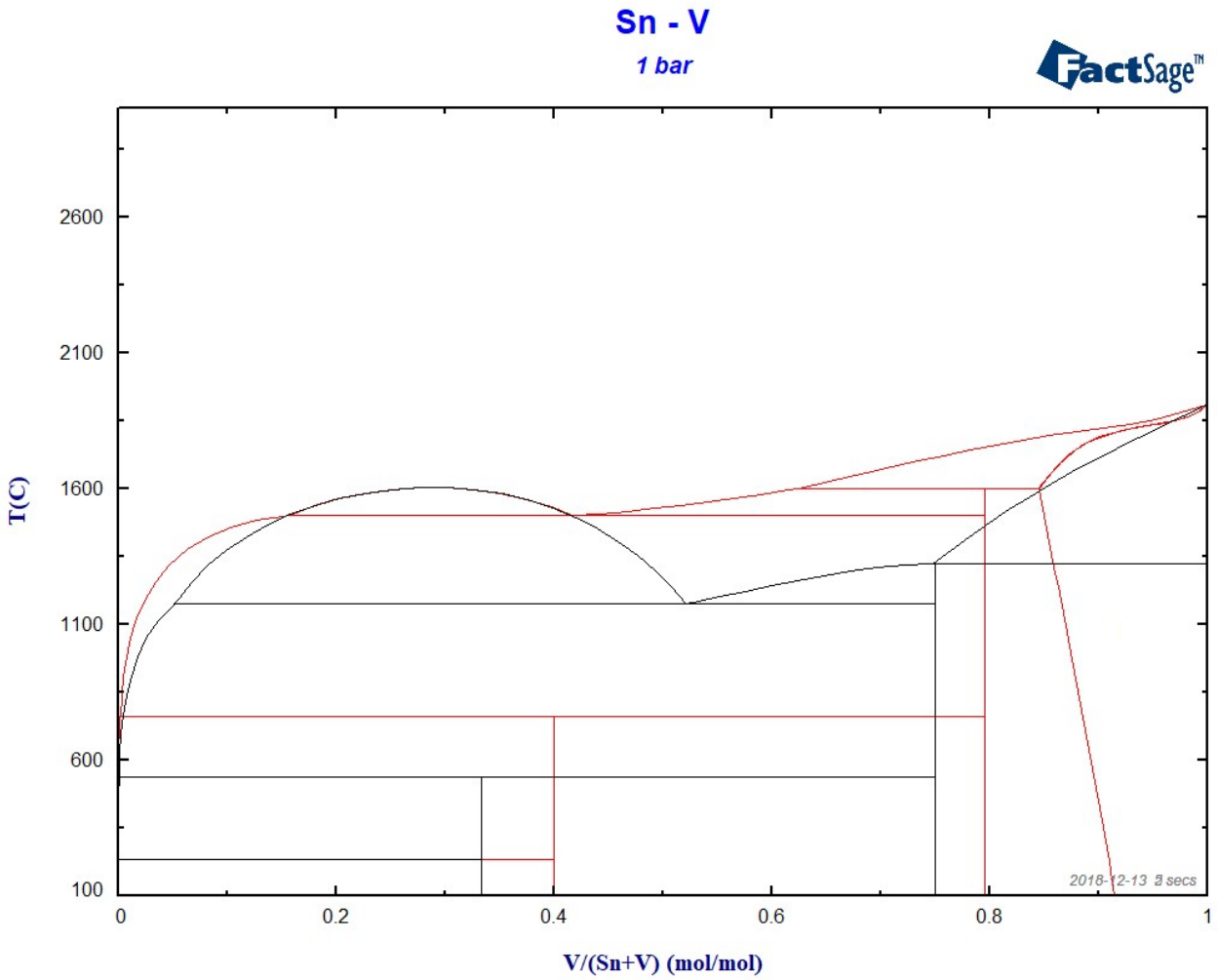

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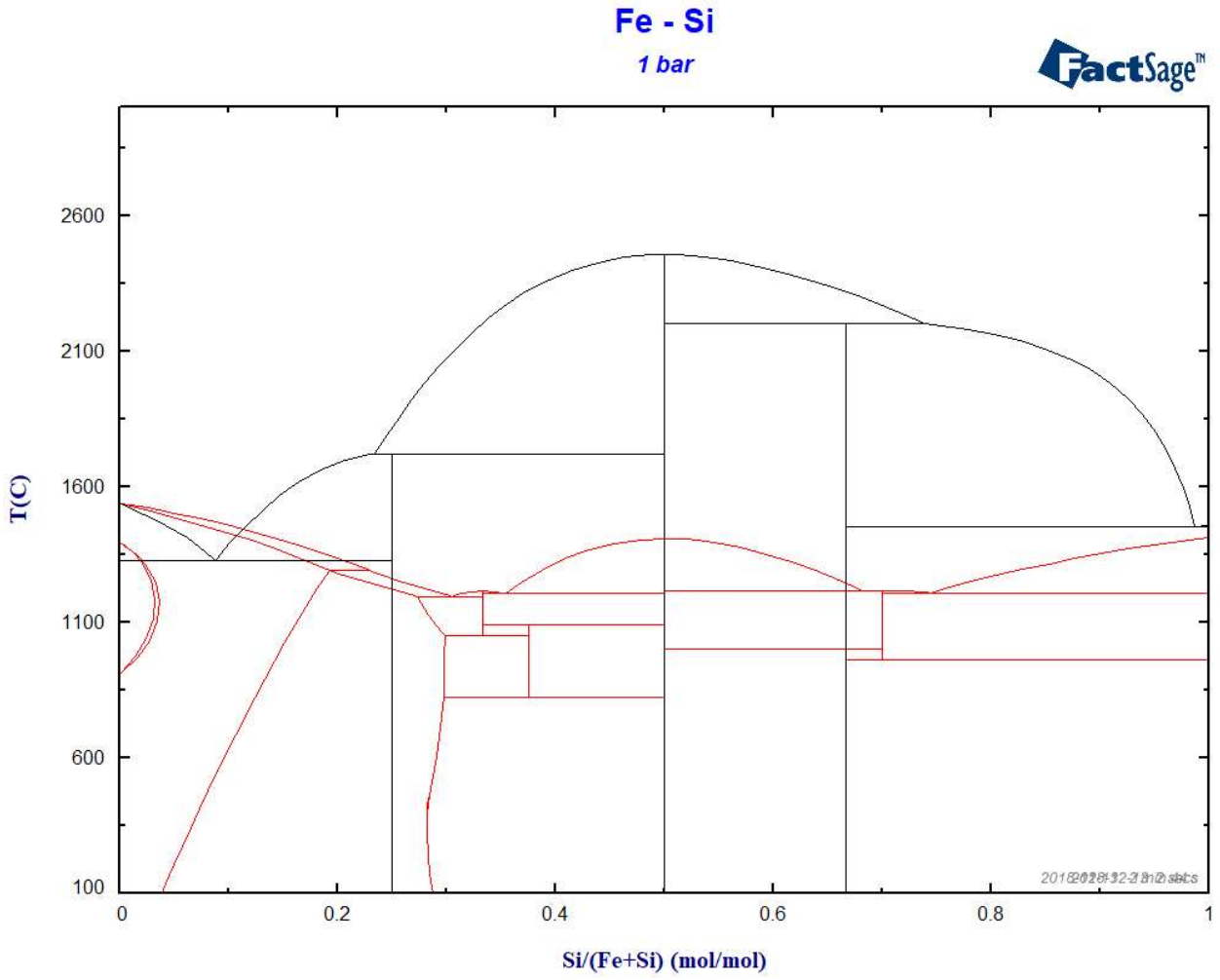

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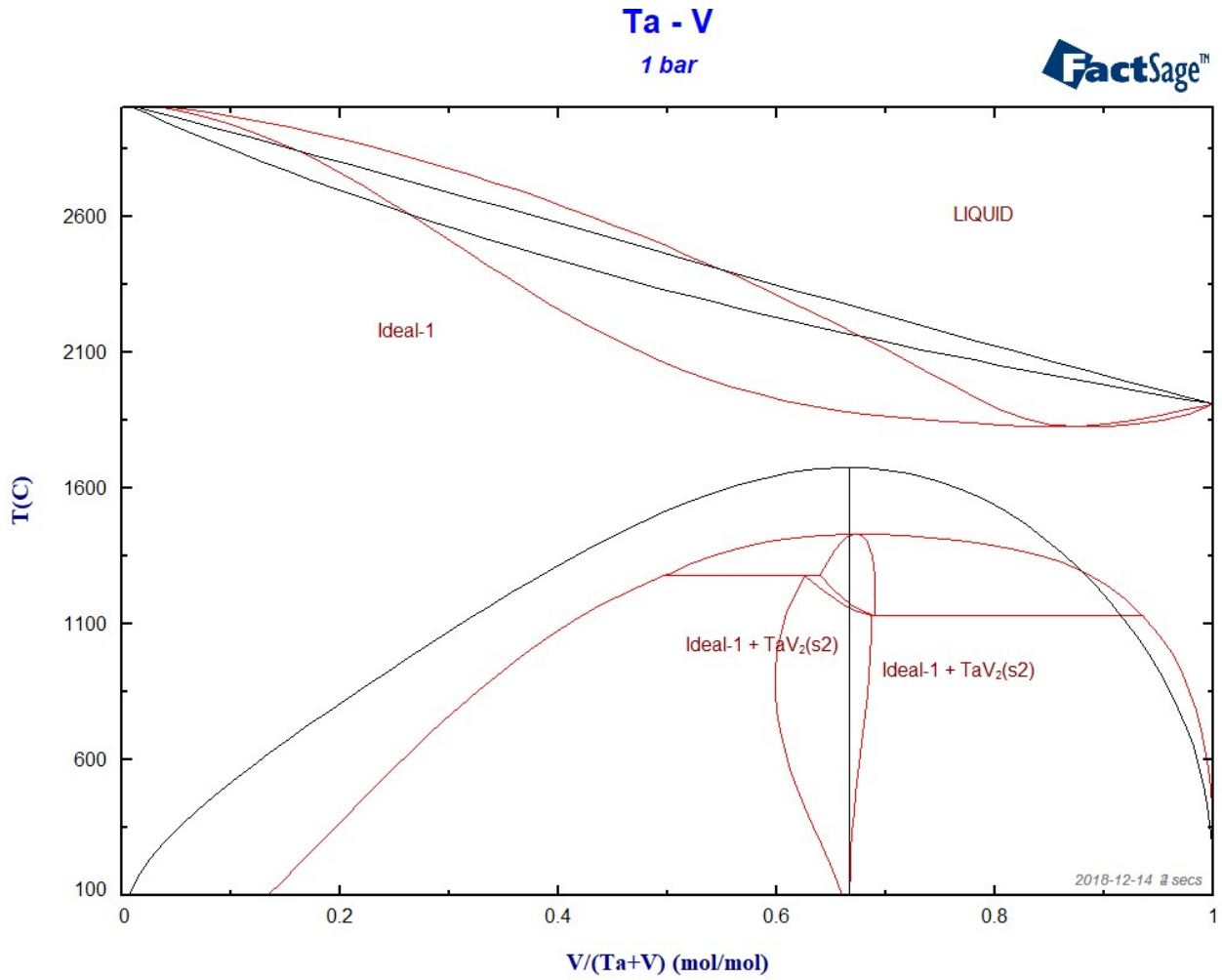
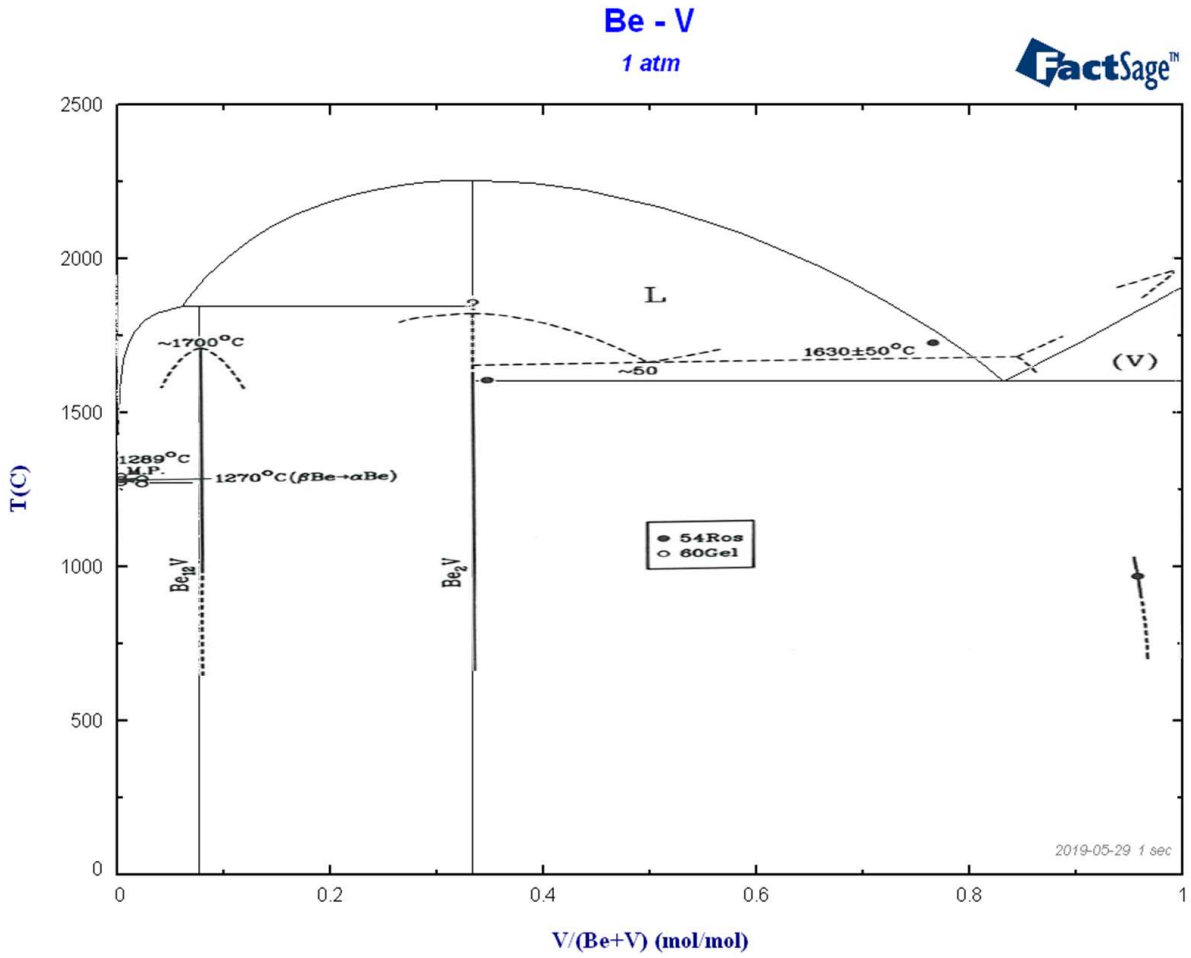
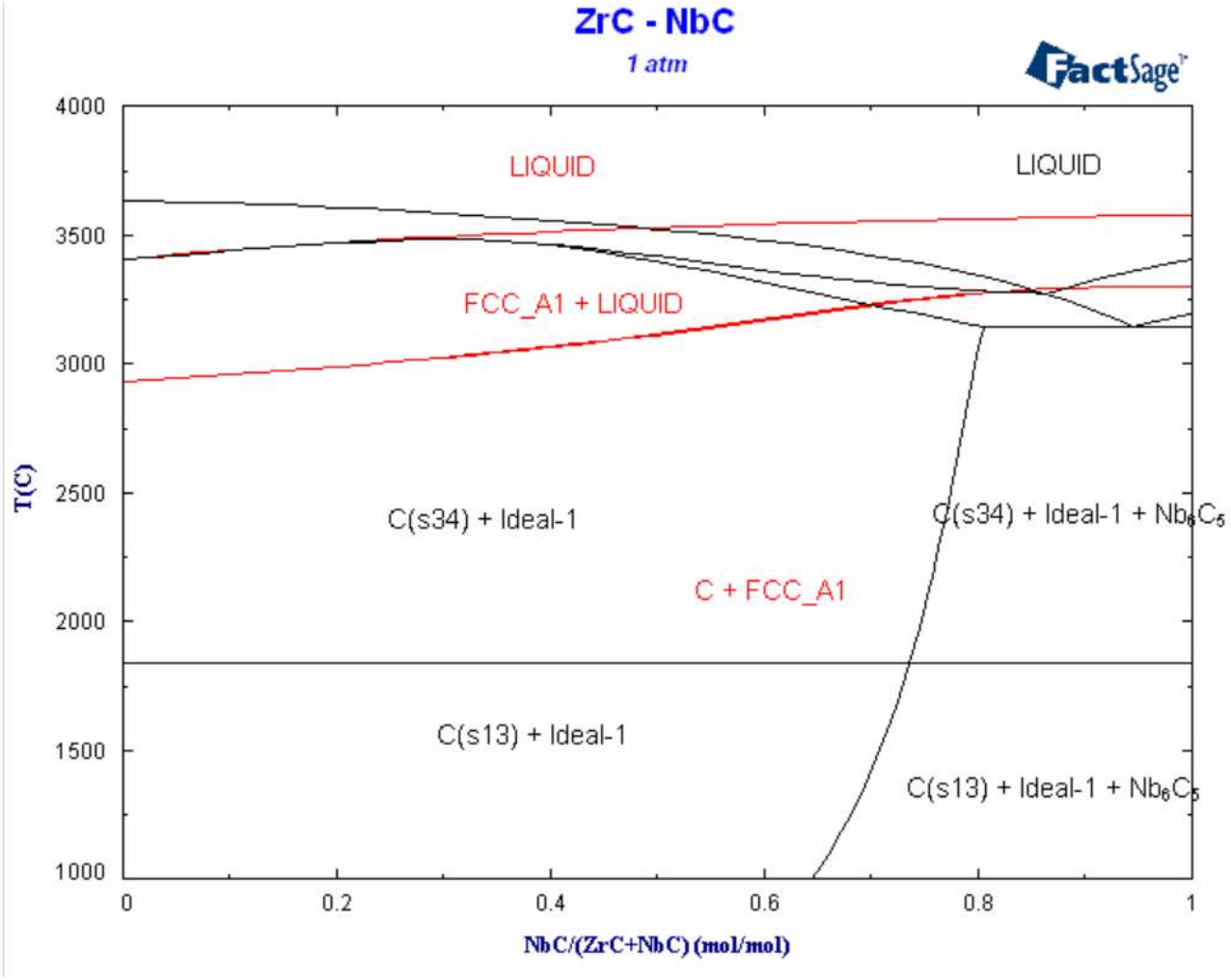


Accuracy of aiMP (black) vs. P*hase Diagrams of Binary Beryllium Alloys, ASM1987*



Accuracy of aiMP (black) vs. SpMCBN (red)

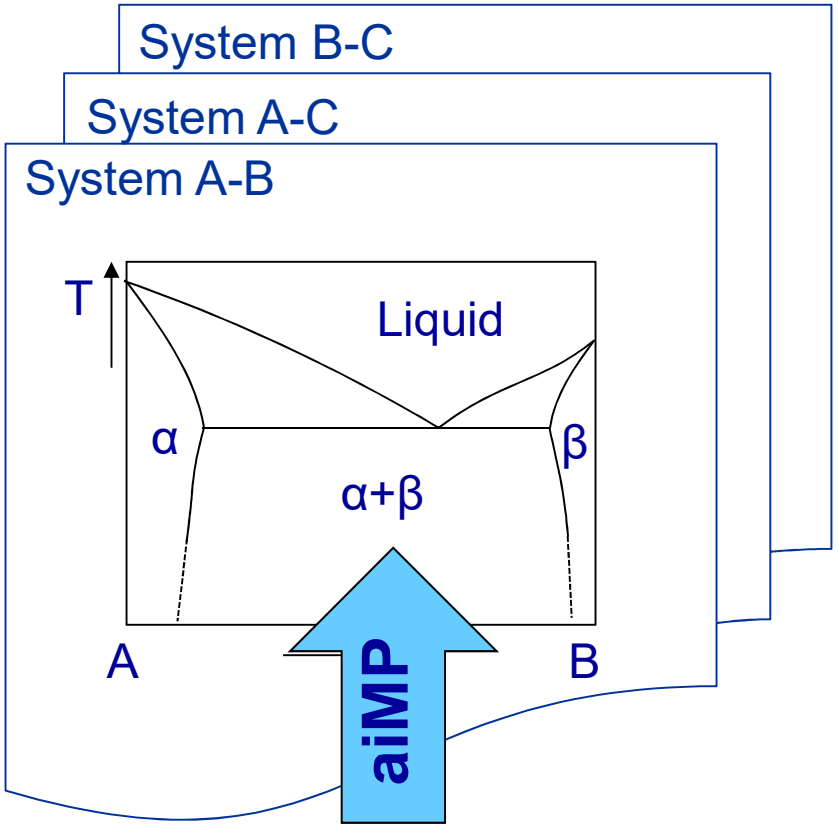


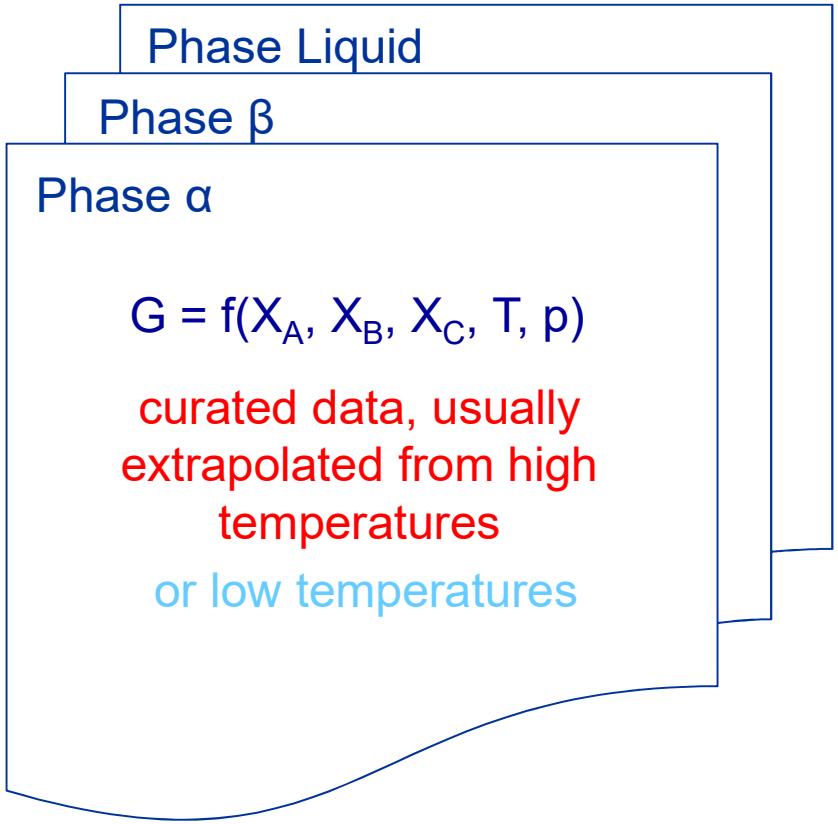
Another reason…

"Several years have now elapsed since I first became aware that I had accepted many false opinions for true, and that consequently what I afterward based on such principles was highly doubtful; and from that time I was convinced of the necessity of undertaking once in my life to rid myself of all the opinions I had adopted, and of commencing anew the work of building from the foundation, if I desired to establish a firm and abiding superstructure in the sciences."

Descartes, Meditations on First Philosophy (1641)
http://www.wright.edu/~charles.taylor/descartes/meditation1.html

What is the CalPhaD (Calculation of Phase Diagrams) method?





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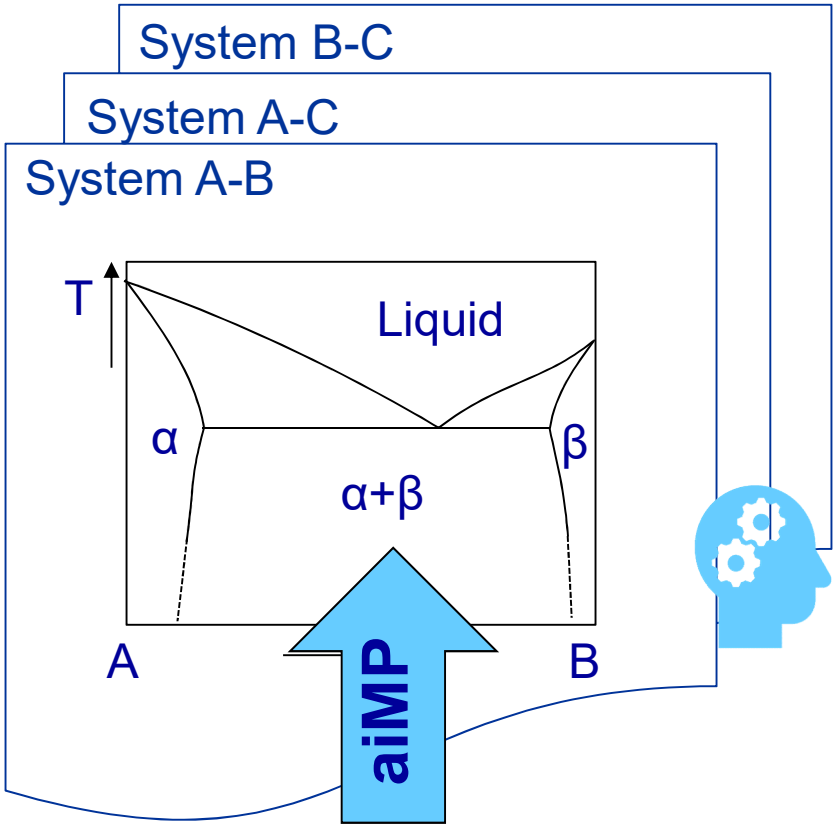

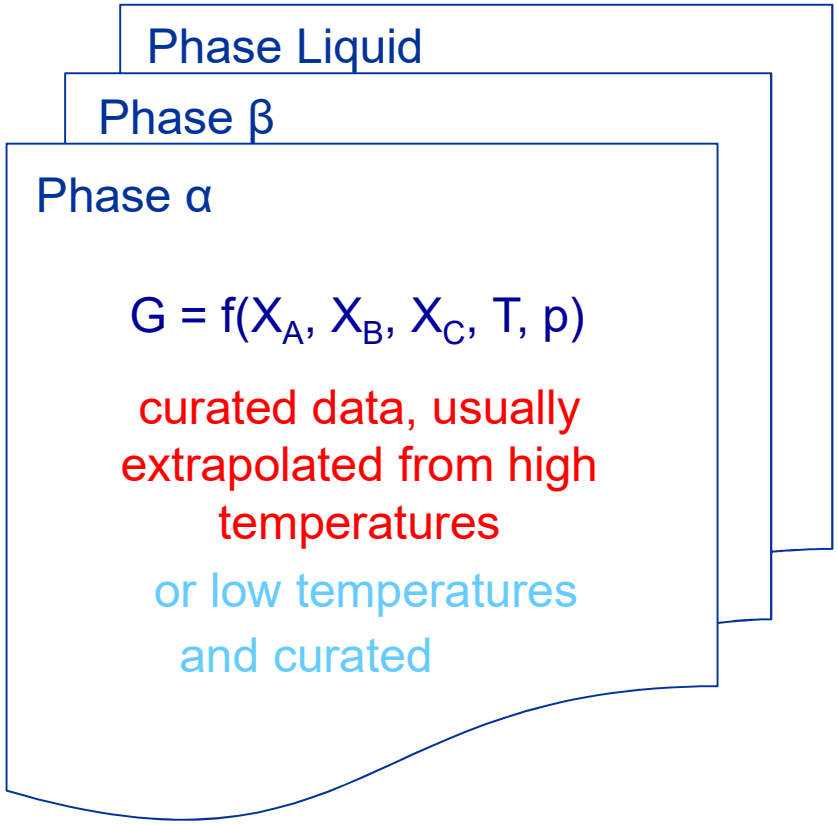

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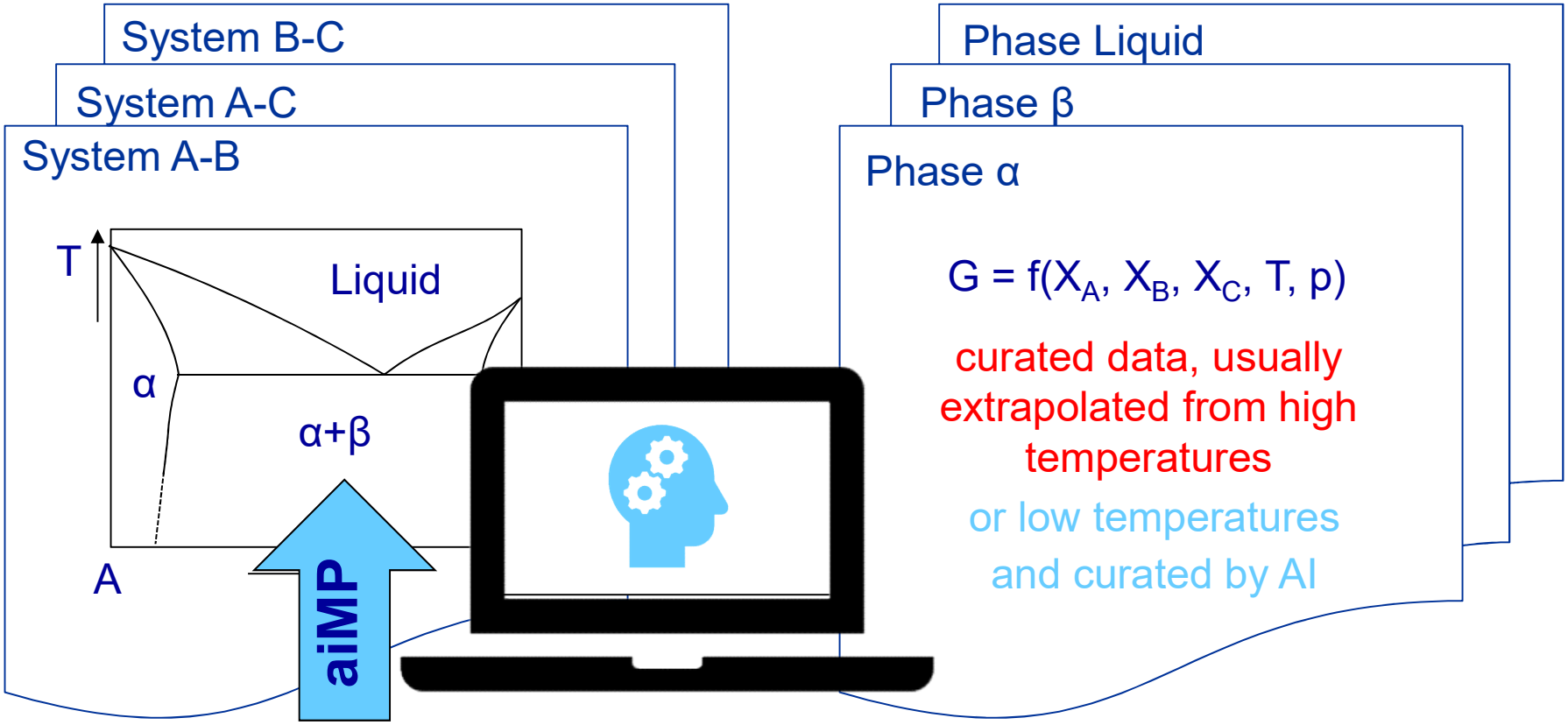

Roadmap

1. Metals
2. Carbides, Nitrides, Borides, Oxides
3. Suflides, salts…

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
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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

Thank you for your attention!

Part of the work has been supported by the German Federal Ministry of Education and Research (BMBF) in the framework of the project QuaResPro (From Quantum Mechanics to Ressource-efficient Product Desing, KMU-Innovativ 033RK058A).

Thank you

– and see you next year!

22nd GTT-Technologies Users‘ Meeting on June 24th to 26th 2020