Computational thermochemistry for sustainable metallurgy

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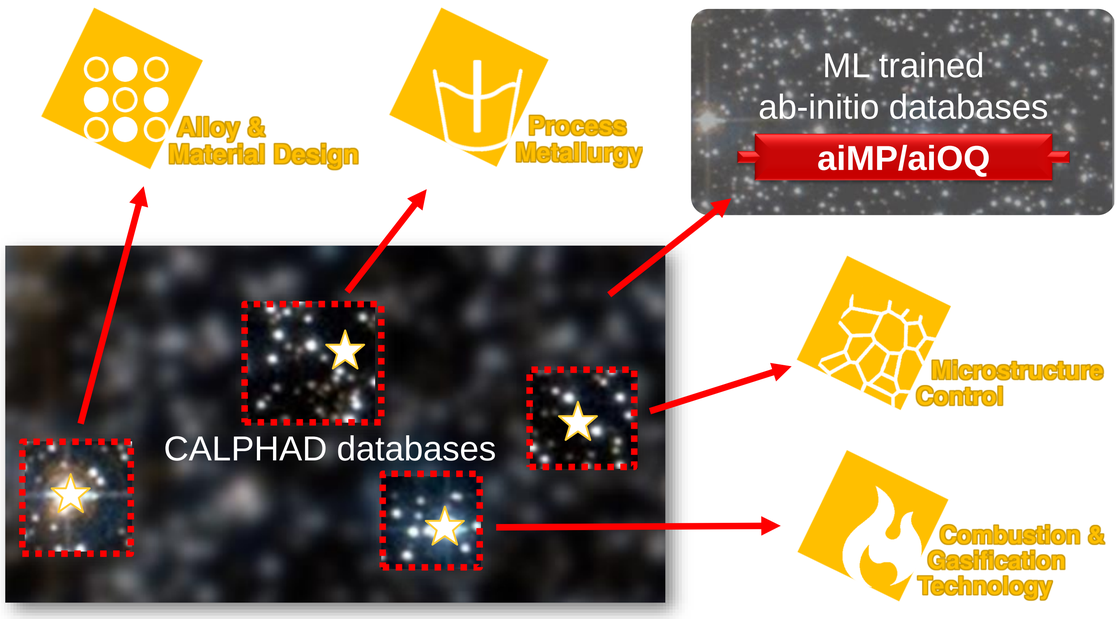
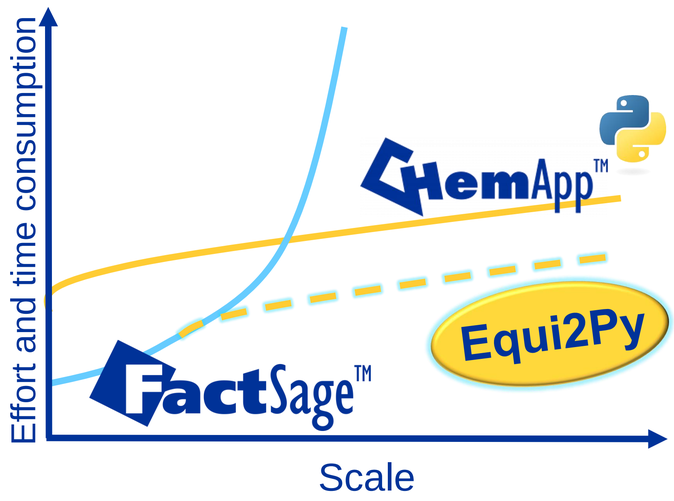
At GTT-Technologies, we help you to navigate in chemical space.

Thermochemical databases = Map of chemical space



Source: Image from NASA (Hubble telescope)

ChemApp is a programmer's library that permits the calculation of complex, multicomponent, multiphase chemical equilibria and their associated extensive property balances. With the Equi2Py module in FactSage 8.3, you can effortlessly set up thermochemical systems and smoothly transition to the ChemApp for Python scripts, reducing the complexity of setting up thermochemical experiments for anyone, even those with no programming experience.

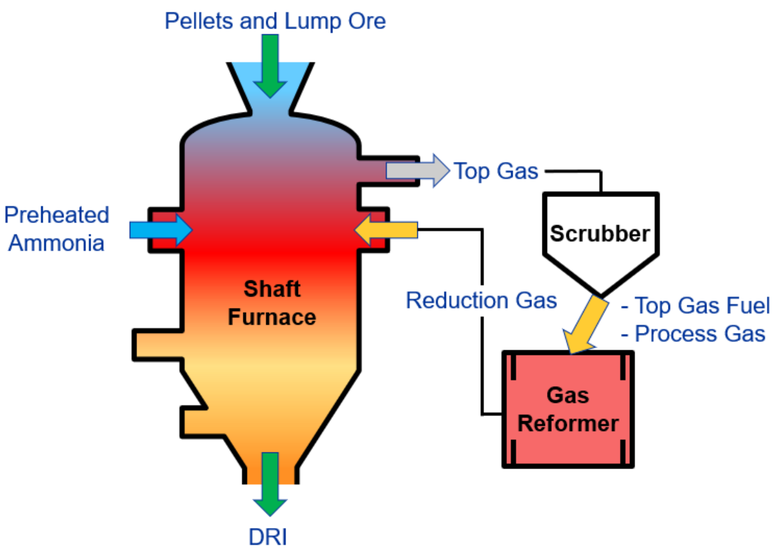


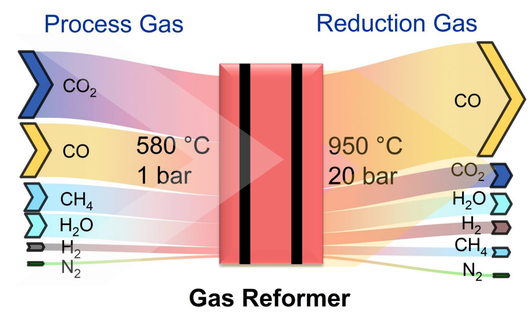
	FactSage™	ChemApp™
Programming knowledge needed?	No	Yes
Time needed to learn basic usage	1 week	1 month
Time needed to set up a calculation	2 min	10 min
Time needed to repeat an analysis	1 min	1 sec
Number of equilibrium calculations	< 10^3	< 10^7
Access to databases	FactSage databases	Excerpts via FactSage (.cst)

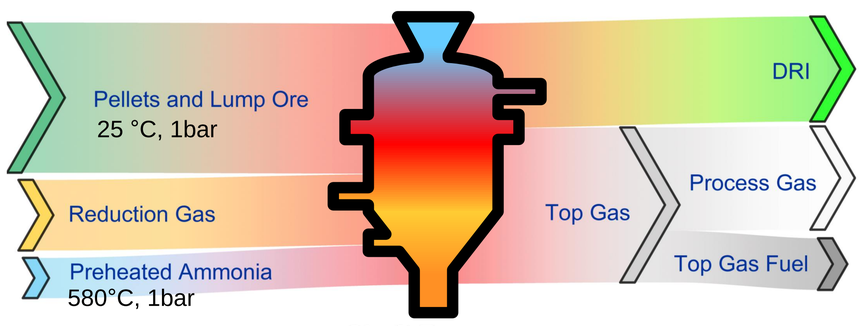
Equi2Py

Metallurgical process modelling including full solution thermodynamics

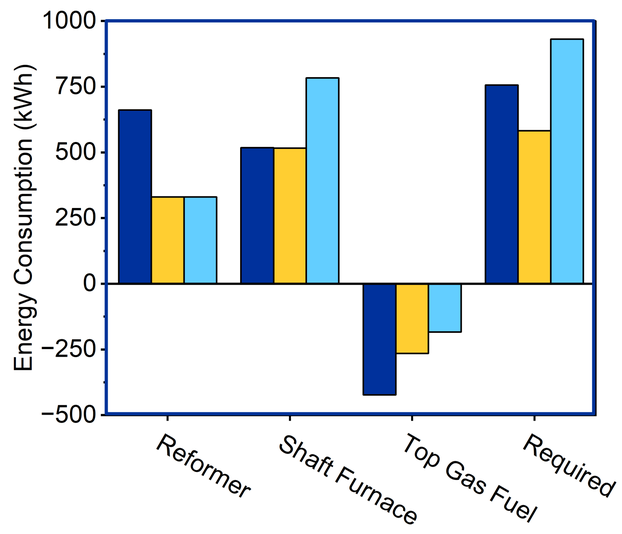
Stream calculations in ChemApp for Python







Recovered Heat and Energy Consumption at Midrex Furnace Unit
1 tonne of Hematite reduced to 0.96 metallization degree

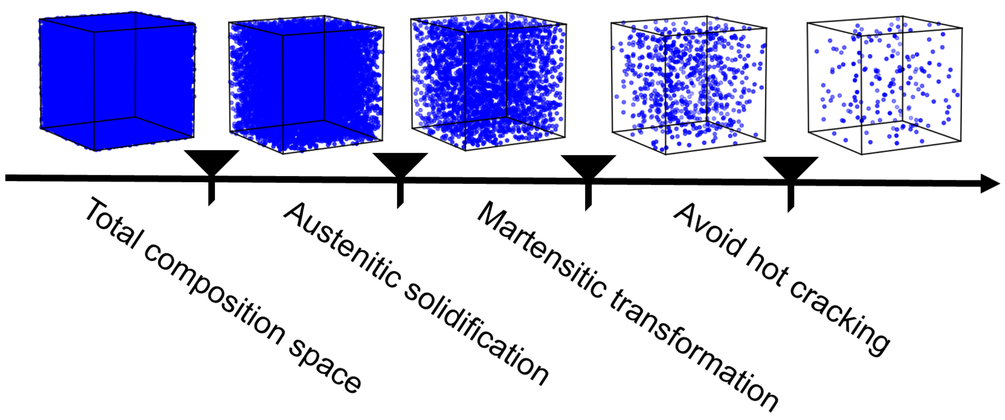


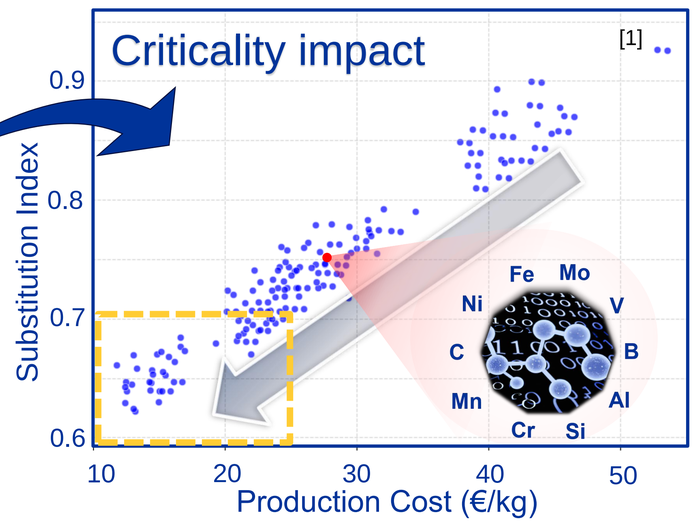
Integration of direct reduction furnaces into the plant flowsheet requires considering certain data for estimation or simulation. Stream calculation in ChemApp for Python allows setting initial conditions in addition to general boundary conditions. This enables quick calculation of heat balances and modeling scenarios like mixing hot air with a cold aqueous solution.

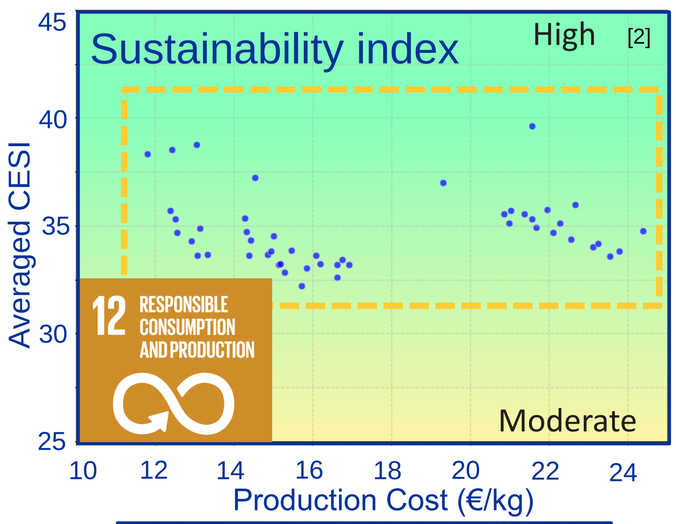
Process informed alloy design

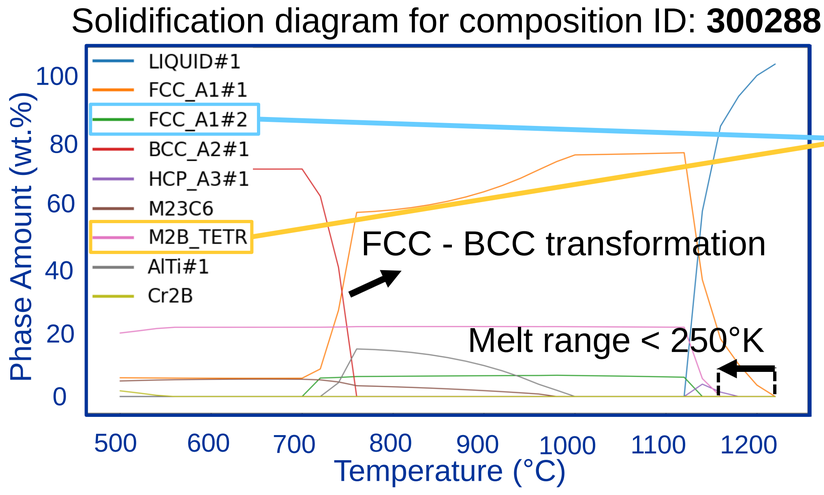
High throughput screening with ChemApp

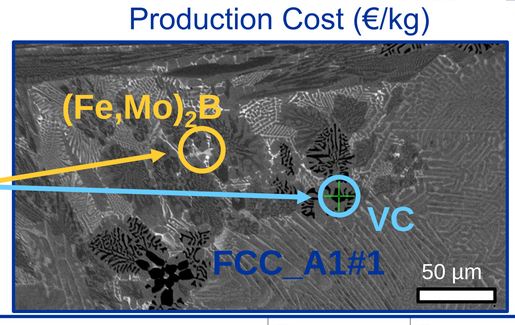
765,000 compositions were assessed based on materials and process criteria, resulting in the identification of **168** promising hardfacing alloy compositions after high-throughput screening.











Property	Predicted	Calculated
Liquidus T (°C)	1209	1195
Solidus T (°C)	1127	1162
T_{ms} (°C)	205	207 - 228
Production cost (€/kg)	22	-
Density (g/cm³)	7.8	-

[1] European Commission, Study on the Critical Raw Materials for the EU 2023 – Final Report. Results derived from Substitution indexes (SI) used for calculating the supply risk and economic importance.
[2] Smith, L et al. (2021). A Chemical Element Sustainability Index. Resources, Conservation and Recycling, 166, 105317. CESI framework consist of the Human Development Index, the Global Warming, the Recycling Rate and the National Economic Importance.

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