Thermodynamic modelling software and data at GTT-Technologies

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GTT-Technologies, Herzogenrath, Germany

Thermodynamic Software

Thermodynamic Databases

Consulting Services

GTT in a nutshell

Thermodynamic Software

- FactSage (with CRCT)
- ChemApp
- ChemSheet
- SimuSage
- Process models

Thermodynamic Databases

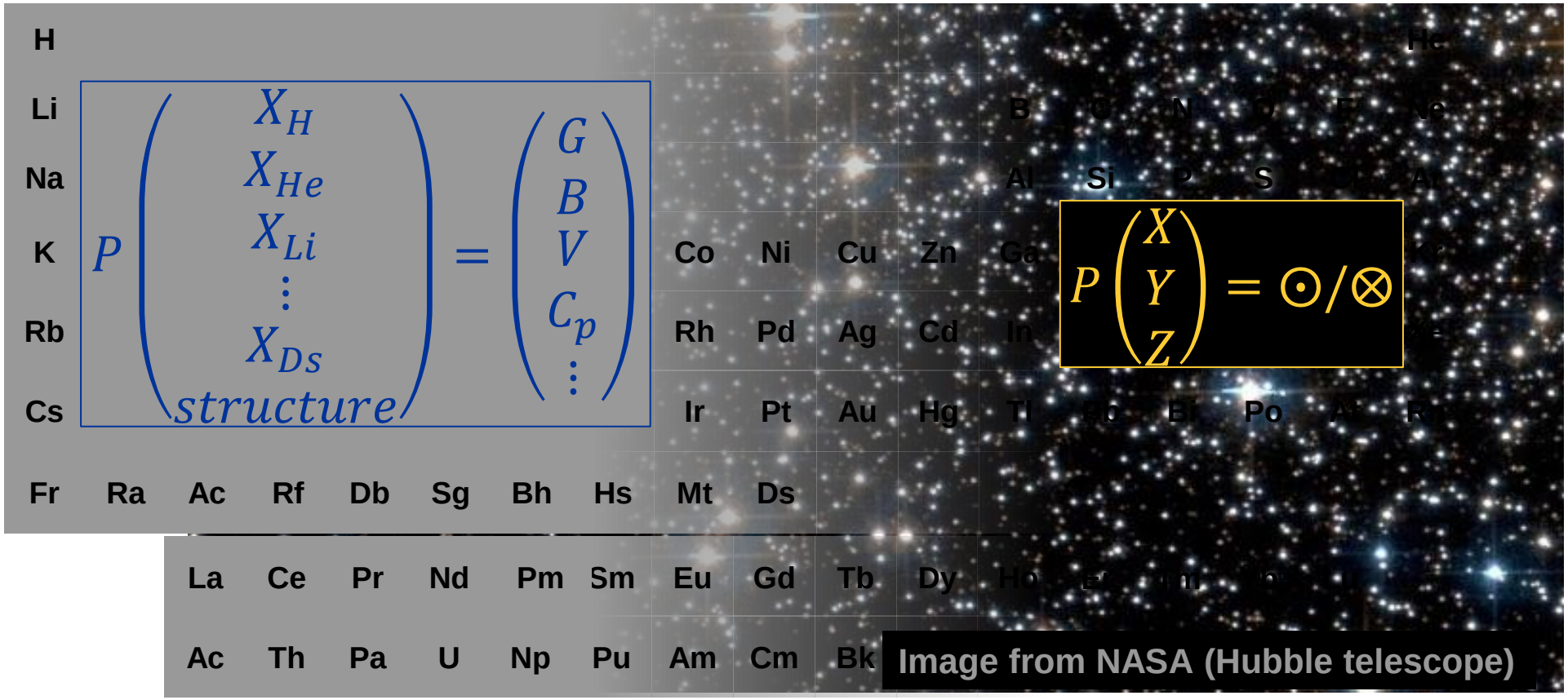
- FACT (by CRCT)
- GTOx
- SGTE
- aiMP, aiOQ

Consulting Services

- Partner in public project
- Application calculations
- Database development
- Teaching

Thermodynamics as navigation tool in Materials Science

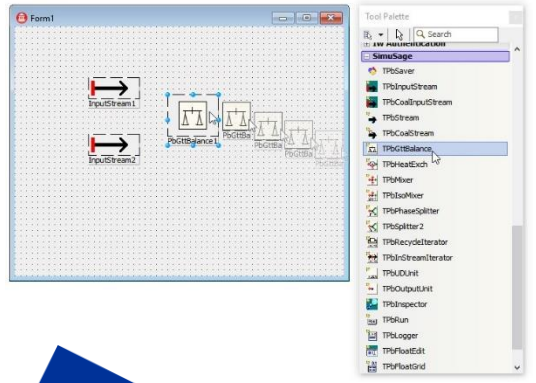
How do you navigate?



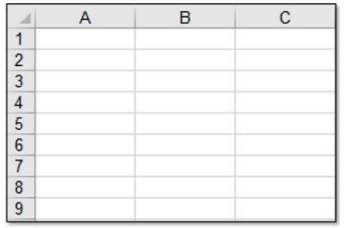
GTT-Technologies
in cooperation with CRCT, Polytechnique Montreal, Canada

FactSage™

ChemApp™



SimuSage™



ChemSheet™

Thermodynamic Databases

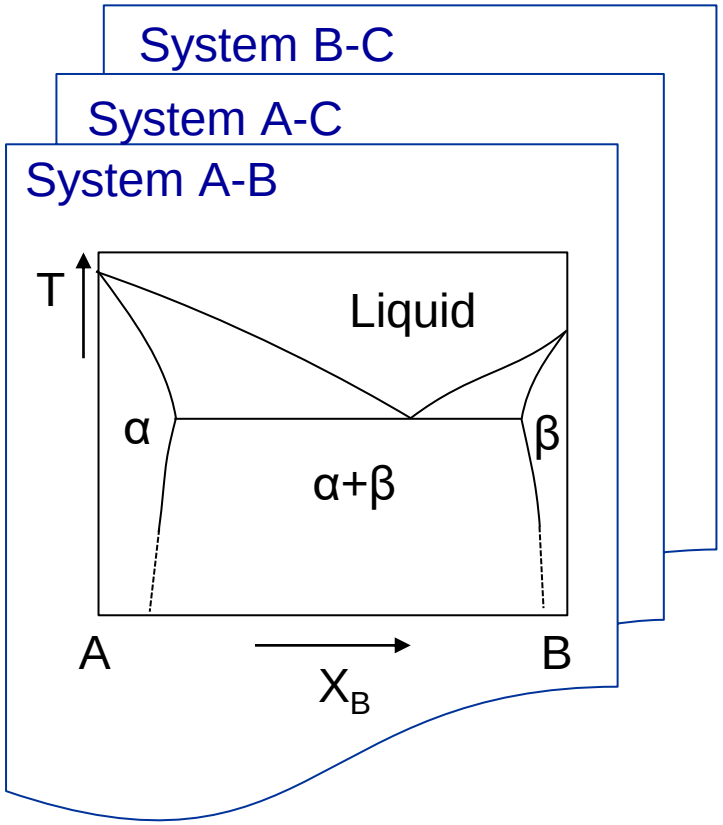
GTT-Technologies
in cooperation with CRCT, Polytechnique Montreal, Canada

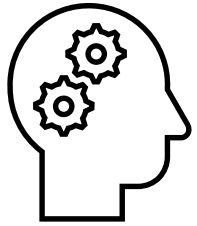
- Slags and oxides
- Steels
- Light metals (Al, Mg, [Ti, Li])
- Copper
- Lead
- Sulfides and mattes
- Salts
- Refractories (Carbides, Nitrides, Silicides)
- Noble metals
- Solders

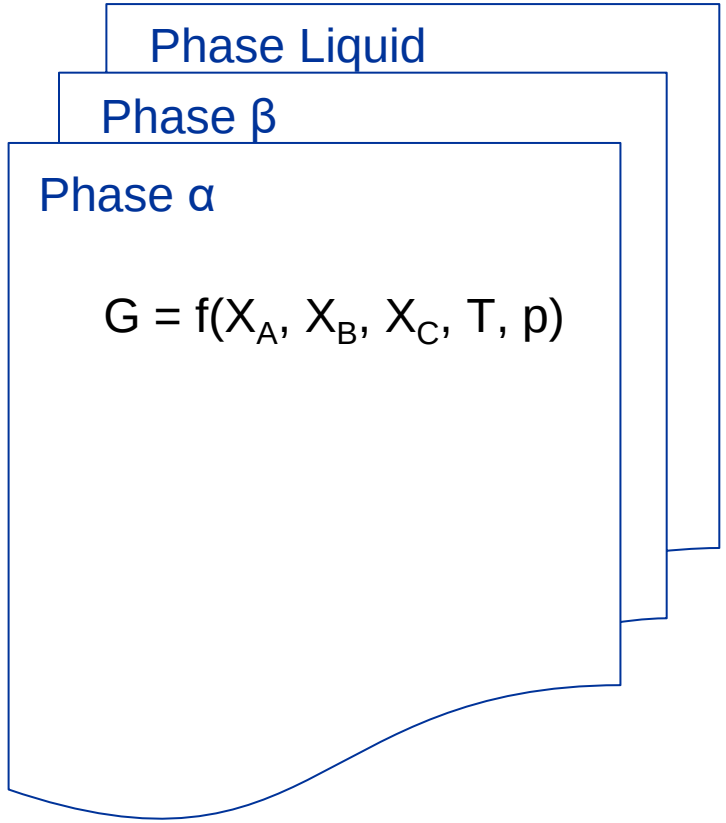
- Nuclear materials
- Pulp and paper
- Fertilizer
- Materials Project at high T (ML-based)
- (and user requests)

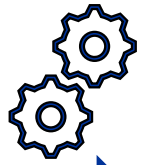
More than 7000 phase diagrams freely available under factsage.com!

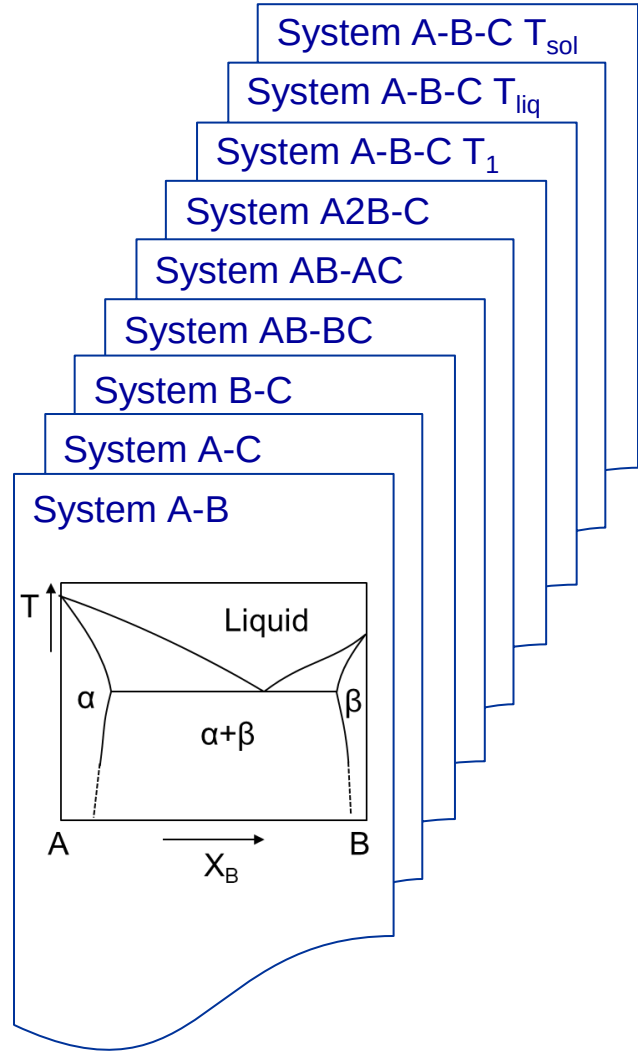
CALPHAD = CALculation of PHAse Diagrams











Phase diagram, experiments

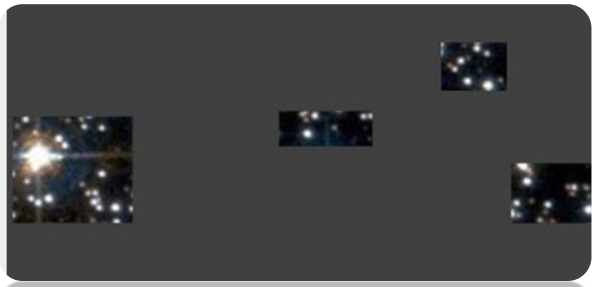
Gibbs energy database

Aktuelle Aktivitäten

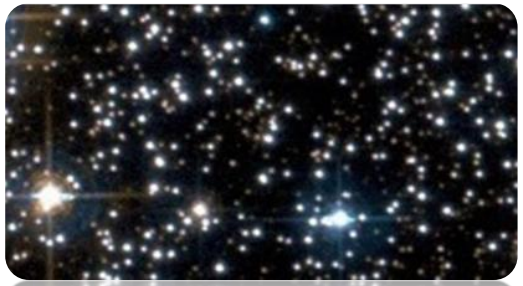
- BMWK-Projekt Verena (2020-): Datenbankentwicklung: Reststoffvergasung, Freisetzung Spurenelemente
- BMWK-Projekt VeRa (2021-): Datenbankentwicklung: Biomasseverbrennung
- BMWK-Projekt PCM-II (2021-): Datenbankentwicklung: Salze und Salz-Hydrate als Wärmespeicher
- ZIM-Projekt Software-basiertes Materialdesign von Hartstoffschichten (2022-): High-throughput-Rechnungen, Cloud computing, Legierungsentwicklung
- Euratom-Projekt Scorpion (2022-): Identifizierung von Beschichtungslösungen für Accident-tolerant nuclear fuels
- Beantragt:
  - BMWK-Projekt FesTES: Datenbankentwicklung Salze als feste Wärmespeicher, u.a. Korrosion
  - SFB-1394 „Structural and Chemical Atomic Complexity: From Defect Phase Diagrams to Material Properties”: Transferprojekt (mit Tilmann Hickel, BAM und Ulrich Kerzel, RWTH)
  - Materialdigital: Glasagent (mit Schott, BAM u.a.)
- Wissenschaftliche Kooperationen, Kontakte:
  - RWTH Aachen (alle ProfesorInnen der Fachguppe Materialwissenschaft und Werkstofftechnik)
  - MPIE (Neugebauer, Raabe)
  - RU Bochum (ICAMS)
  - NOMAD CoE/FairMat, DGM (FA Circular Materials, FA Thermodynamik und Kinetik, FA Modelling, Simulation and Data)

Aktuelle Aktivitäten: KI4MAT-Bezugspunkte

- Zwei große Themen:
  1. Karte des chemischen Zusammensetzungsraumes vollständig erforschen.



ML → Materialdaten



  2. Vom „Kartenanbieter“ zum „Navigationssystem-Anbieter“

ML → Materialdaten, Beschleunigung

GTOx content: 17 metals + 7 anion groups

MeOx – Me – MeS – $MeSO_4$ – $MeCO_3$ – MeF – MeCl – $MeCrO_4$

MeOx = Al_2O_3-CaF_2-CaO-CrO-Cr_2O_3-Cu_2O-CuO-FeO-Fe_2O_3-K_2O-Na_2O-Li_2O-MgO-MnO-Mn_2O_3-NiO-P_2O_5-SiO_2-SrO-TiO_2-Ti_2O_3-V_2O_3-V_2O_5-ZnO

Me = Al, Ca, Cu, Cr, Fe, K, Li, Mg, Mn, Na, Ni, Si, Sr, Ti, V, Zn + C, P, S, O

MeS = Al_2S_3, CaS, CuS, CrS, FeS, K_2S, MgS, MnS, Na_2S, NiS, ZnS

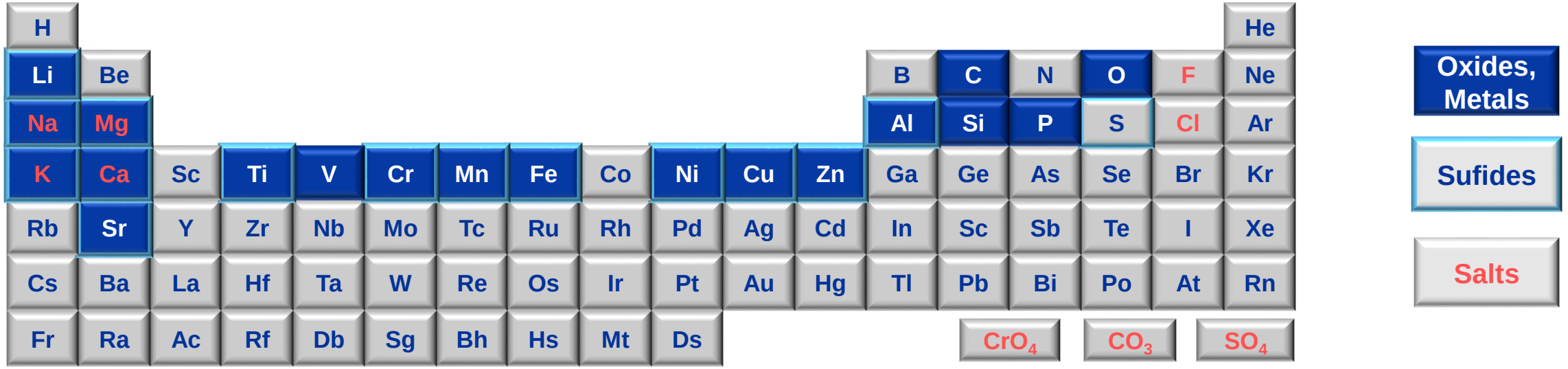
$MeSO_4$ = $CaSO_4$, $MgSO_4$, K_2SO_4, Na_2SO_4, $NiSO_4$

$MeCO_3$ = $CaCO_3$, K_2CO_3, $MgCO_3$, Na_2CO_3

MeF = AlF_3, CaF_2, MgF_2

MeCl = $CaCl_2$, KCl, $MgCl_2$, NaCl

$MeCrO_4$ = $CaCrO_4$, K_2CrO_4, Na_2CrO_4, $SrCrO_4$



Challenge: Recovery of minority elements

Figure 3 shows the recovery rates of only 20 elements using recycling rou
all of the 46 elements in the Fairphone 2, these 20 have been selecte
depletion rate and social and/or environmental impact in their mining c
recycling of these metals more urgent.

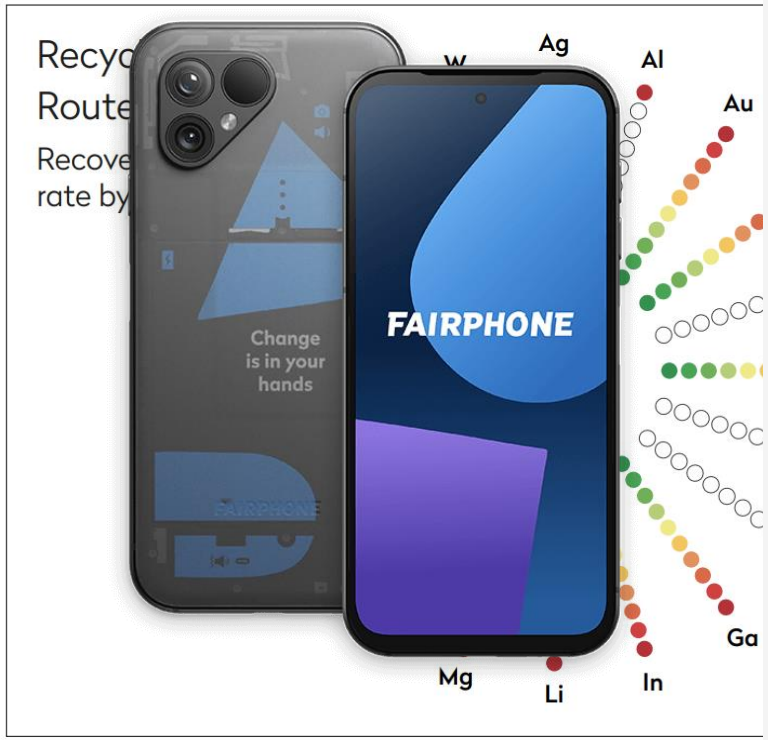
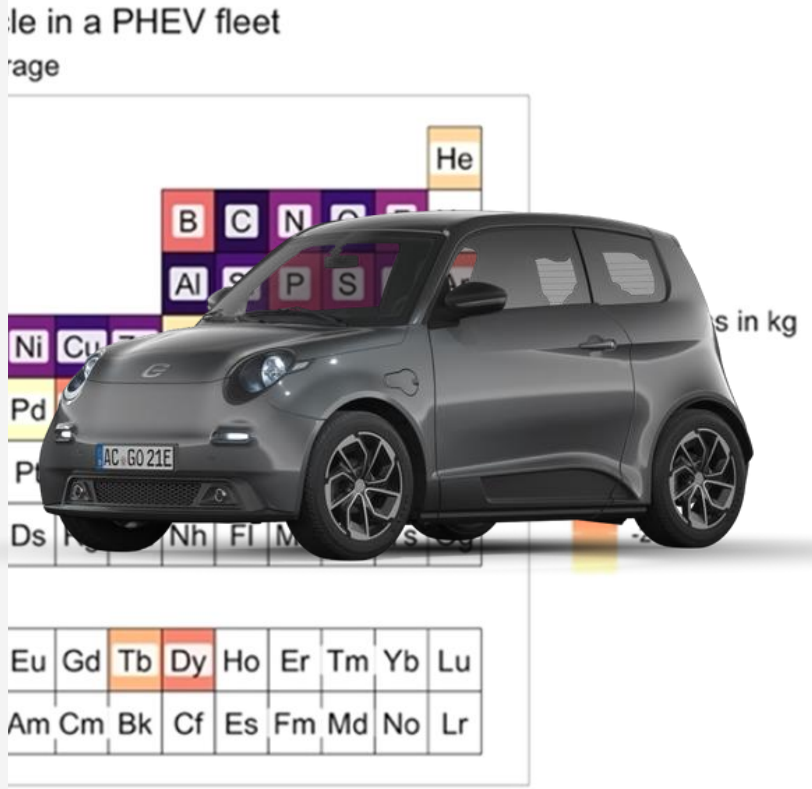


Figure 3:
Materials Flower for Recycling Route 1 (Total Smelting & Metal refining); develope

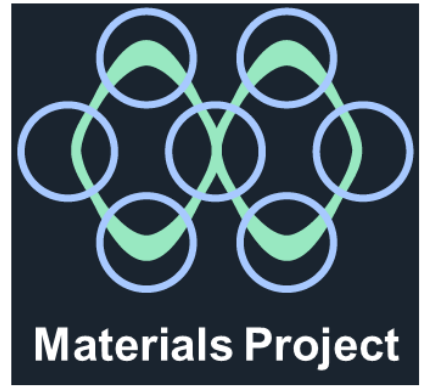
www.fairphone.com/en/2017/02/27/recyc



2000 compounds, 76 elements > 1 mg
org/10.1021/acs.est.1c00970

Maps of chemical space: Ab initio + ML → CalPhaD

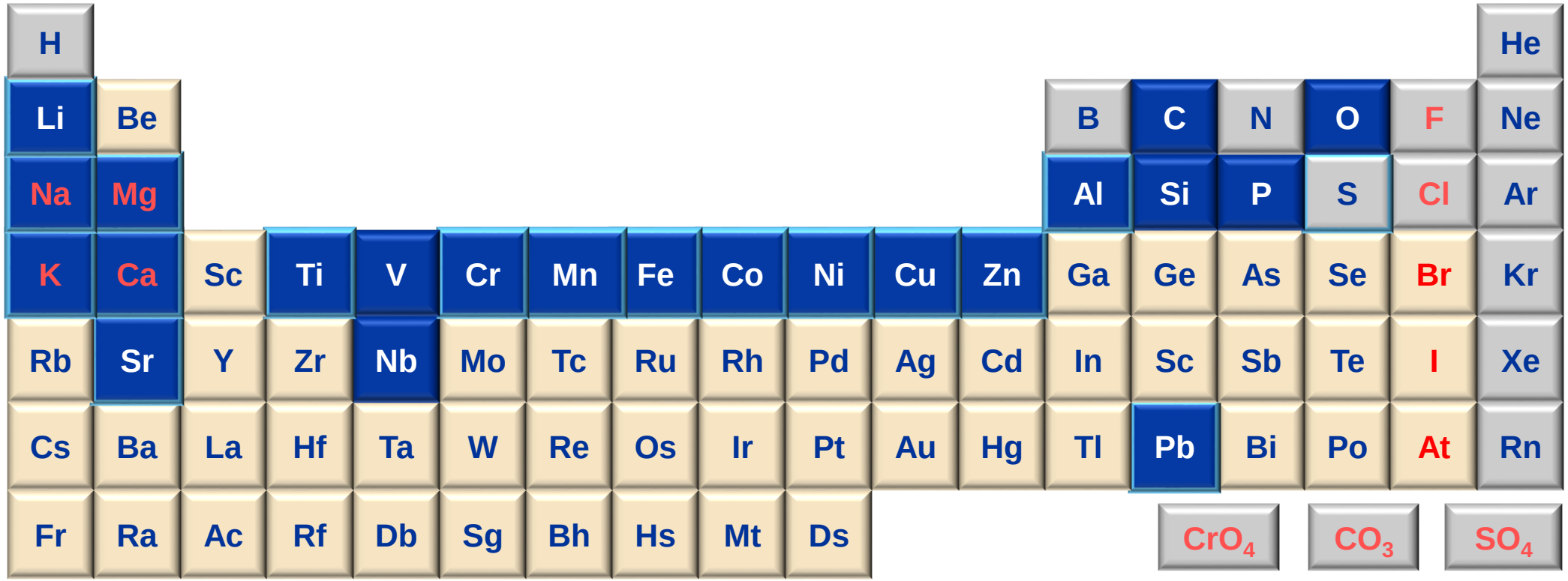
- aiMP (ab initio materialsproject.org): 128‘000 compounds
- aiOQ (ab initio OQMD.org): 718‘000 compounds
  - ΔH_f^{0K} from materialsproject.org / oqmd.org [1,2]
  - consistency modifications for ΔH_f^{298K}
  - machine learning for C_p
  - machine learning for S^{298K}
  - DFT calculated enthalpy of mixing in FCC, BCC, HCP for ~1400 binary systems
- First commercial CalPhaD database relying on ab initio + ML [3]



[1]: Jain et al., APL Materials, 1 (2013) 011002.
[2]: Saal et al., JOM 65 (2013) 1501.
[3]: https://gtt-technologies.de/data/#aimp-ab-initio-materials-project

Vision: aiMP + GTOx

→ **Seamless combined use of aiMP and GTOx to navigate chemical space**

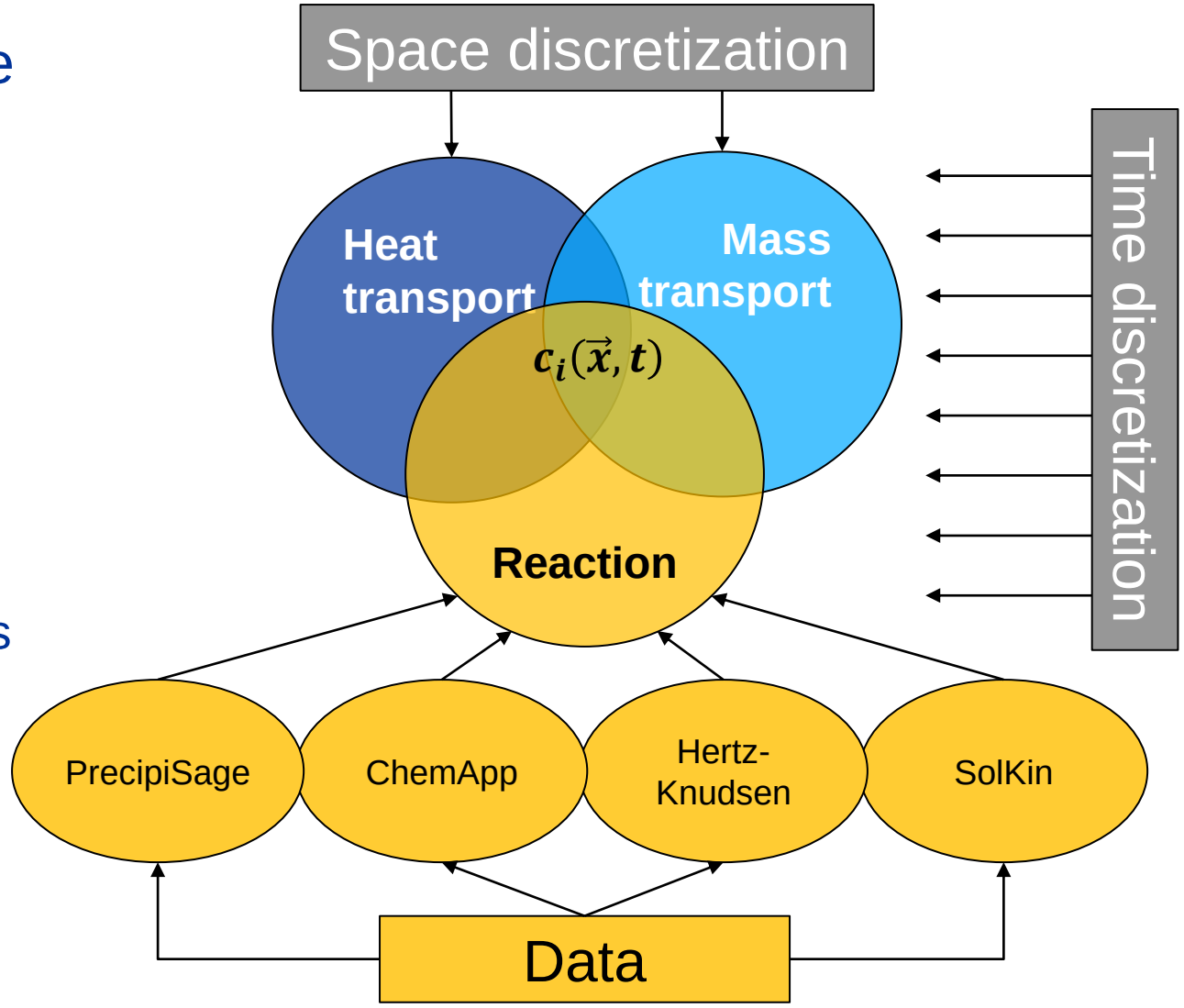


Road to kinetic software @GTT

Going beyond equilibrium and steady state calculations: space and time

- Space: FVM model framework
  - Spatial discretization
  - Consider extensive properties i.e. heat, mass
  - One evolution equation per chemical species
  - 1D (later 2D)

- Time: FVM model framework + reaction kinetics
  - PrecipiSage → Precipitation and phase transformation
  - Equilibrium incl. constrained equilibrium → ChemApp
  - Evaporation → Hertz-Knudsen
  - SolKin → Solidification
  - …

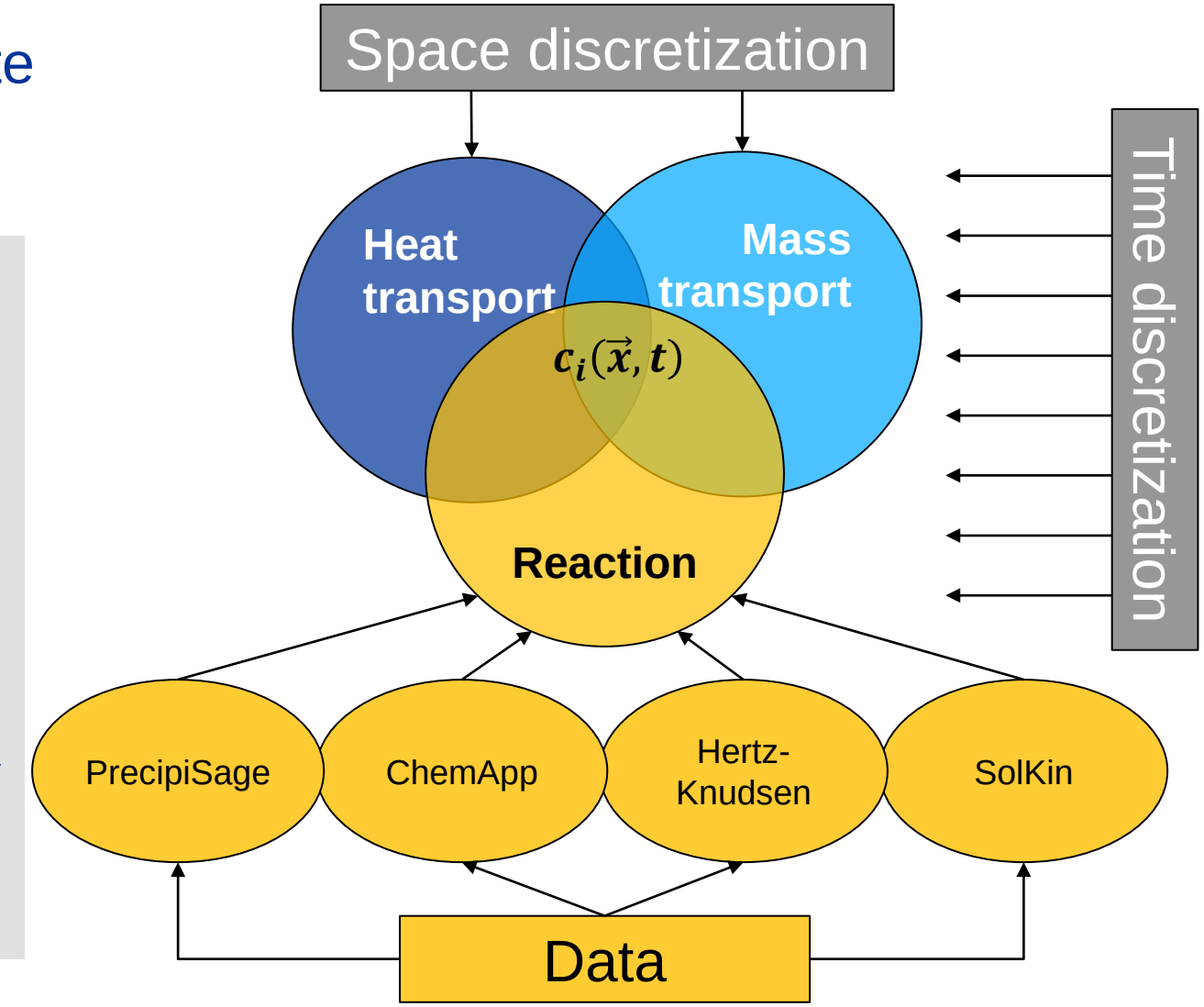


Road to kinetic software @GTT

Going beyond equilibrium and steady state calculations: space and time

Für GTT neue Klassen von Materialdaten: Dichte, Viskositäten, Diffusivitäten, Reaktionsgeschwindigkeiten
→ Schätzungen ausreichend!

Beschleunigung:
Active-learning ML-Modelle als on-the-fly Ersatz für rechenintensive physikalische Modelle.



Thank you for your attention!

If you have any question, please contact me:

mtb@gtt-technologies.de

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