# Automated Calphad Optimization Workflow

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## Motivation:

Automate optimization of simple binary metallic systems
- systems with intermetallics and/or
- systems with liquid miscibility gaps
- no systems with solid solutions (yet)

in order to
- create “good enough“ liquid descriptions in aiMP with minimum effort
- deepen our understanding of inaccuracies in aiMP
- learn what is necessary to create liquid and solid solutions in aiMP

## Strategy:

systems with intermetallics
AlCa, AlSr, CaNi, CaPb, LiSi, MgSi, NiSr, PbSr, ZnSr, PbLi (unsuccessful)
systems with liquid miscibility gaps:
CaK, CrK, CrNa, CrPb, CuK, PbAl, PbCu, PbFe, PbMn, PbNi, PbSi, PbZn, VNa

Create starting data file
- SGTE unaries pure elements
- SLIQ GTOx starting parameters
- aiMP intermetallics

↓

Generate .exp files of different CO recipes using Chemapp for python

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Generate parameters .json file using python code

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Create .opt file
1. .dat file
2. .exp files
3. .json parameter file
4. set hyperparameters

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Run .opt file

↓ Adjust boundary conditions repeat x5

Create new .opt file

↓

Adjust parameter selection

↓

Run .opt file

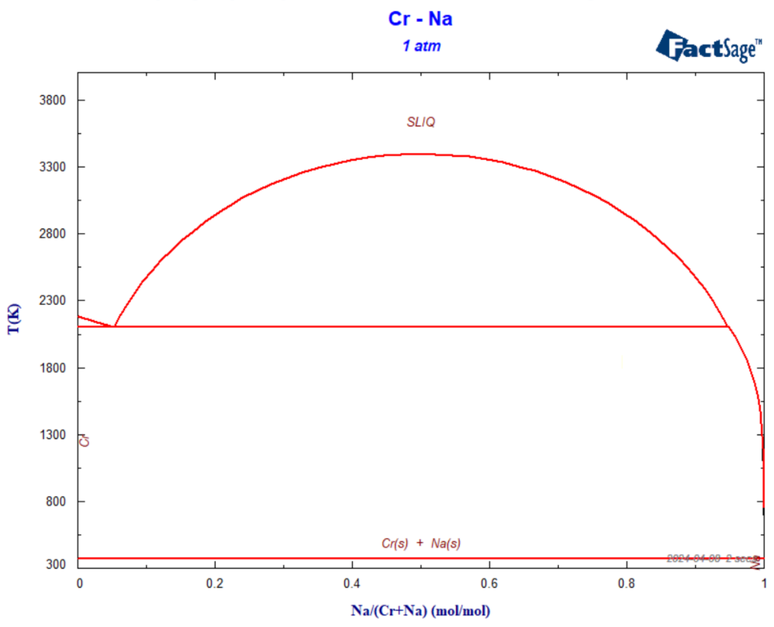
↓

Check final .opt file

## Results:

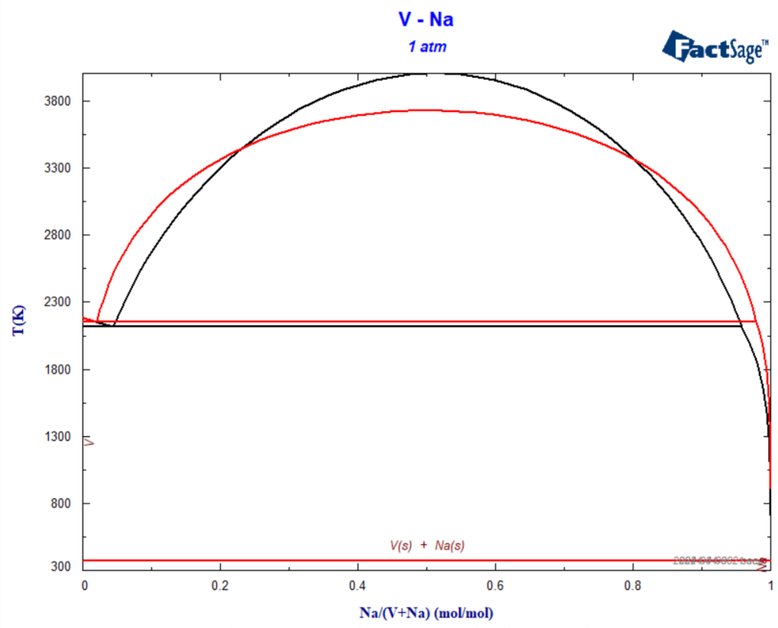
Black: automated optimization results
Red: normal calphad results in FactSage

### Miscibilty gap system with best agreement:



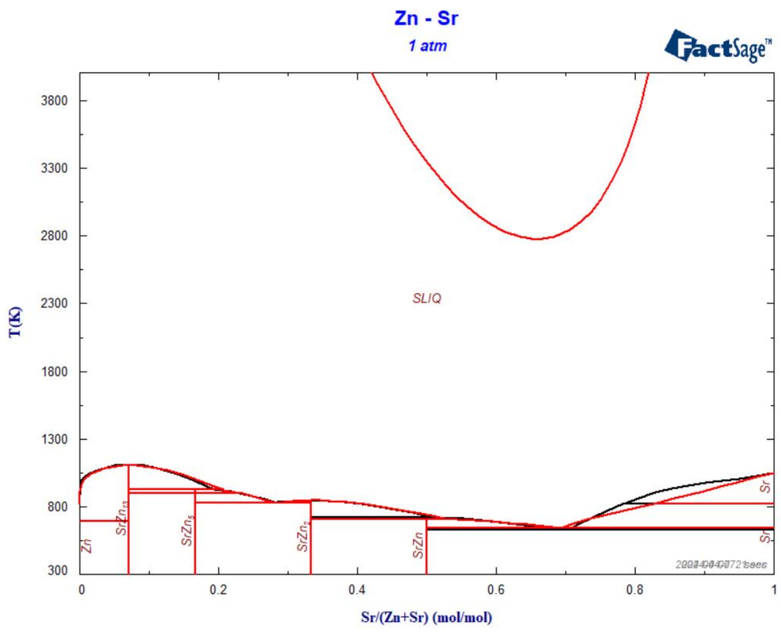

Best miscibility gap result

### Miscibilty gap system with worst agreement:



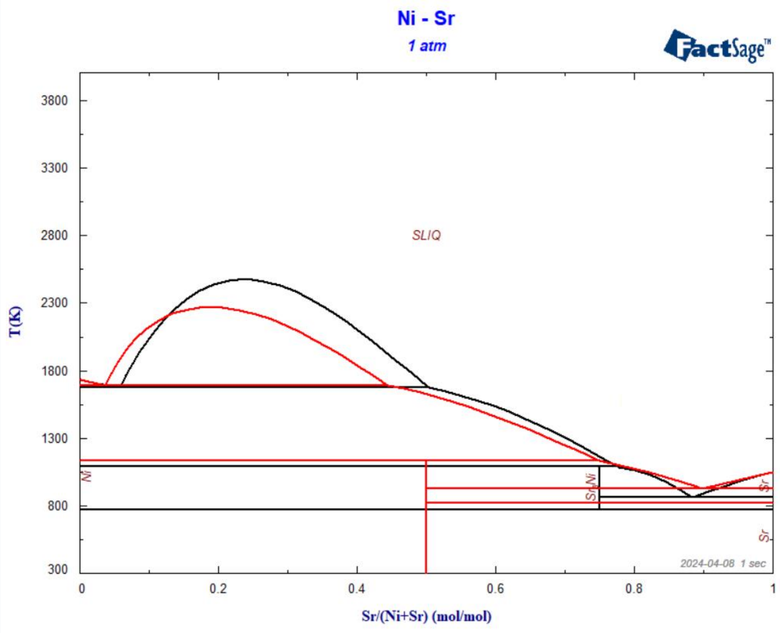

Not enough experimental data for accurate L2 parameter fit, worsens the fit

### Intermetallic system with best agreement:




- Stabilized and fit all intermetallics
- Avoided the high temperature inverse miscibility gap

### Intermetallic system with least agreement:




- Missing the NiSr intermetallic
- Automated optimization stabilized a different intermetallic to fit the solidus temperatures

→ Data formats used in Calphad Optimizer enable development of workflows
→ Successfully optimized 22 systems with 78 intermetallics in a single workflow
→ Run time for all 22 optimizations 150 min on desktop PC (run in parallel)

## Next Steps:

1. Increase experimental data sources
2. Study Error Sum contributions from Calphad Optimizer
3. Check whether changes in $\Delta H_f^{298}$ and $S^{298}$ for aiMP intermetallics point towards systematic errors
4. Automate a method to introduce mixed associates when necessary
5. Optimize 60 miscibility gap and intermetallic containing systems
6. Start optimizing 11 systems containing the fcc solid solution phase

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