



Deeper Understanding of Phase Diagrams Through Visualisation

Ruan Theron, **Andrea Steyn**, Johan Zietsman
GTT User's Meeting
June 2019

Content

Background
Core Concepts
Binary Phase Diagrams
Ternary Phase Diagrams
Methodology

Background

New process development

Process improvement and design

Failure analysis

RapidThermo aims to reduce computation time of equilibrium calculations.

Background

Presentation Purpose

Share how we are using visualization to improve our understanding and insight.

Background

Why This Matters

Engineers in SA enter work place with a limited understanding of thermochemistry.

advancing through insight

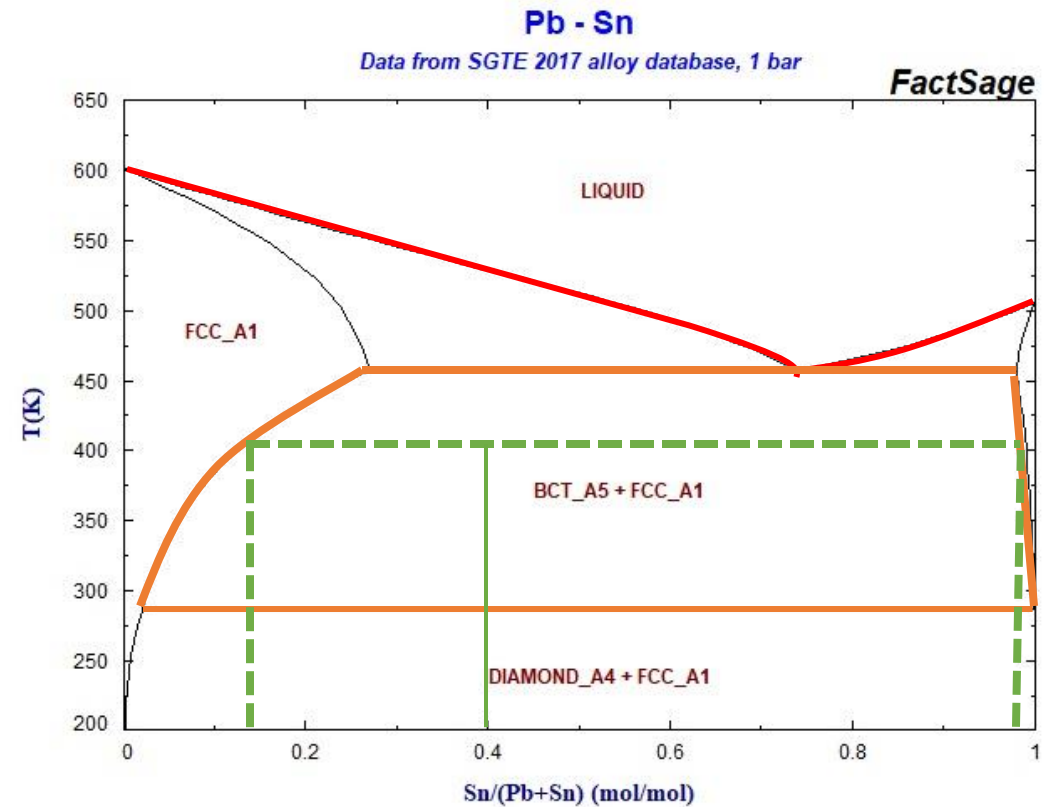
Importance of 2nd law and thermochemistry to all we do.

Core Concepts

Core Concepts

Phase Diagrams

- Zero fraction lines
- Phase regions
- Lever rule



Core Concepts

Gibbs Free Energy Minimisation

Gibbs energy of a system decreases in the course of spontaneous change:

$$\Delta G_{\text{system}} < 0$$

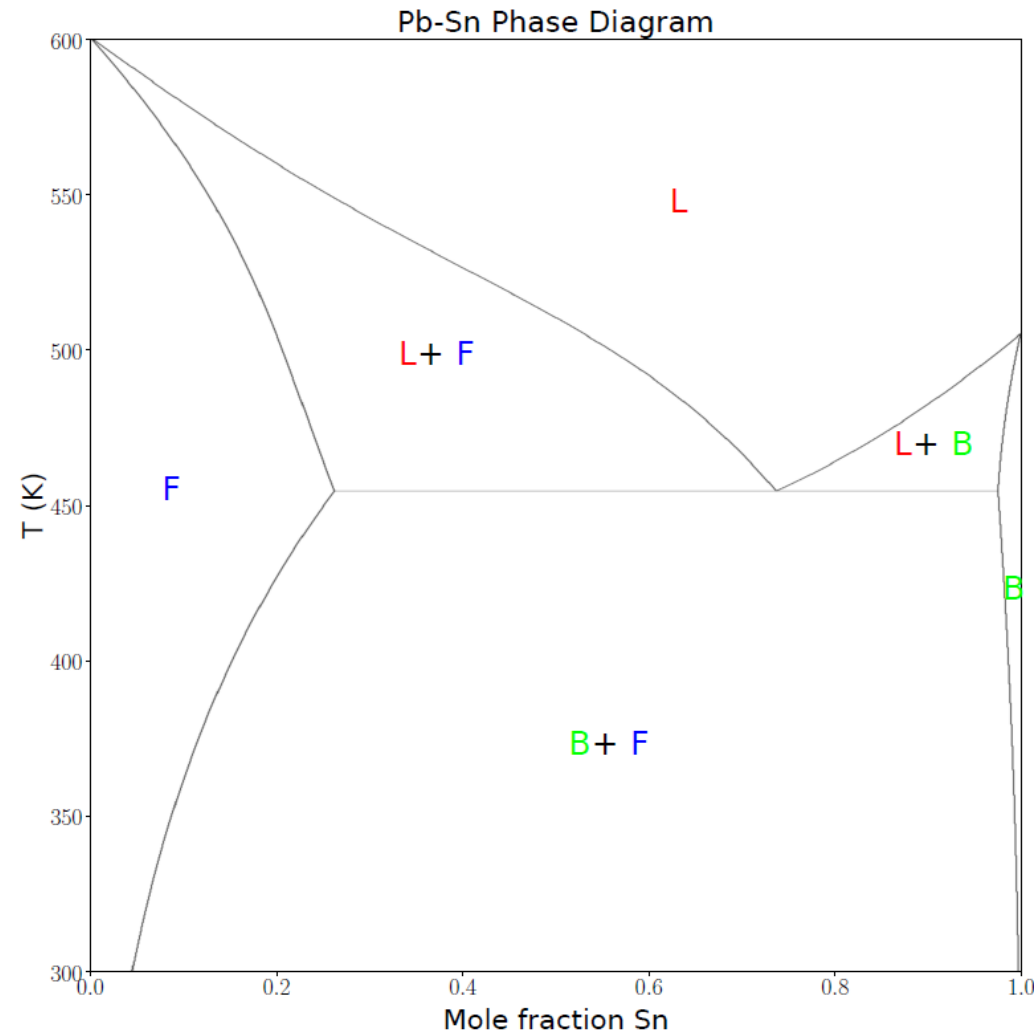
System with n_{ph} phases:

$$G_{\text{system}} = \sum_{\text{ph}=1}^{n_{\text{ph}}} G^{\text{ph}}$$

Binary Phase Diagram

Binary Phase Diagrams

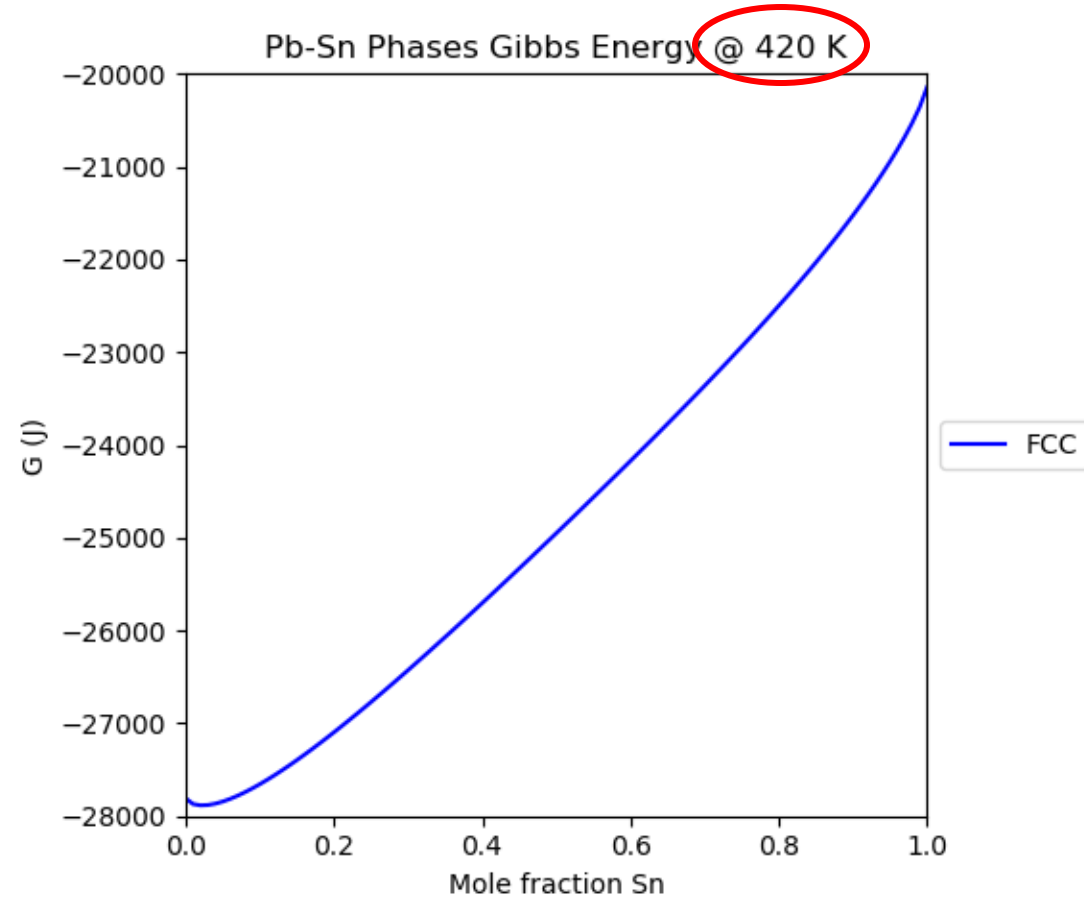
PbSn



Phases:
FCC (F)
BCT (B)
Liquid (L)

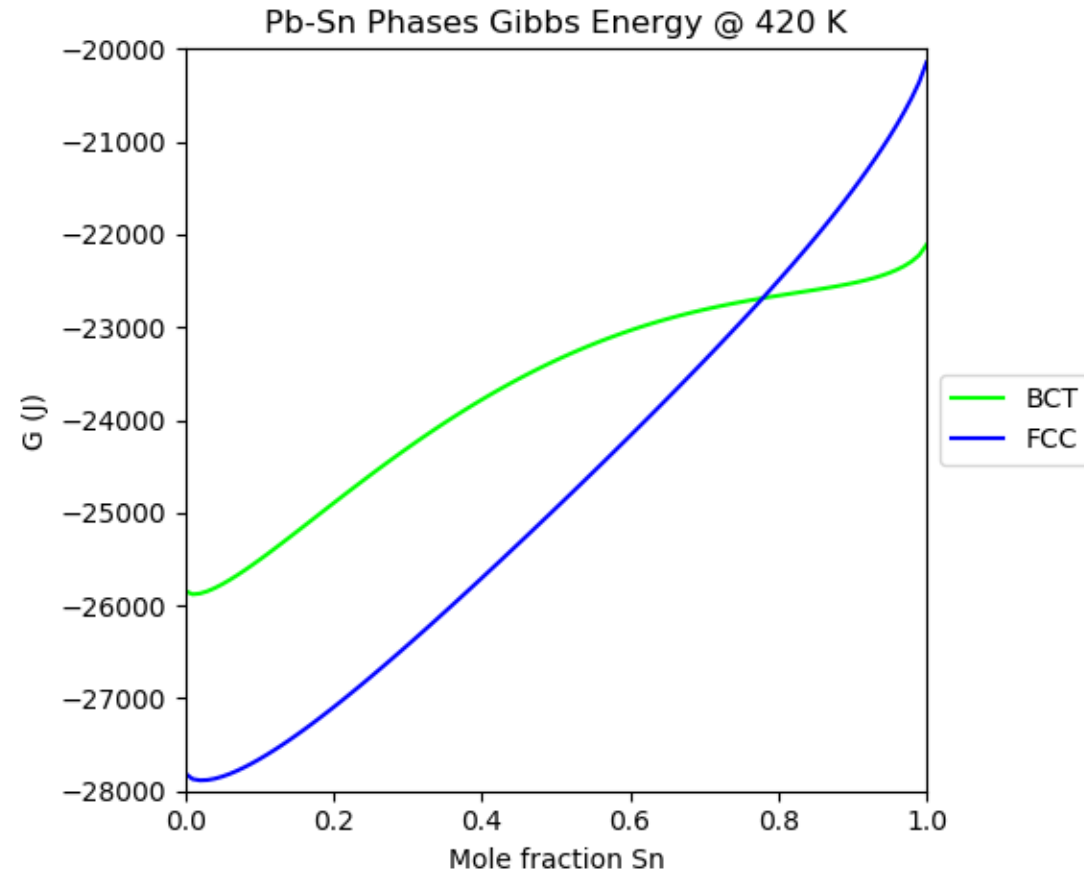
Binary Phase Diagrams

PbSn – Gibbs Energy per Phase



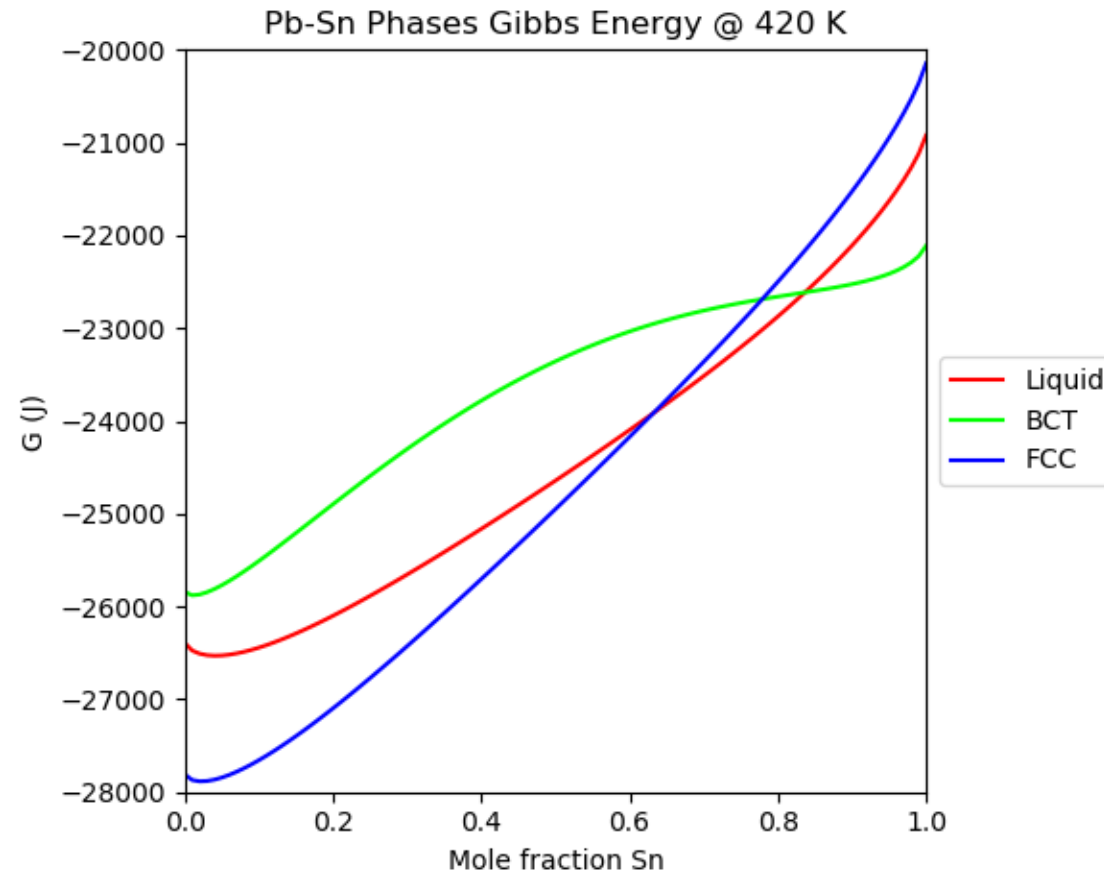
Binary Phase Diagrams

PbSn – Gibbs Energy per Phase



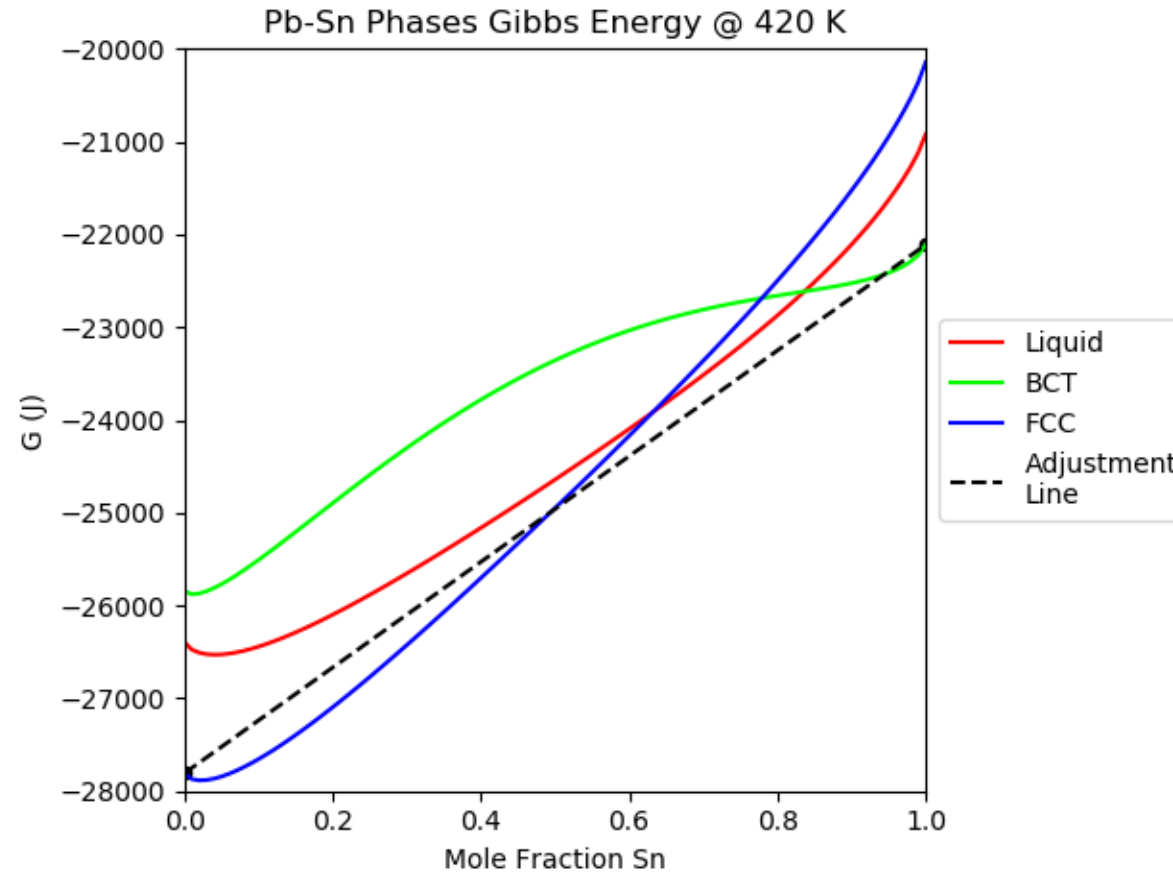
Binary Phase Diagrams

PbSn – Gibbs Energy per Phase



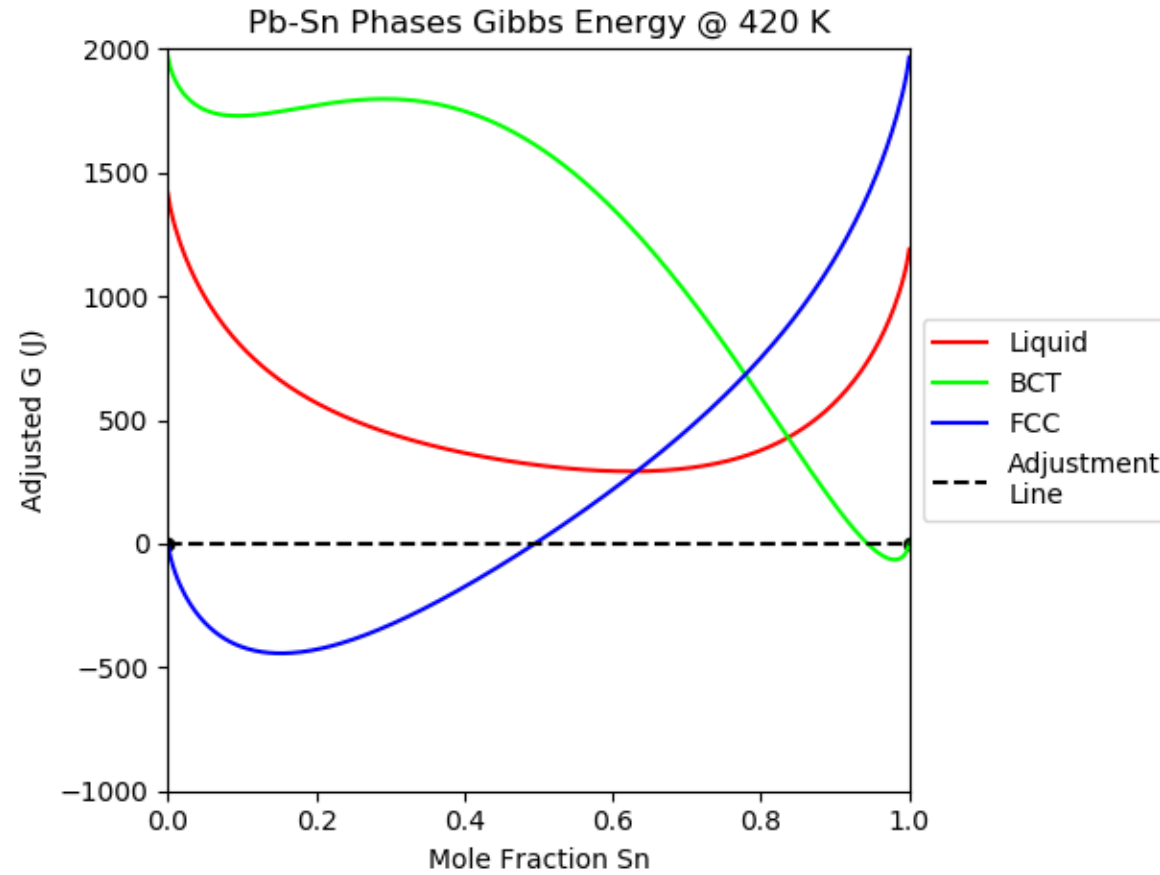
Binary Phase Diagrams

PbSn – Gibbs Energy Adjustment



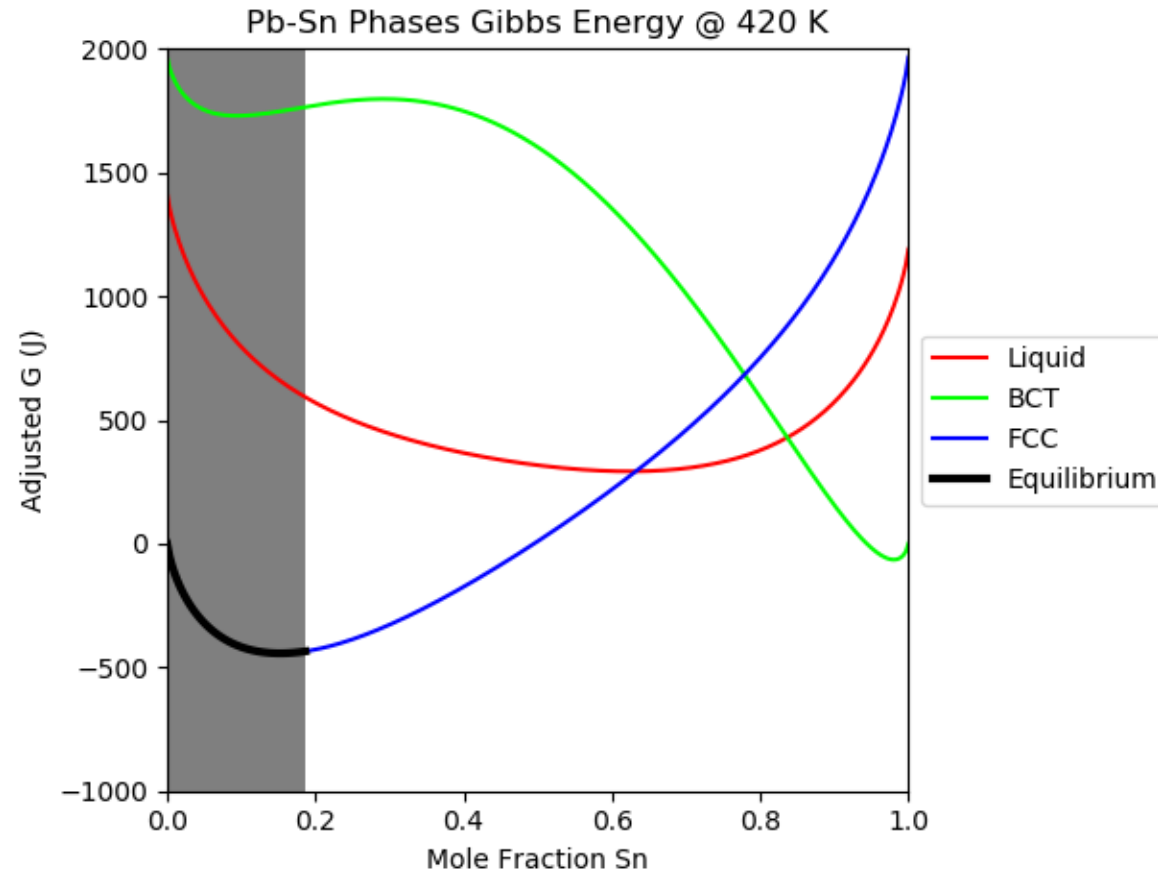
Binary Phase Diagrams

PbSn – Adjusted Gibbs Energy



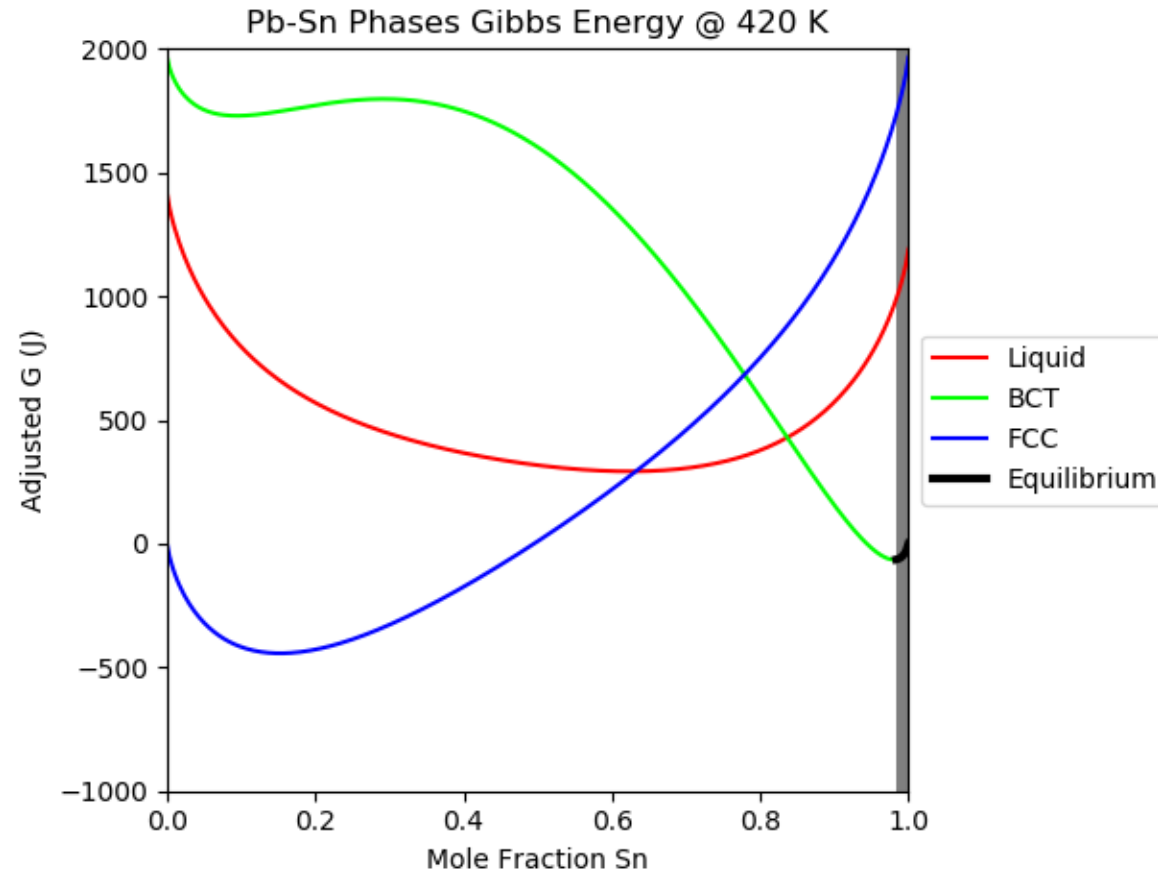
Binary Phase Diagrams

PbSn – Gibbs Energy Minimisation



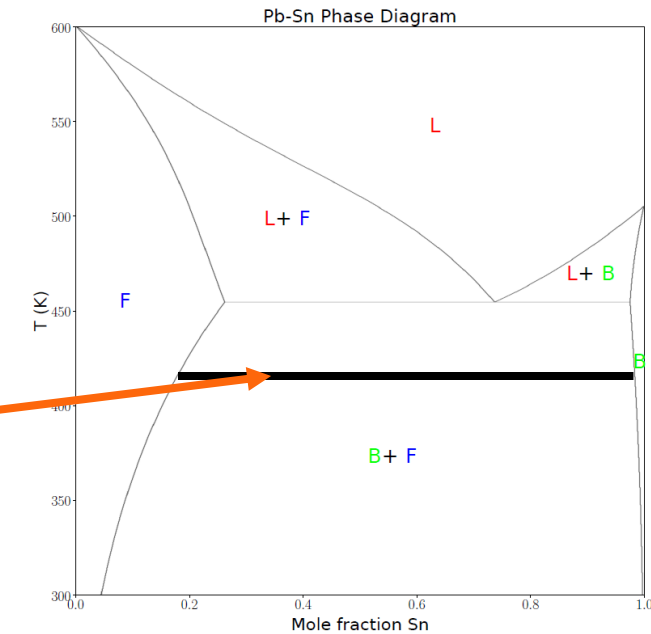
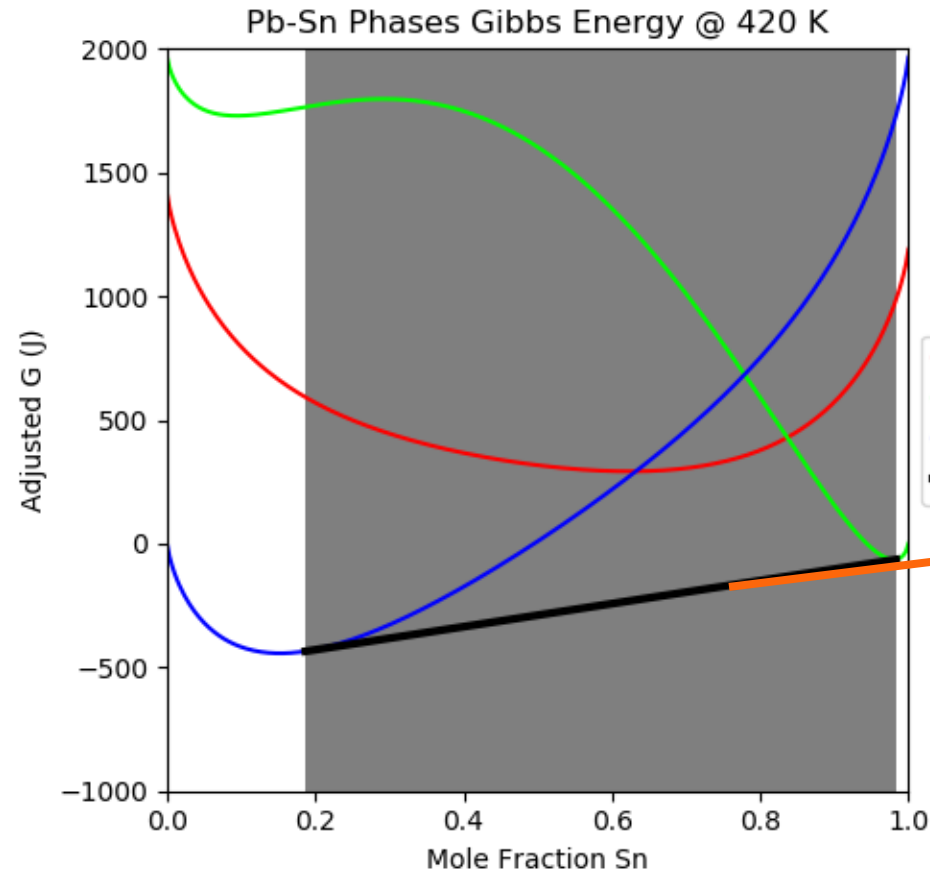
Binary Phase Diagrams

PbSn – Gibbs Energy Minimisation



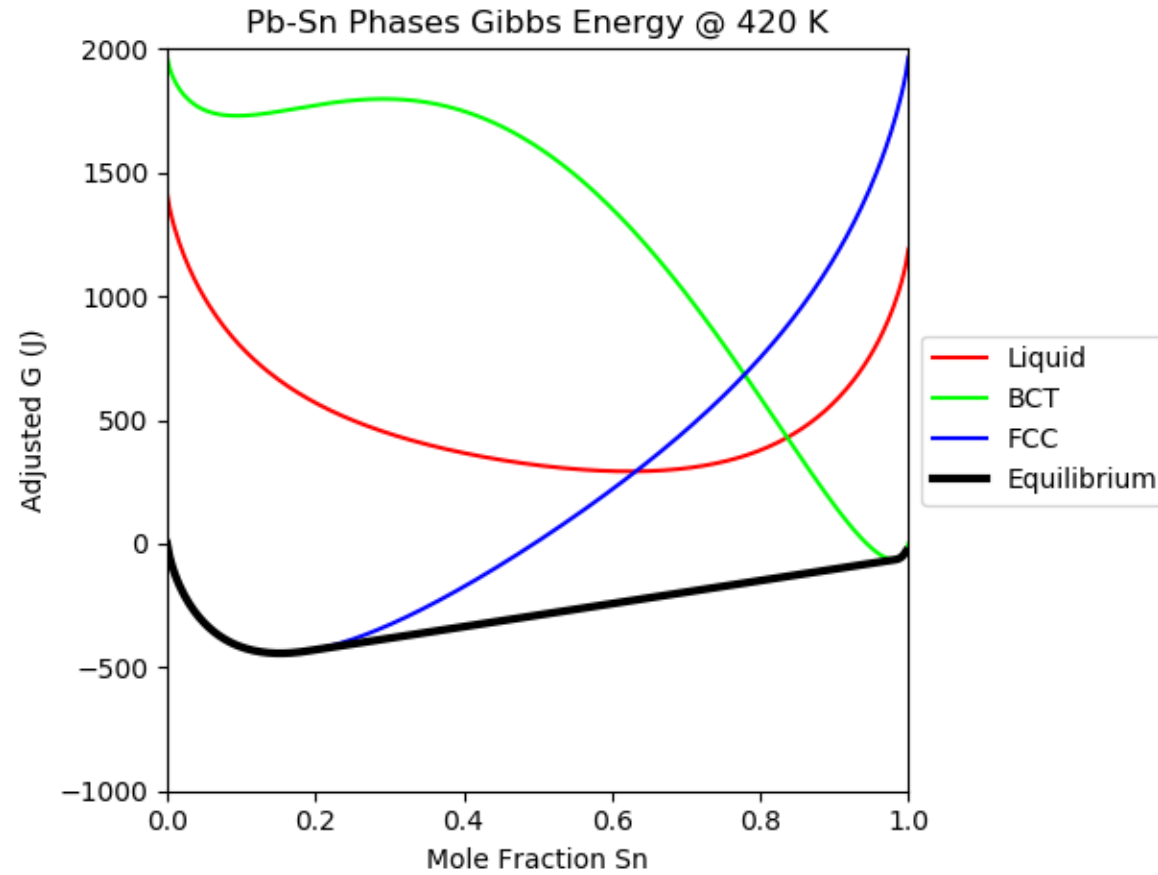
Binary Phase Diagrams

PbSn – Gibbs Energy Minimisation



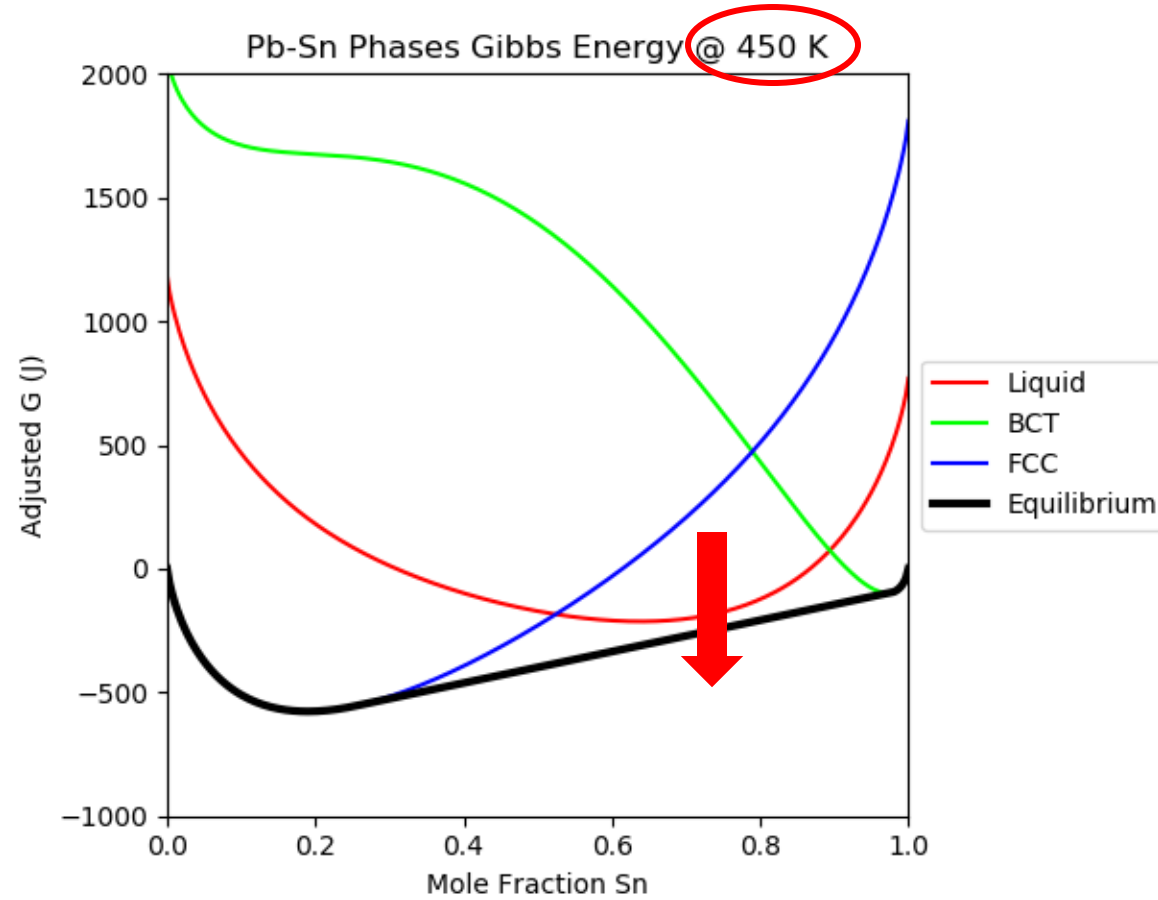
Binary Phase Diagrams

PbSn – Gibbs Energy Minimisation



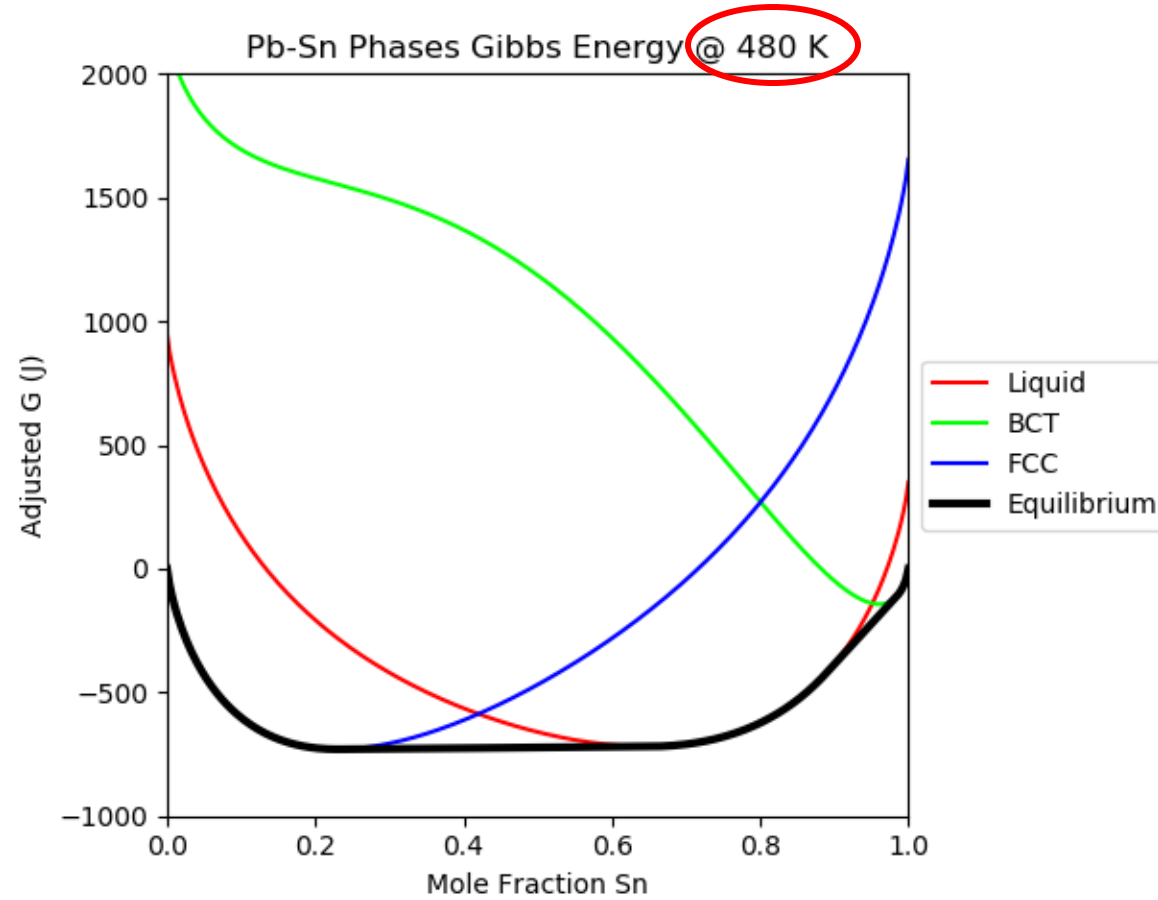
Binary Phase Diagrams

PbSn – Gibbs Energy at Higher Temperature



Binary Phase Diagrams

PbSn – Gibbs Energy at Higher Temperature



Binary Phase Diagrams

PbSn – Interactive Diagram

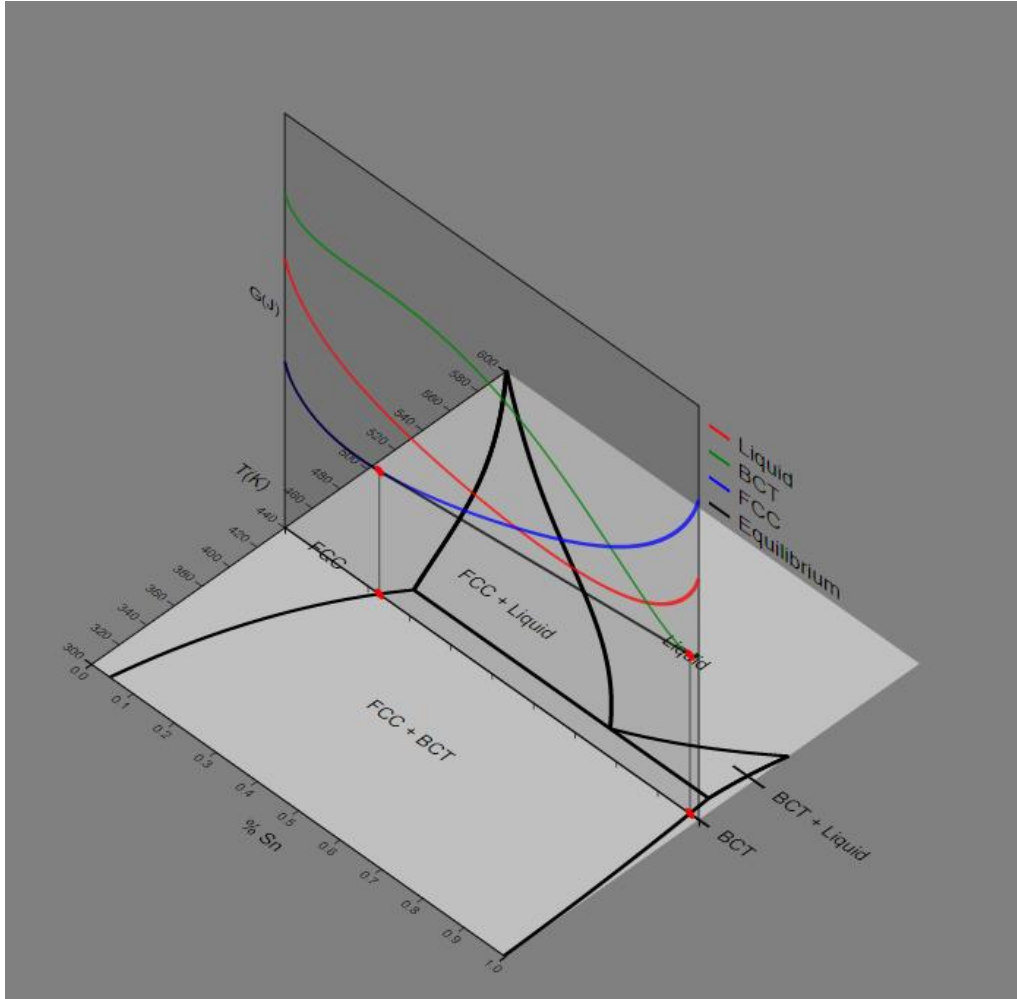
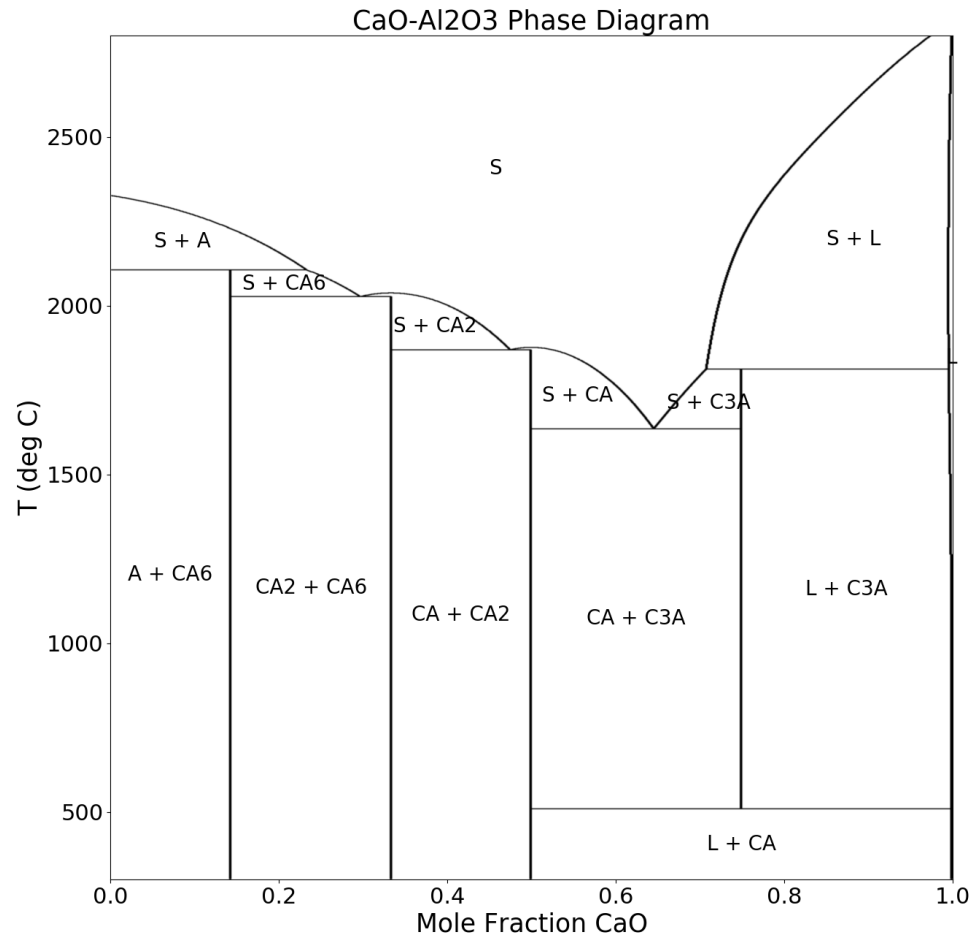


Diagram can be viewed on
Ex Mente's website:

<https://www.ex-mente.co.za/pbsn-interactive-diagram>

Binary Phase Diagrams

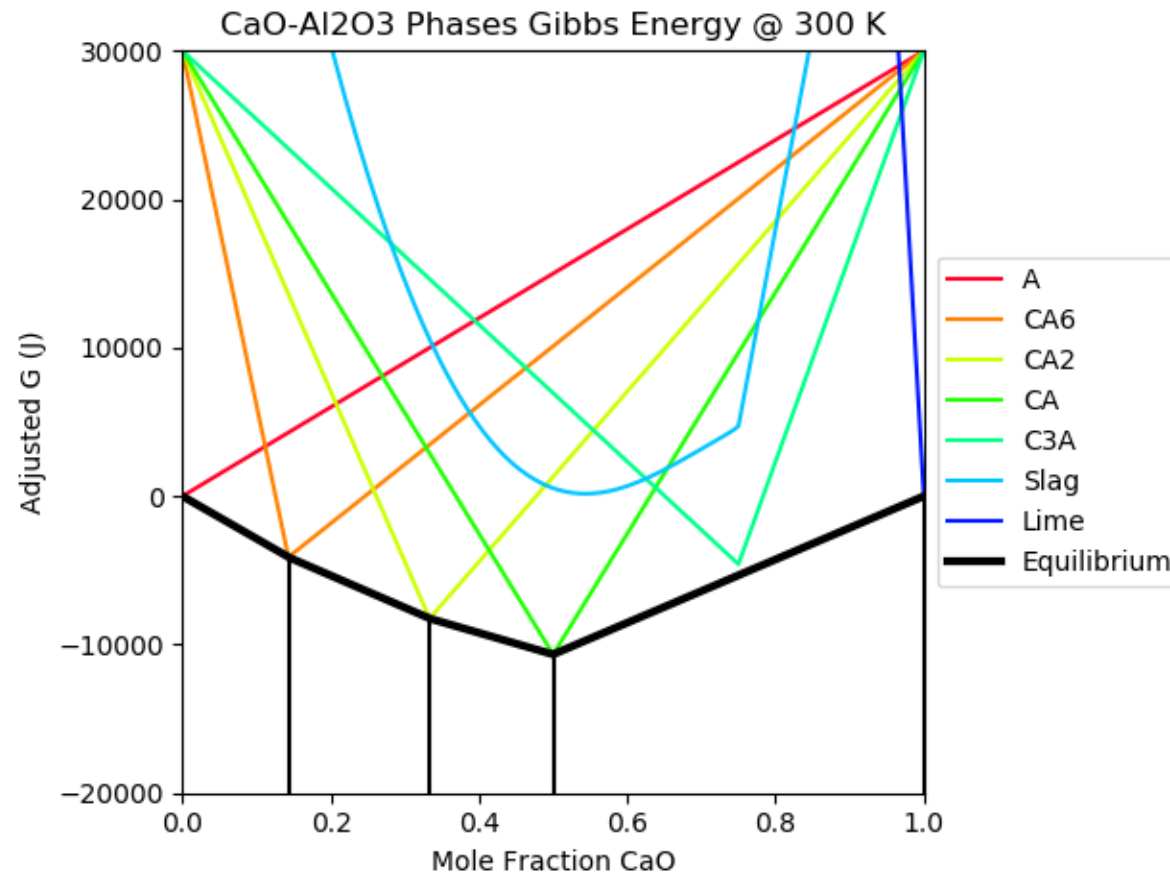
CaO-Al₂O₃



Phases	Abbreviations
Al ₂ O ₃	A
CaAl ₁₂ O ₁₉	CA6
CaAl ₄ O ₇	CA2
CaAl ₂ O ₄	CA
Ca ₃ Al ₂ O ₆	C3A
Lime	L
Slag	S

Binary Phase Diagrams

CaO-Al₂O₃: Gibbs Energy Minimisation



Binary Phase Diagrams

CaO-Al₂O₃ – Interactive Diagram

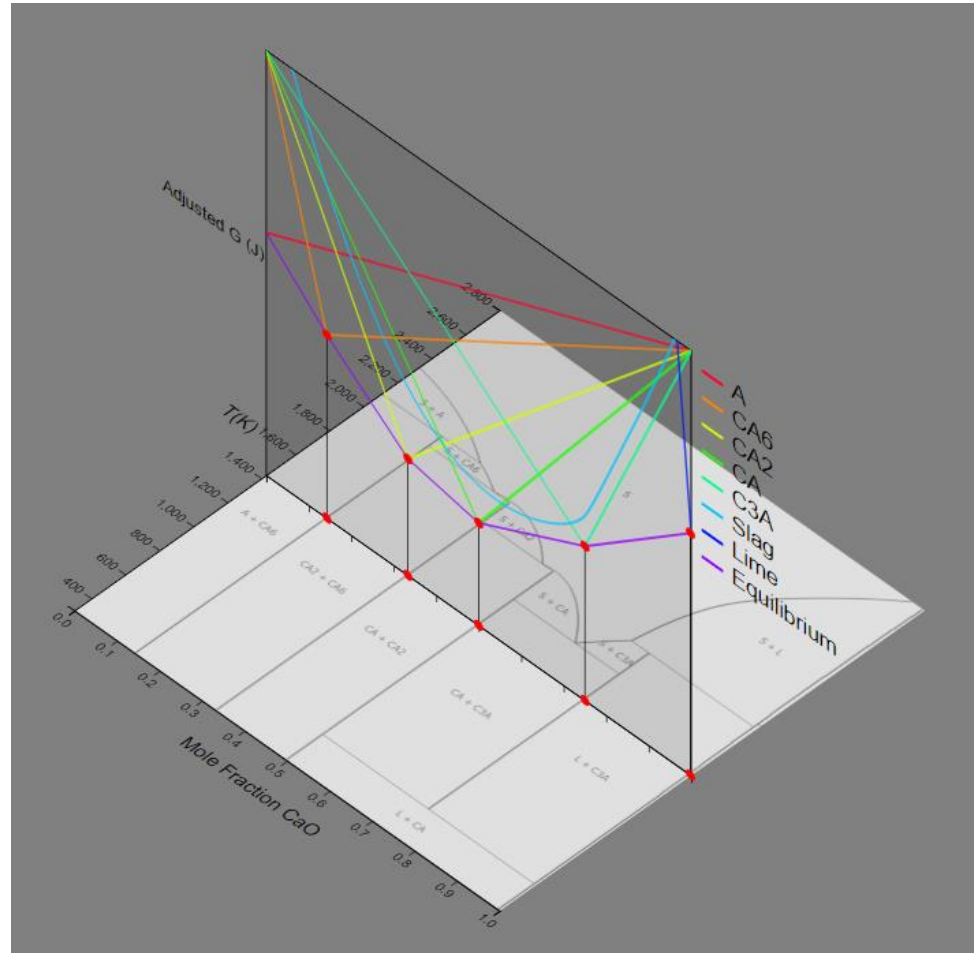


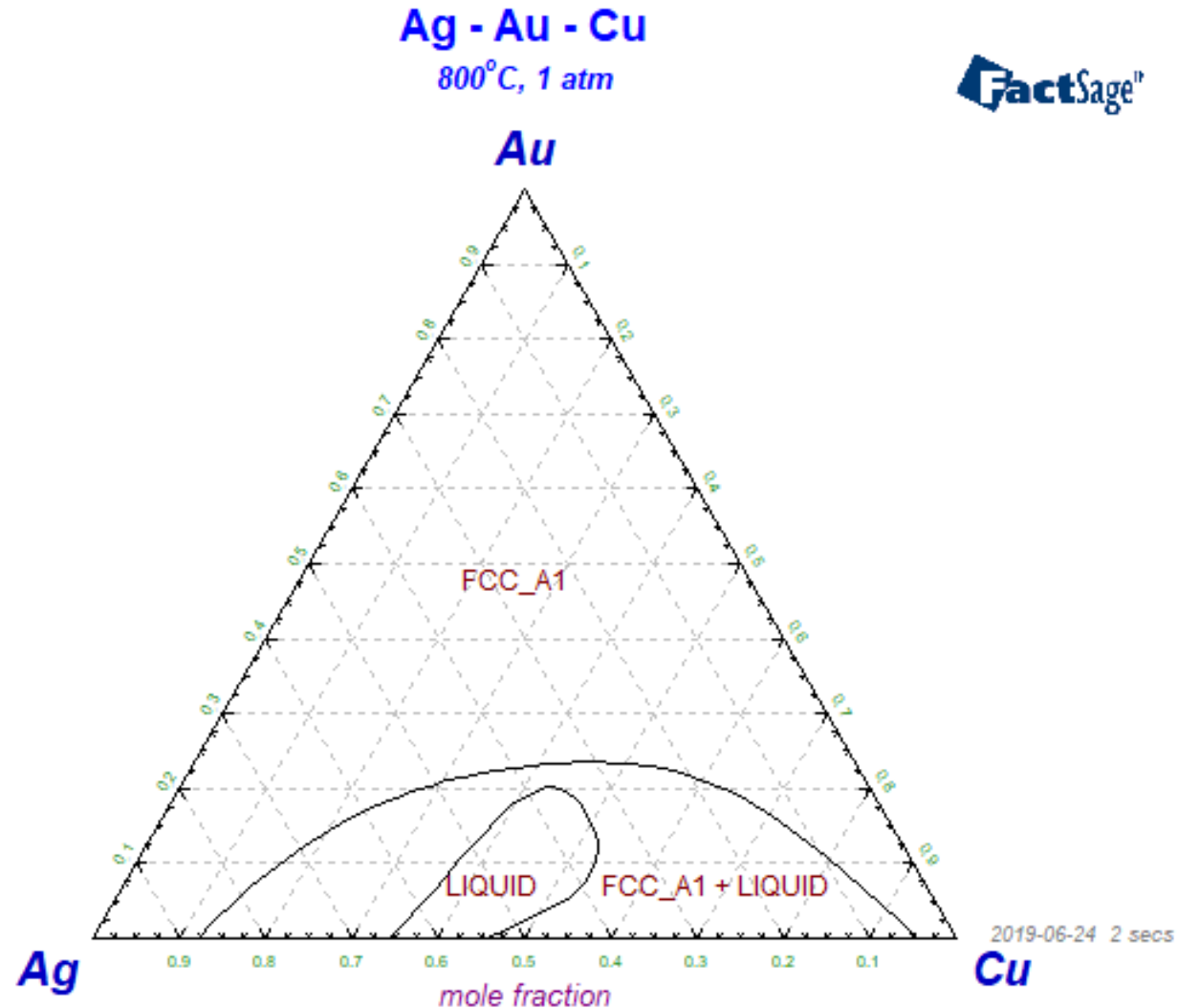
Diagram can be viewed on
Ex Mente's website:

<https://www.ex-mente.co.za/cao-al2o3-interactive-diagram>

Ternary Phase Diagram

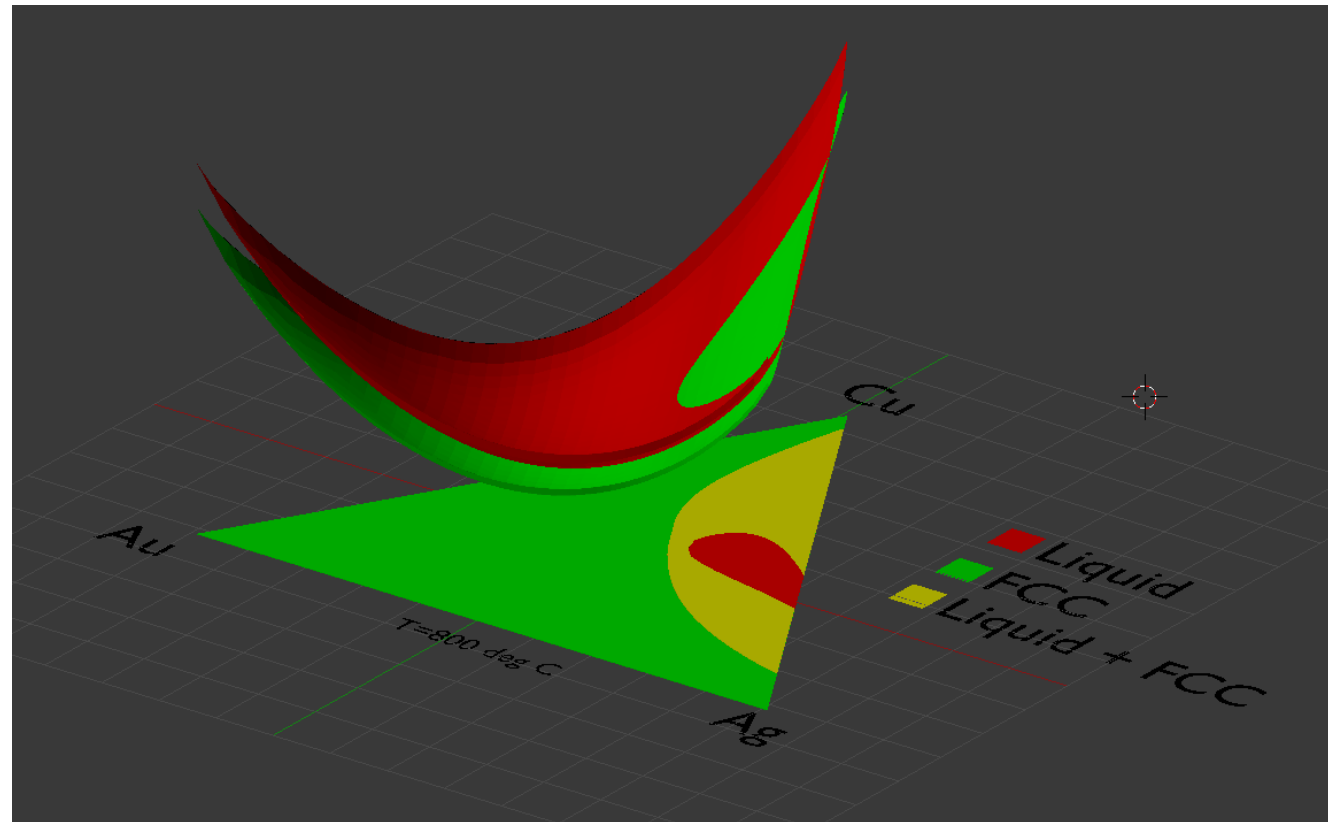
Ternary Phase Diagrams

Ag-Au-Cu



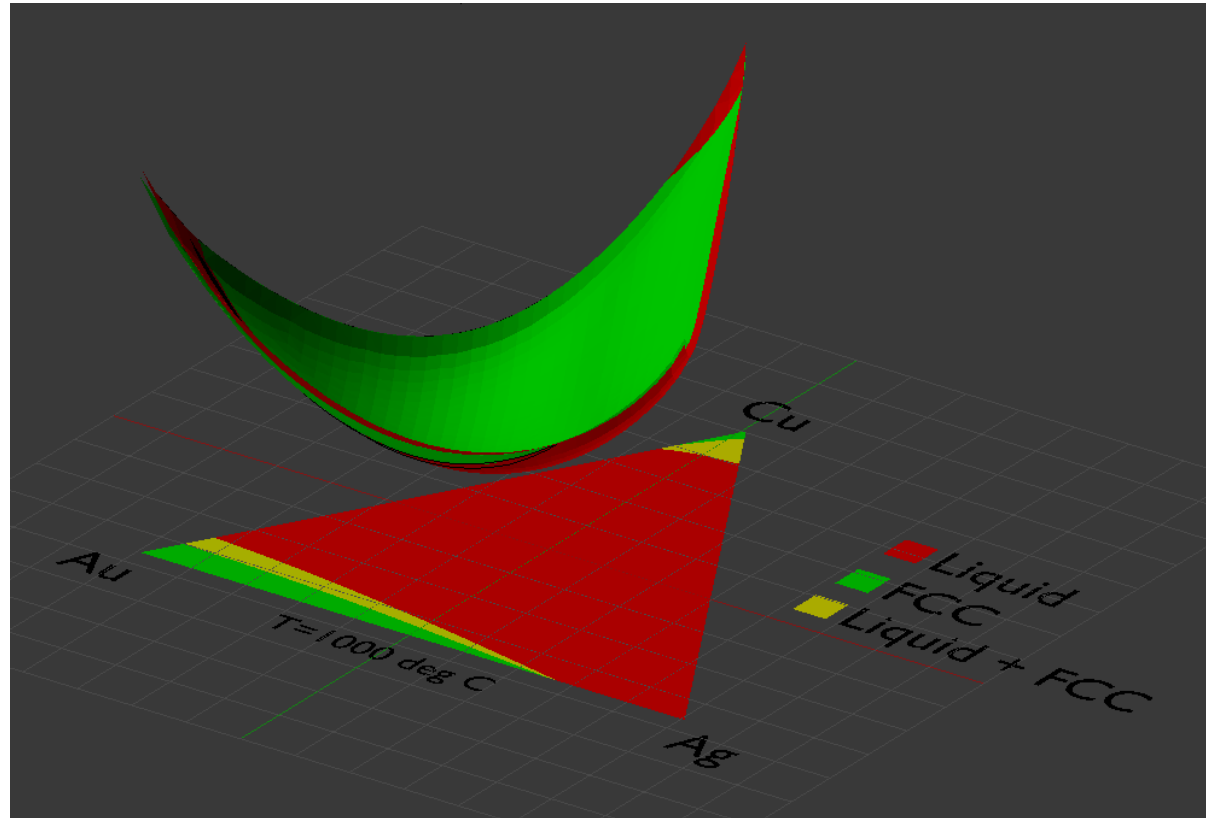
Ternary Phase Diagrams

Ag-Au-Cu $T = 800^{\circ}\text{C}$



Ternary Phase Diagrams

Ag-Au-Cu $T = 1000^{\circ}\text{C}$



Methodologies

Methodologies

- Data Generation

All data was generated with ChemAppPy

- Data Transformation was conducted with Python

- Additional tools:

- D3 for 2D visualisation
- Blender for 3D visualisation

Conclusion

We are still exploring different ways on how to visualise thermochemistry concepts

Continued work:

- 3D phase diagrams
- 4D phase diagrams
- RapidThermo

5-component (5D) accelerated equilibrium calculations

Thank You