

# Introduction to pycalphad

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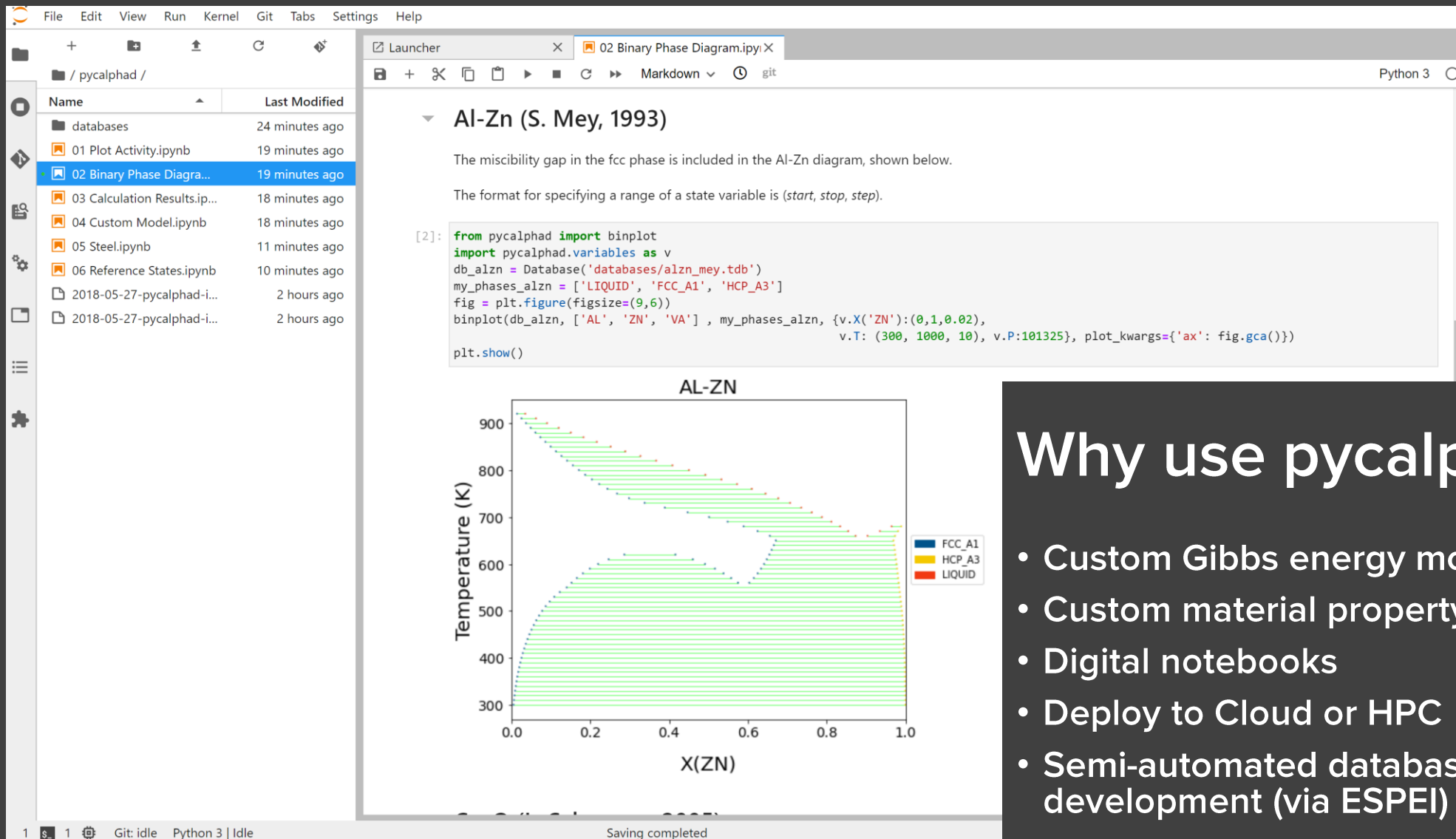
PyCalphad/ESPEI Virtual Workshop



# pycalphad = Python + CALculation of PHAse Diagrams

- pycalphad is software for designing thermodynamic models, calculating phase diagrams and investigating phase equilibria.
- Using CALPHAD-based models, pycalphad predicts properties of materials, including
  - Transition (e.g., melt) temperatures, phase fractions, solidification, degradation, corrosion, etc.
  - Anything that can be connected to a chemical or thermodynamic process
- Free and open source at [pycalphad.org](https://pycalphad.org)





## Why use pycalphad

- Custom Gibbs energy models
- Custom material property models
- Digital notebooks
- Deploy to Cloud or HPC
- Semi-automated database development (via ESPEI)

# Notable Features in pycalphad 0.9

- Improved performance, nearly zero calculation start time
- Preliminary support for ‘local’ equilibrium calculations
- User-specified reference states
- Binary and ternary phase diagram plotting
- T, P,  $\mu_i$ ,  $x_i$  conditions with multiple components
- Step/map calculation, global minimization
- Support for associates and ionic liquids
- IHJ and Xiong magnetic models
- Order-disorder model, Two-state model, Einstein model
- Windows, Mac, and Linux support



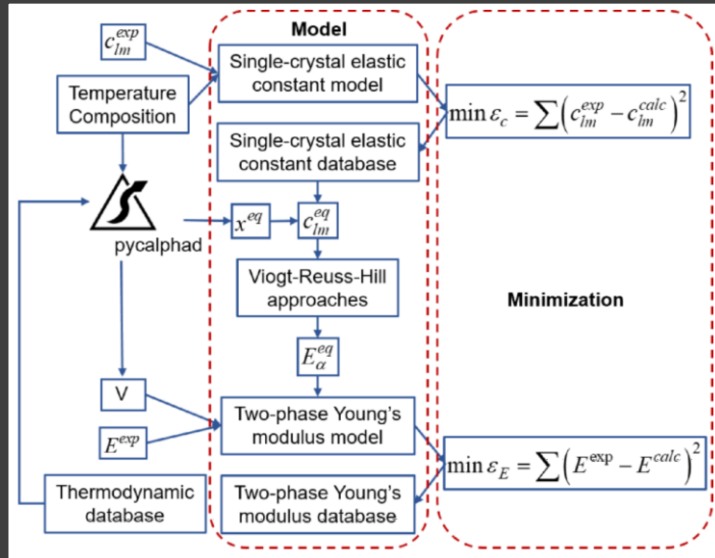
# Current Limitations in pycalphad 0.8

- In progress: “Advanced” conditions (e.g., amount of a phase)
- In progress: Quasichemical model
- A few TDB features are unsupported (Option “B”, Option “F”, STATUS\_BITS, etc...)
  - Contact us: we can usually help you work around the issue



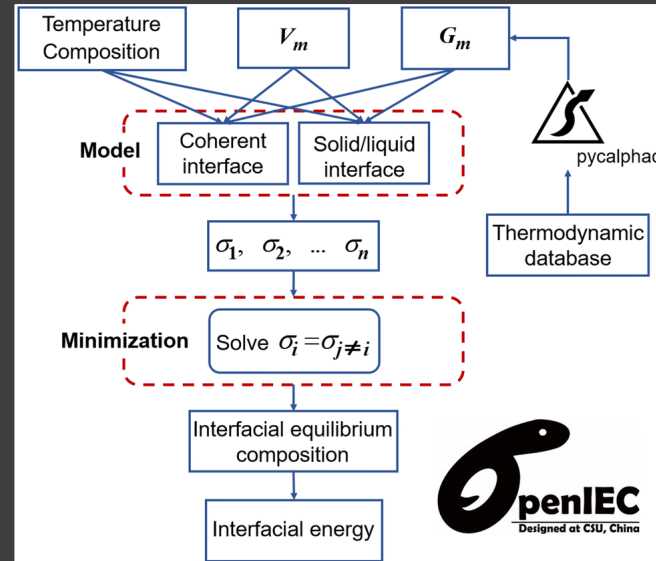
# PyCalphad Community Selected Use Cases

## Two-phase Elastic Constants



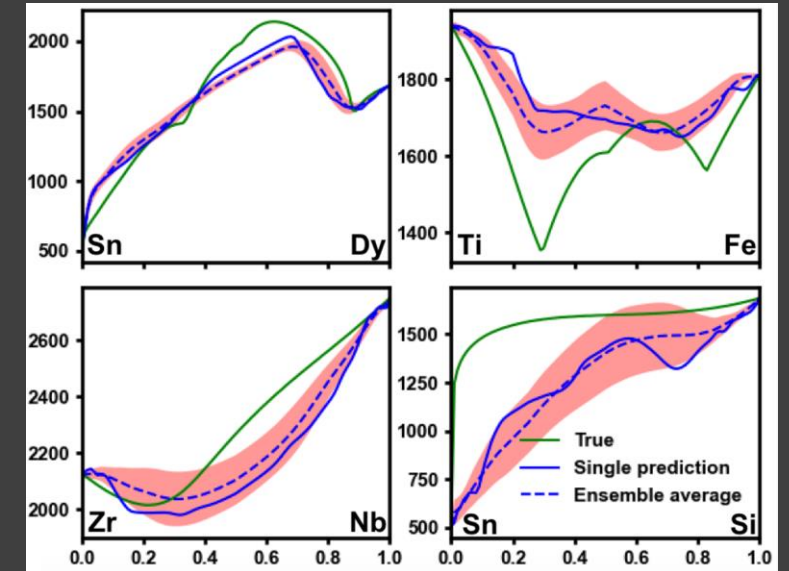
Y. Shang, et al., *Materialia* **8**, 100500 (2019)  
doi: 10.1016/j.mtla.2019.100500

## Interfacial Energy



S. Yang, et al., *J. Mat. Sci.* **54**, 10297–10311 (2019)  
doi: 10.1007/s10853-019-03639-w

## Machine Learning



P. Guan and V. Viswanathan (2020)  
arXiv:2010.14048v1



# Contact Us

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[pycalphad.org](http://pycalphad.org)

Chat with us on Gitter!

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