Calphad Optimizer in FactSage 8.2 – Introduction and Demonstration

Bruno Reis, Florian Tang, Philipp Keuter, Moritz to Baben
GTT-Technologies

Calphad optimizations consist of three steps: The collection and evaluation of experimental data, the setup of sensible thermochemical models and the actual optimization. The new Calphad Optimizer in FactSage makes the last step easy by providing the Calphadian with extensive feedback to control the optimization. Main benefits of using the Calphad Optimizer:

- Access to all thermochemical models in FactSage, including quasichemical models
- Easy input of experimental data, e.g. by predefined recipes and test option
- Access to two different optimizers (Gaussian Process and NOMAD)
- Extensive feedback on error (per data group and data point) and sensitivity of parameters
- An intuitive Graphic User Interface