

# TAOS

## The Alloy Optimization Software

### Description

The Alloy Optimization Software (TAOS) has been developed at LLNL to be a powerful, user-friendly tool that allows for computational design of optimal alloys on commodity computers. It does not require users to have domain expertise in computational materials science.

On just commodity stand-alone computer hardware, TAOS allow users to design new materials with a targeted property (e.g., melting temperature, freezing range, phase formed) under applied constraints (e.g. phases to avoid, minimum melting temperature) in minutes to hours (depending on the constraint optimization criteria). Its intuitive graphical user interface (GUI) allows for rapid screening of desired alloy compositions from a large multidimensional composition space down to a manageable number of experimental targets.

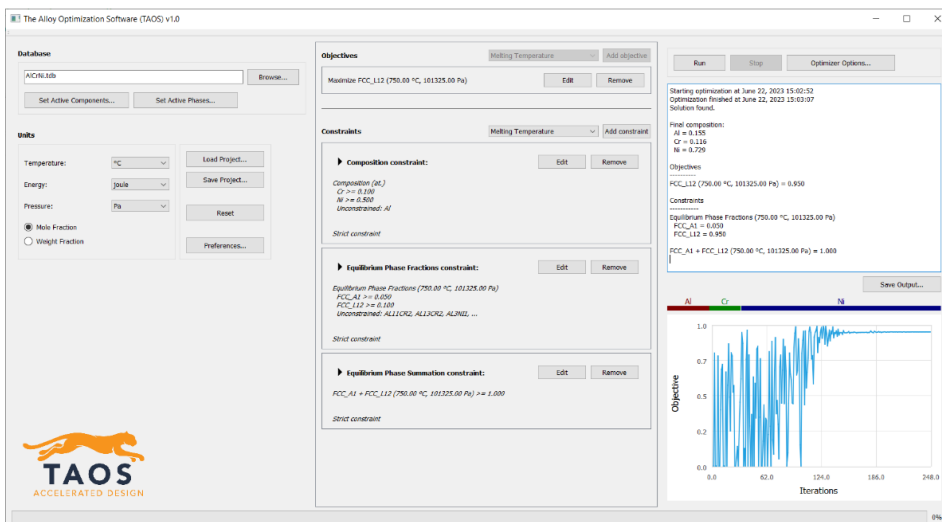
TAOS is based on the use of CALPHAD (CALculation of PHase Diagrams) thermodynamic databases, integrates the pycalphad thermodynamic engine to work as a self-consistent software with unencrypted databases, and automatically interacts with the Thermo-Calc software and commercial databases through TC-python (being provided by [www.thermocalc.com](http://www.thermocalc.com)). Note that Thermo-Calc products are not included in TAOS.

The technology is currently being packaged in a user-friendly way to allow for broad application as a commercial tool. LLNL is seeking interested end user licensees.

### Category

Software

### Learn more



### Advantages

TAOS is an easy-to-use, automated, cross-platform software with a GUI that supports rapid iteration for efficient screening of target compositions.

- It can be run by non-specialists on commodity computers.
- An approximately 10x reduced cost and at least 2x reduced time to market for alloy designs.
- Automates the search for optimal alloys over a large multicomponent phase space. In comparison, typical competitive calculations are constrained to a single alloy composition per calculation and often a small numbers of alloy components.
- Offers a broader software compatibility and more features than currently available alloy design tools.

### **Applications**

TAOS is tuned for applications in operational alloy development environment and is aimed at users engaged in alloy design and production using conventional and advanced manufacturing (AM).