

# Phase Diagrams with Thermo-Calc

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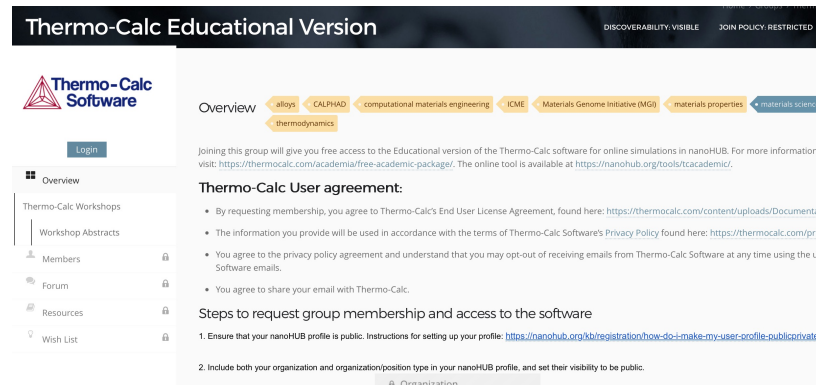
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# Running Thermo-Calc on nanoHUB

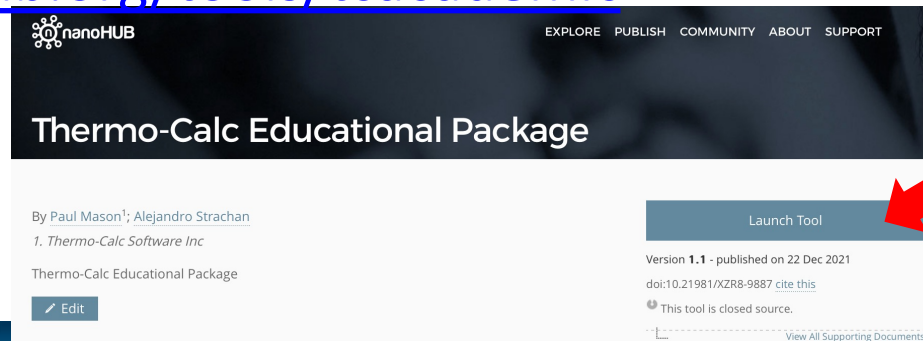
The academic version of Thermo-Calc is freely available on nanoHUB

STEP 1: Login to nanoHUB & request membership to the Thermo-Calc group: <https://nanohub.org/groups/tcacademic>



The screenshot shows the 'Thermo-Calc Educational Version' page. At the top, it says 'DISCOVERABILITY VISIBLE' and 'JOIN POLICY RESTRICTED'. The Thermo-Calc Software logo is on the left. The main content area has a navigation bar with categories: alloys, CALPHAD, computational materials engineering, ICME, Materials Genome Initiative (MGI), materials properties, and thermodynamics. Below this, there is a 'Login' button and a sidebar with 'Overview', 'Thermo-Calc Workshops', 'Workshop Abstracts', 'Members', 'Forum', 'Resources', and 'Wish List'. The main text area contains a 'Thermo-Calc User agreement' section with bullet points and a 'Steps to request group membership and access to the software' section with numbered instructions.

STEP 2: Once you are admitted: launch the tool <https://nanohub.org/tools/tcacademic>



The screenshot shows the 'Thermo-Calc Educational Package' tool page on nanoHUB. The page header includes 'nanohUB' and navigation links: 'EXPLORE', 'PUBLISH', 'COMMUNITY', 'ABOUT', 'SUPPORT'. The main title is 'Thermo-Calc Educational Package'. Below the title, it says 'By Paul Mason<sup>1</sup>; Alejandro Strachan' and '1. Thermo-Calc Software Inc'. There is an 'Edit' button. On the right side, there is a 'Launch Tool' button with a red arrow pointing to it. Below the button, it says 'Version 1.1 - published on 22 Dec 2021', 'doi:10.21981/XZR8-9887 cite this', and 'This tool is closed source.' At the bottom right, there is a link to 'View All Supporting Documents'.

# ThermoCalc Demo

Thermo-Calc Educational Package

Thermo-Calc - Educational Version 2021a

File Tools Window Help

New Open Save Switch to Console Mode

Project Configuration Results

My Project

Wizards

Quick Start

Templates

Single Point Equilibrium One Axis Equilibrium

Scheil Solidification Simulation Binary Calculation

Select Templates

Scheduler

Scheduled Jobs

Phase Diagram Ternary Diagram

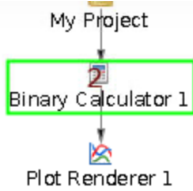
# Select Databases

The screenshot shows the Thermo-Calc Educational Package interface. The main window is titled "Binary Calculator 1" and is part of a project named "My Project". The "Databases" dropdown menu is set to "TCBIN: TC Binary Solutions v1.1", which is highlighted by a red arrow. Below the dropdown menu, there are tabs for "Elements", "Phases and Phase Constitution", "Data Sources", and "Description". The "Elements" tab is selected, showing a periodic table of elements. The "Calculation Type" is set to "ZE VA /-".

The interface also includes a "Project" panel on the left showing a tree view of the project structure, a "Scheduler" panel at the bottom left, and a "Results" panel on the right showing "Plot Renderer 1".



# Calculation



TCBIN: TC Binary Solutions v1.1

Elements    Phases and Phase Constitution    Data Sources    Description

|                     |    |    |    |    |    |    |    |    |    |    |    |    |           |    |    |    |    |    |    |    |    |  |    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|---------------------|----|----|----|----|----|----|----|----|----|----|----|----|-----------|----|----|----|----|----|----|----|----|--|----|--|--|--|--|--|--|--|--|--|--|--|--|--|--|
|                     |    |    |    |    |    |    |    |    |    |    |    |    |           |    |    |    |    | ZE | VA |    |    |  |    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|                     |    |    |    |    |    |    |    |    |    |    |    |    |           |    |    |    |    | /- |    |    |    |  |    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| H                   |    |    |    |    |    |    |    |    |    |    |    |    |           |    |    |    |    |    |    |    |    |  | He |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Li                  | Be |    |    |    |    |    |    |    |    |    |    |    |           |    |    | B  | C  | N  | O  | F  | Ne |  |    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Na                  | Mg |    |    |    |    |    |    |    |    |    |    |    |           |    |    | Al | Si | P  | S  | Cl | Ar |  |    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| K                   | Ca | Sc | Ti | V  | Cr | Mn | Fe | Co | Ni | Cu | Zn | Ga | Ge        | As | Se | Br | Kr |    |    |    |    |  |    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Rb                  | Sr | Y  | Zr | Nb | Mo | Tc | Ru | Rh | Pd | Ag | Cd | In | <b>Sn</b> | Sb | Te | I  | Xe |    |    |    |    |  |    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Cs                  | Ba | *  | Hf | Ta | W  | Re | Os | Ir | Pt | Au | Hg | Tl | <b>Pb</b> | Bi | Po | At | Rn |    |    |    |    |  |    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Fr                  | Ra | ** | Rf | Db | Sg | Bh | Hs | Mt | Ds | Rg | Cn | Nh | Fl        | Mc | Lv | Ts | Og |    |    |    |    |  |    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| * Lanthanide series |    |    | La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho        | Er | Tm | Yb | Lu |    |    |    |    |  |    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| ** Actinide series  |    |    | Ac | Th | Pa | U  | Np | Pu | Am | Cm | Bk | Cf | Es        | Fm | Md | No | Lr |    |    |    |    |  |    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

Calculation Type

- Phase diagram
- Gibbs energy curves    Temperature    Kelvin    1000.0
- Activity curves    Temperature    Kelvin    1000.0
- Phase fractions    Mole fraction    0.0

Help    Add Predecessor    Calculate Phase Diagram    Create New Successor



# Plots

Project Configuration Results

My Project  
Binary Calculator 1  
Plot Renderer 1

Scheduler  
Scheduled Jobs

Configuration  
Binary Calculator 1

Databases  
TCBIN: TC Binary Solutions v1.1

Elements Phases and Phase Constitution Data Source

Calculation Type  
 Phase diagram  
 Gibbs energy curves Temperature Kelvin  
 Activity curves Temperature Kelvin  
 Phase fractions Mole fraction

Results  
Plot Renderer 1

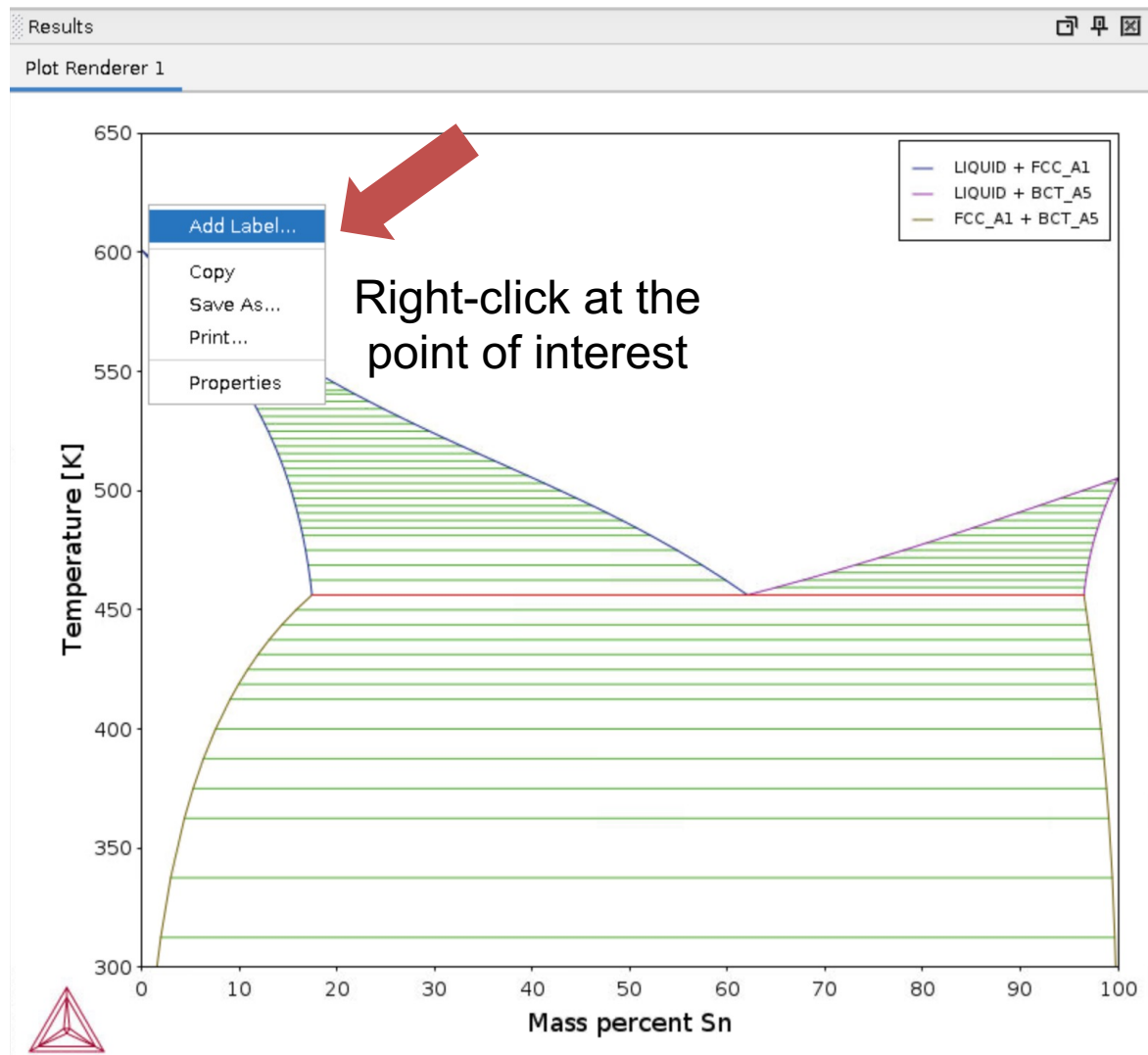
Drag the window to resize the plot; do NOT close it

Temperature [K]

Mass percent Sn

Legend:  
— LIQUID + FCC\_A1  
— LIQUID + BCT\_A5  
— FCC\_A1 + BCT\_A5

# Label phases in Thermo-Calc





# Solidification

