Scientific Research on the Cloud

materials square

www.matsq.com

Cutting-Edge Materials Simulation Techniques

We provide state-of-the-art materials simulation tools through MatSQ. We're constantly improving our existing services and adding new simulation methods.

Professional Consulting & Technical Support

Professional consultants(Ph.D.) are ready to support your materials simulation needs from start to finish.

Everything on the Cloud

Don't worry about the computing resources and licensing. MatSQ uses cloud computing to handle projects of any scale.

Reduce R&D Expenses

Minimize Trial & Errors

In Silico Approach

What if we could definitly reduce the number of experimental attempts? Introduce simulation and obtain results without experiment!

Reasonable R&D

Simulation can screen promising one among the tremendous possibilities. Conduct your experiments only with highly potent samples!

Find Good Starting Points

Modeling

Design the experiment to theoretical model

Atomic · Molecular Simulation

Perform atomic-scale simulation for cause investigation and experimental scheme

Result Analysis

Determine the proper experimental condition from the results analysis

Verify Origins of Failure

Display Materials

Defect analysis of oxide semiconductor. Find the structure stability depends on the temperature.

Solar Cell Materials

Obtain heterostructure properties to improve efficiency.
Calculate various optical properties

Battery Design

Analysis using simulation methodologies (DFT, MD, FEM, etc.) to find the origins of the degradation of batteries

materials square

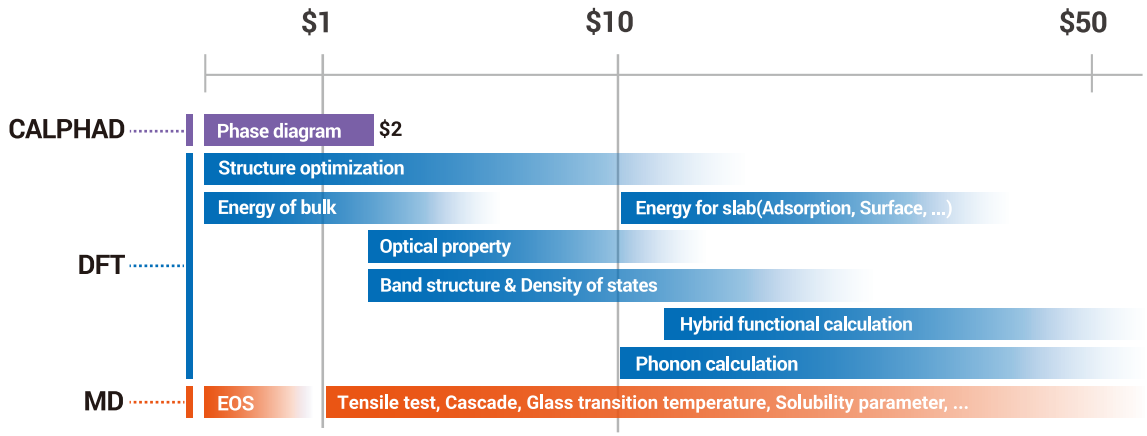
SERVICE URL www.matsq.com
CONTACT support@matsq.com

Price (DFT/MD)

MatSQ Pricing

PAY-AS-YOU-GO: Computing Resources

$0.25 per core hour



Subscription

Unlimited Plan

	GRAPHITE-100 ACADEMY	GRAPHENE-330	FULLERENE-660	DIAMOND-990
	$ 100	$ 330	$ 660	$ 990
CPU Hour Credits per month	2,000 hrs	1,000 hrs	2,500 hrs	6,000 hrs
Unlimited Core with One dedicated HPC	-	8 cores	18 cores	24 cores
Storage Basic 100GB	-	+100 GB	+200 GB	+500 GB

Subscription

Support Plan

Pro

$ 1,250 per month

- ✔ Technical support (Email/Chatting)
- ✔ Online basic tutorial + Meeting (3hr)
- ✔ Modeling
  - Workflow consulting
  - Input parameter optimization
- ✔ Result Analysis
  - Scientific visualization service

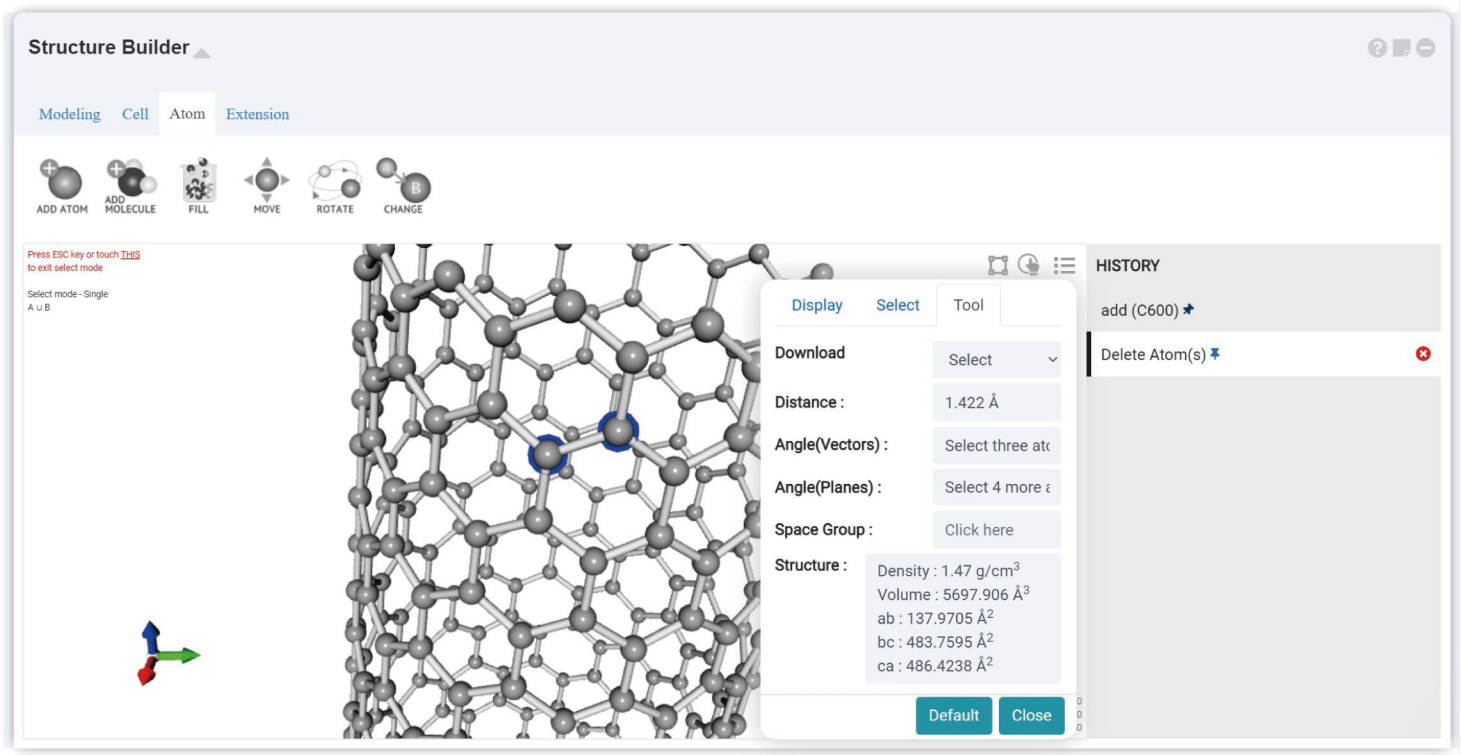
Business

$ 2,500 per month

- ✔ Technical support (Email/Chatting)
- ✔ Online basic tutorial + Meeting (5hr)
- ✔ Modeling
  - Workflow consulting
  - Input parameter optimization
  - Input script consulting
  - Simulation advice
- ✔ Result Analysis
  - Scientific visualization service
  - Result analysis consulting

Modeling FREE

'Structure builder' is a powerful and intuitive DFT modeling tool.
You can easily generate structure and check the DFT model in the visualizer.



Manipulator

Applications

Battery

- Design next generation battery
- Battery degradation simulation
- Battery charge capacity / Voltage / Speed

Structural Materials

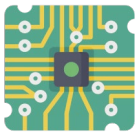
- Stability under extreme conditions
- Ionic & Electronic transport behavior
- Calculation of optical properties
- Thermal resistivity

Solar Cell

- Design highly-efficient solar cell
- Resolve stability and toxicity issue
- Transmittance, absorption coefficient

Display

- OLED and QD Display
- Stability under thermal stress
- Verify origins of failure



Semiconductor

- Stability of new memory
- Electronic transport behavior
- Current-voltage relation

MatSQ Materials DFT

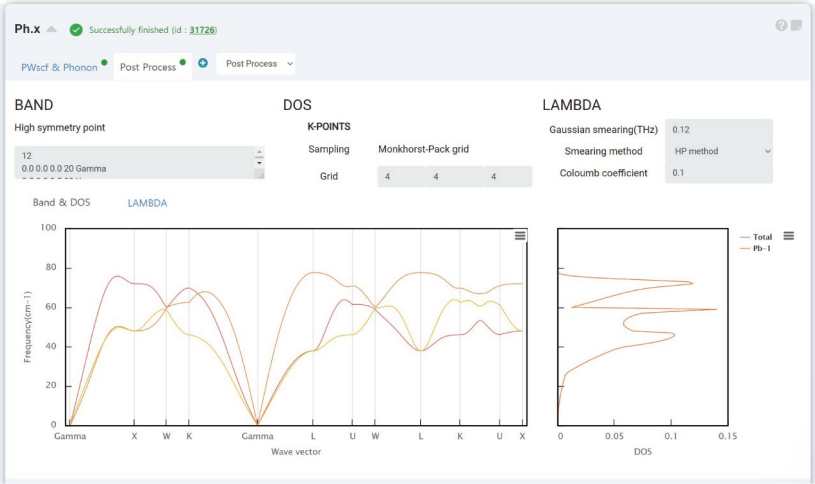
DFT Density Functional Theory

GUI for Quantum ESPRESSO

Quantum ESPRESSO for DFT simulation is provided with fully optimized calculation parameters and various pre/post-processing modules.

Simulation on the Cloud

Materials Square is powered by cloud computing servers. You can make simulation on the cloud and pay-as-you-go.



Available Properties

Structural Relaxation

Energetics

Cohesive Energy
Adsorption Energy
Surface Energy
Stacking Fault Energy

Electronic Structure Calculation

Partial/Local Density of States
Band Structure
Fatband(Projected Band Structure)
Charge Density

Mechanical Properites

Bulk Modulus
Elastic Constants
Stress-Strain Curve

Vibrational Properties

Phonon Density of States
Phonon Dispersion
Dielectric Constants
Effective Charge
Electron-Phonon Coefficient

Optical Properties

Dielectric Function
Absorption Coefficient
Refractive Index
Join Density of States

MD Classical Molecular Dynamics

MatSQ Materials MD

GUI for LAMMPS

MD simulation is performed using LAMMPS with fully optimized calculation parameters and various pre/post processing modules.

Simulation on the Cloud

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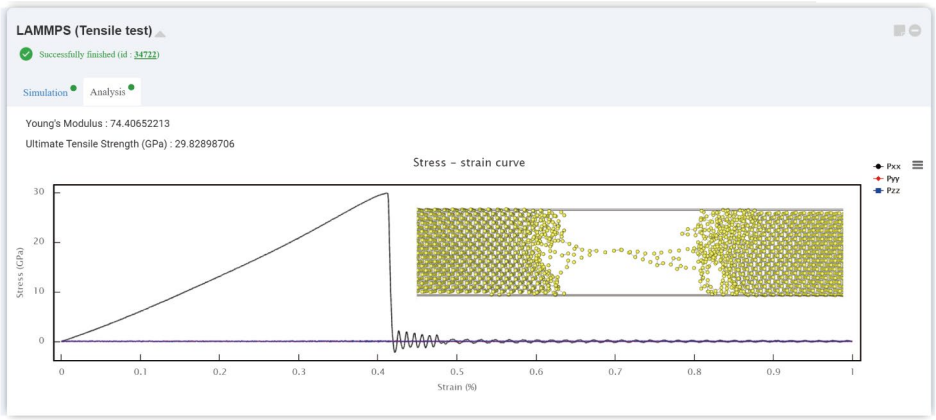


Available Properties

Trajectory Analysis

Trajectory Movie
MSD, RDF, ADF,
Molecular Counting

Energetics

Kinetic/Potential Energy
Temperature Profile

Cascade Simulation

Antisite Counting

Thermal Conductivity

Lattice Thermal Condcutivity
Heat Flux

Equation of States

Bulk Modulus

Dislocation Simulation

Structure Analysis
Stress-strain Curve

Tensile Test

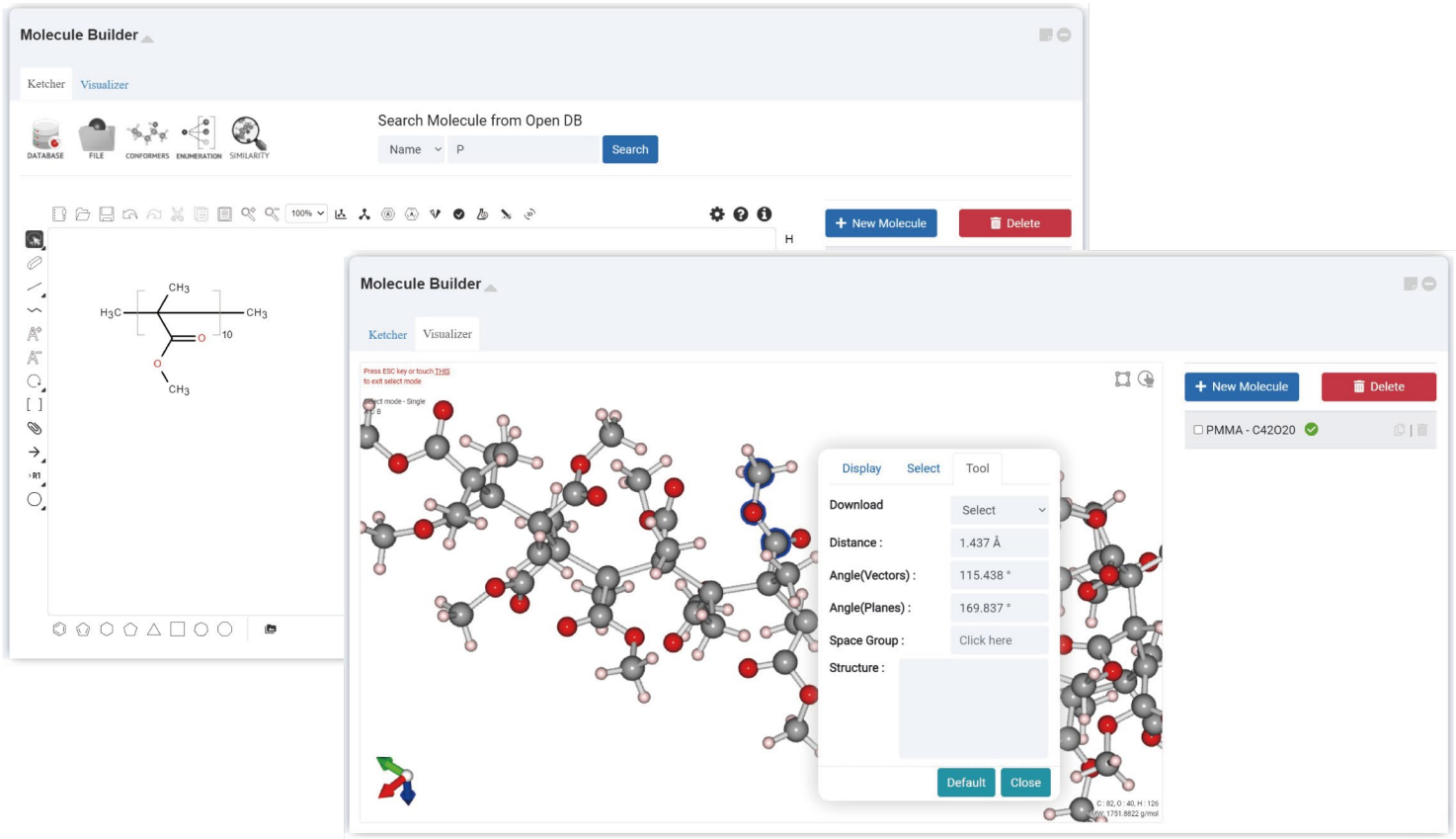
Stress-strain Curve
Young' Modulus
Ultimate Tensile Strength

Melting/Quenching

Custom LAMMPS Input

Modeling FREE

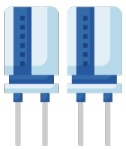
'Molecule builder' is a powerful, intuitive and engaging molecule modeling tool.
You can easily draw molecule using ketcher and convert the structure to the 3D model.



Applications

Catalyst

- Development of organic/inorganic catalyst
- Calculation of catalytic effect
- Refining high efficiency process technology

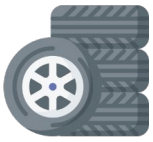


Conducting Materials

- Solid-state battery electrolytes
- Battery charge capacity / Voltage / Speed
- Design highly-efficient solar cell
- Capacitors

Display

- Electronic device transparent electrode
- OLED and QD display materials
- Stability of thermal stress



Elastomer

- Design new rubber materials
- Elastomer nanocomposite
- Thermal stability
- Prediction of mechanical properties

Plastic

- Optimization of various compounds
- Biodegradable polymer materials
- Calculation of polymer properties

DFT Density Functional Theory

MatSQ Chemistry DFT

GUI for GAMESS

GAMESS for DFT simulation is provided with fully optimized calculation parameters and various pre/post-processing modules.

Simulation on the Cloud

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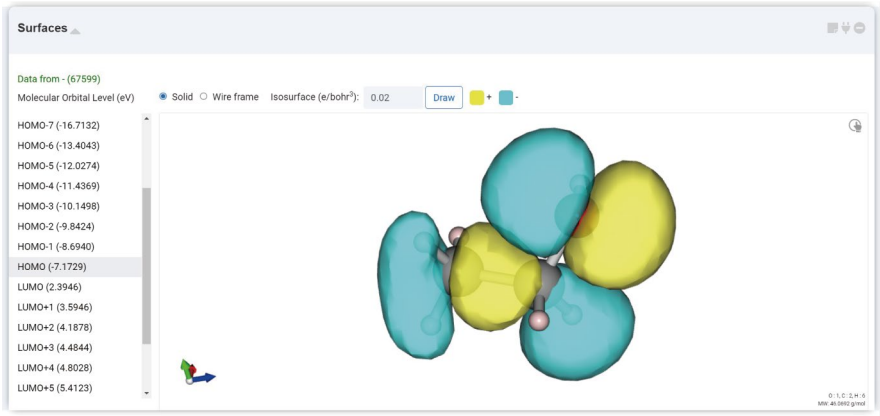

Available Properties

Structural Relaxation

Analysis

Molecular Orbitals Surfaces(HOMO, LUMO, ...)
Charge Population(Mulliken/Lowdin)
Valence Analysis
Bond Order Analysis
Density of States

Vibrational Calculation

IR Intensity
Raman Spectrum

Optical Properties

TDDFT Calculation
UV/Vis Spectrum

Bond Dissociation Energy

Nudged Elastic Band

Intrinsic Reaction Coordinates

MD Classical Molecular Dynamics

MatSQ Chemistry MD

GUI for LAMMPS

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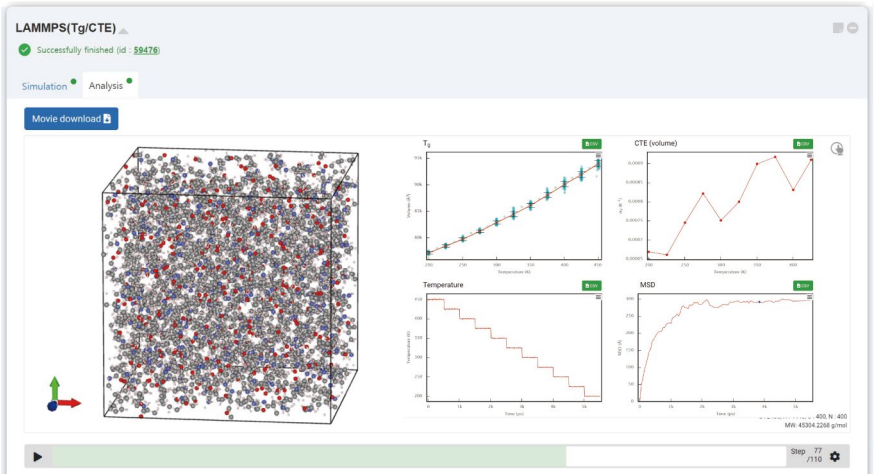


Available Properties

Structural Relaxation(Thermalization)

Analysis

Trajectory Movie
MSD, RDF, ADF

Glass Transition Temperature

Glass Transition Temperature
Thermal Expansion Coefficient

Viscosity

Elastic Properties

Bulk/Young's Modulus
Shear Modulus
Poisson Ratio

Dielectric Constant

Solubility Parameter

Melting/Boiling Point

Vapor Pressure

CALPHAD

Database on the Cloud

We provide several types of thermodynamic database on the cloud. Database is constantly updated.

Pay per Phase Diagram

The price depends on the database you use.
Prices per phase diagram range from $0.01 to $2.

List-Equilibrium

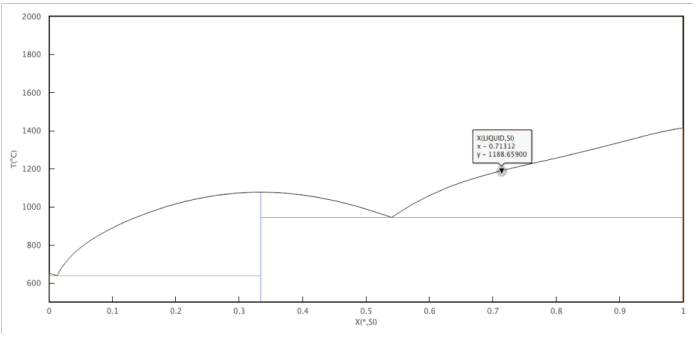
You can calculate the information of each phase according to the temperature condition.

```
Some global data, reference state SER .....:
T=  973.15 K (  700.00 C), P=  1.0000E+05 Pa, V=  3.8131E-06 m3
N=  1.0000E+00 moles, B=  4.8138E+01 g, RT=  8.0913E+03 J/mol
GS= -6.17034E+04 J, GS/N= -6.1703E+04 J/mol, HS=  1.6853E+03 J, S=  651.377 J/K

Some data for components .....:
Component name   Moles     Mole-fr  Chem.pot/RT  Activities  Ref.state
CR             1.8516E-01  0.18516 -7.0852E+00  8.3738E-04  SER (default)
FE             5.1717E-01  0.51717 -5.1354E+00  5.8848E-03  SER (default)
MN             4.3811E-02  0.04381 -9.3274E+00  8.8950E-05  SER (default)
N              1.7183E-01  0.17183 -1.4975E+01  3.1379E-07  SER (default)
NI             8.2020E-02  0.08202 -8.2461E+00  2.6229E-04  SER (default)
```

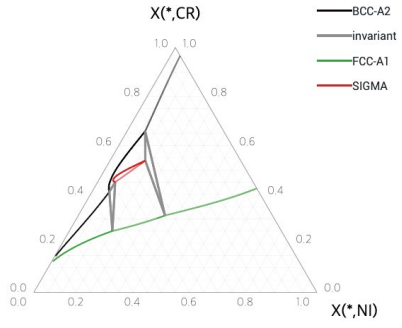
Binary Phase Diagram

You can calculate the phase diagram between two elements.



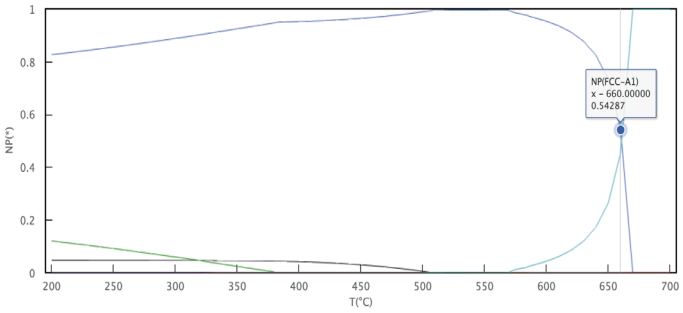
Ternary Phase Diagram

You can calculate the phase diagram between three elements.



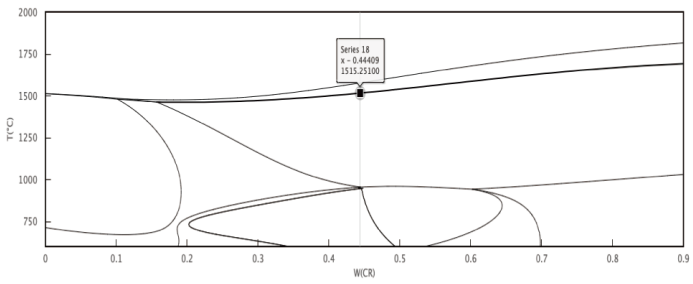
Multi-Component Phase Diagram

You can calculate each phase information of the micro-structure of alloy with various elements added according to the temperature.



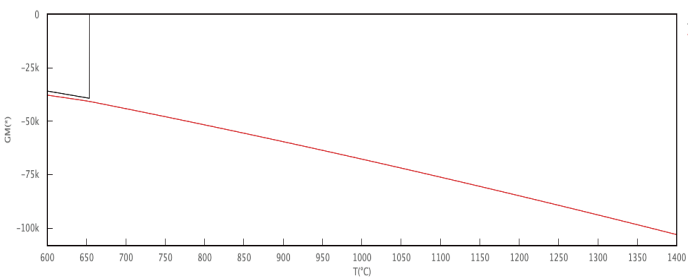
User-Defined Diagram

You can calculate the phase information of alloy according to the custom settings.



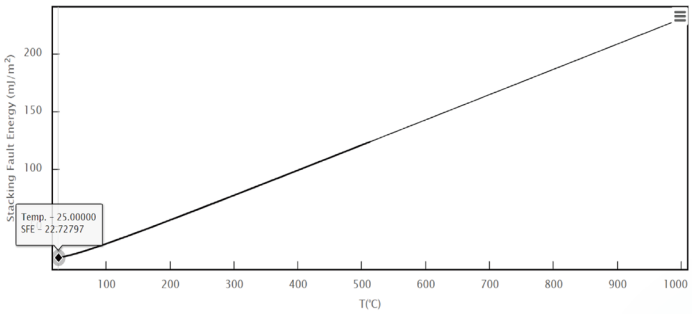
Function Diagram

You can calculate energy function(G, H, S, activity, etc) according to the temperature of composition.



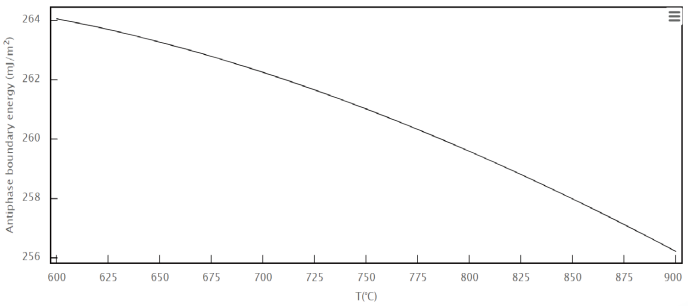
Stacking Fault Energy

You can obtain stacking fault energy only for both austenite steels and Ni-base alloys.



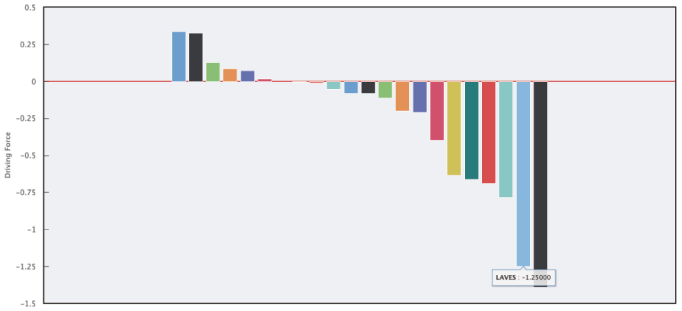
Antiphase Boundary Energy

You can obtain antiphase boundary energy only for Ni-base alloys involving Ni_3Al precipitations.

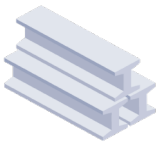


Driving Force

From the matrix phase, you can calculate driving force that represents the degree of appearance of other phases.



Applications



Alloy Design

- Composition-microstructure relation
- Origin of mechanical properties
- Quantification of microstructural factors

Manufacturing Process

- Optimization of heat treatment
- Prediction of mechanical properties
- Martensitic transition

Price

MatSQ CALPHAD

Academy DB — $0.01

Binary System

Thermodynamics information for several binary sytems

Fe-Cr-Mo-Si-V-C System

Thermodynamics information for steel systems (Fe-Cr-Mo-Si-V-C)

Commercial DB — $1.00

MatSQ AL 1.0

Commercial data for Al-base systems

MatSQ HEA 1.0

Commercial HEA databas for Co-Cr-Fe-Mn-Ni-V systems

Commercial DB — $2.00

MatSQ Ni 2.0

Commercial database for Ni-base systems

MatSQ FE 2.0

Commercial database for Fe-base systems(Including Co, Cu, and W)