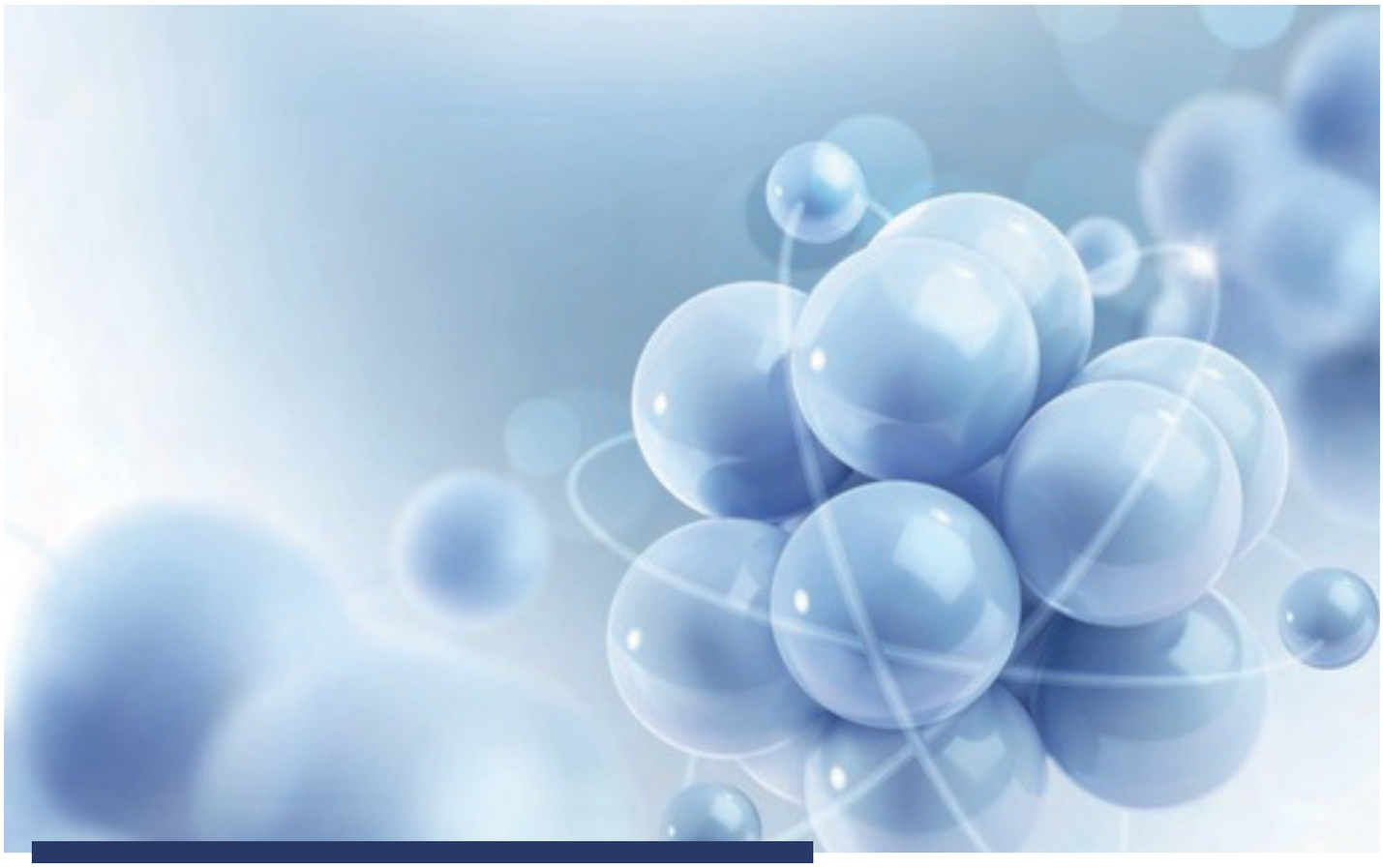
Scientific Research on the Cloud

materials square

www.matsq.com



Everything is on the Cloud

Cutting-Edge Materials Simulation Techniques

Materials Square provides
strictly verified materials research tools
with intuitive user interfaces
Enjoy high-end simulation/ML tools
without any concerns

Professional Consulting & Technical Support

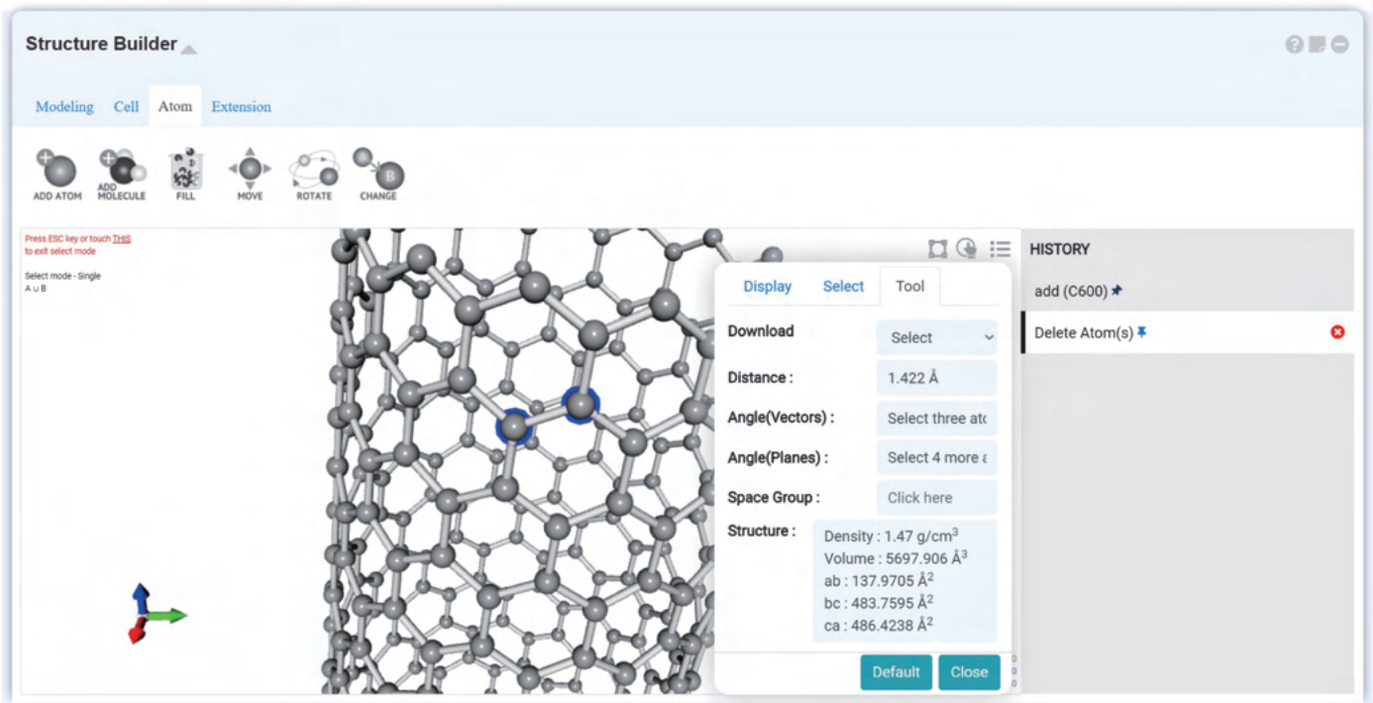
If you need R&D support,
Materials Square's professional
researcher pool is ready for support

High Performance Computer

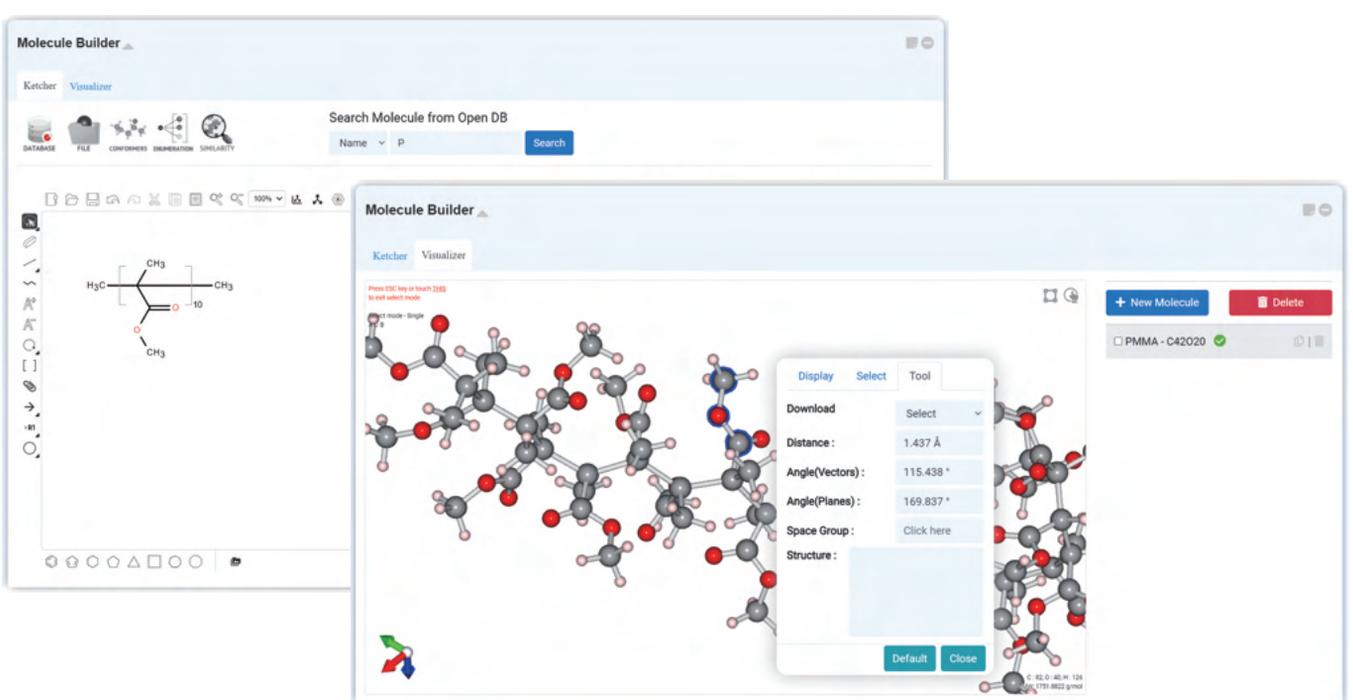
Cloud HPCs are provided as
"pay-as-you-go" pricing model.
Improve your R&D cost efficiency
with Materials Square!

Modeling

Materials Square provides "Molecule Builder" and "Structure Builder" to aid with simulation modeling. Anyone can create structures at the molecular, crystalline, and amorphous levels efficiently and easily.



Manipulator



2 Materials

Applications of Materials Research

Battery

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

Structual Materials

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

Tools of Materials Research

DFT Density Functional Theory

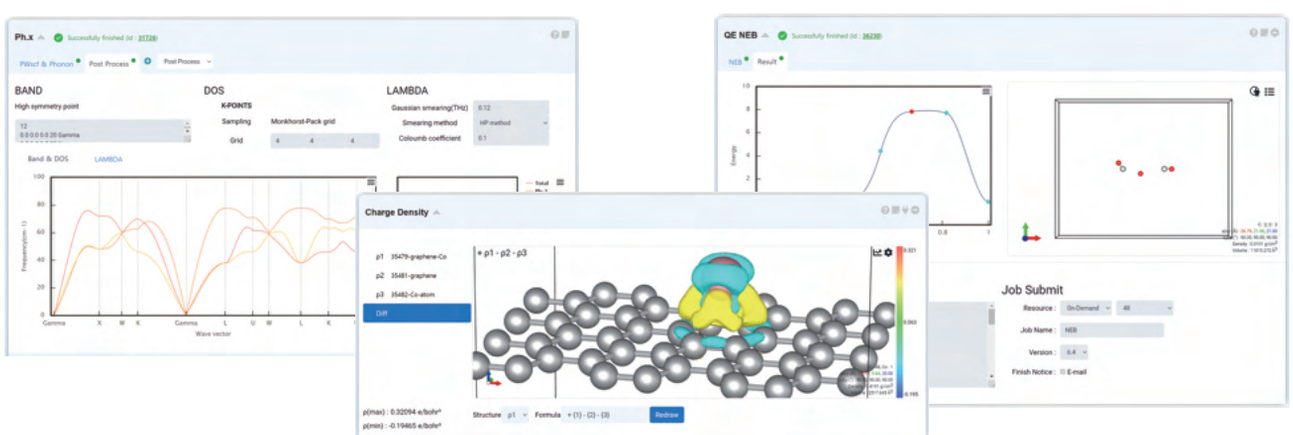
MatSQ Materials DFT

QUANTUMESPRESSO

GUI for Quantum ESPRESSO

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

Calculation Examples



Available Properties

Structual 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

Solar Cell

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

Display

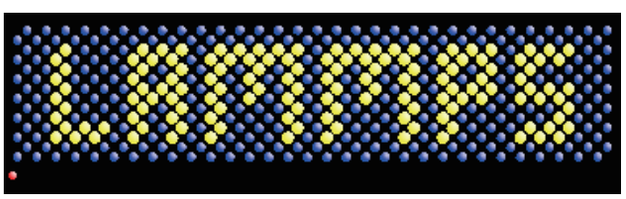
- OLED and QD Display
- Stability under thermal stress
- Verify origins of failure

Semiconductor

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

MD Classical Molecular Dynamics

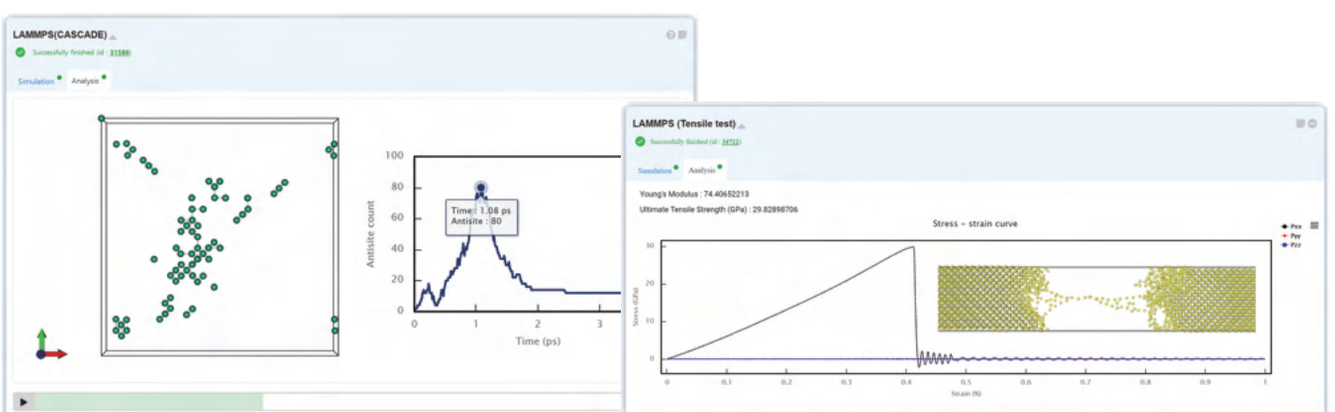
MatSQ Materials MD



GUI for LAMMPS

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

Calculation Examples



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

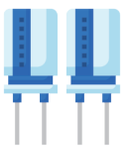
Melting/Quenching

Custom LAMMPS Input

Applications of Chemistry

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

Tools for Chemistry

DFT Density Functional Theory

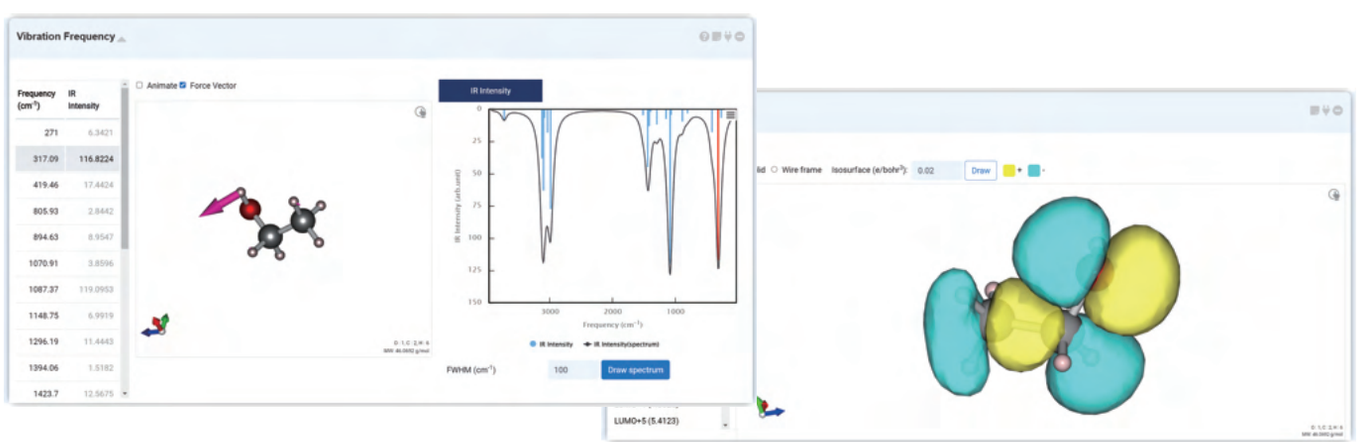
MatSQ Chemistry DFT

GAMESS

GUI for GAMESS

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

Calculation Examples



Available Properties

Structual 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

Display

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

Elastomer

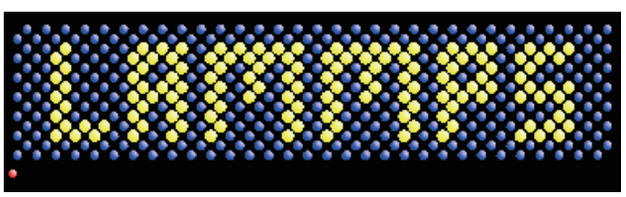
- Design new rubber materials
- Elastomer nanocomposite
- Thermal stability
- Prediction of mechanical properties

Plastic

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

MD Classical Molecular Dynamics

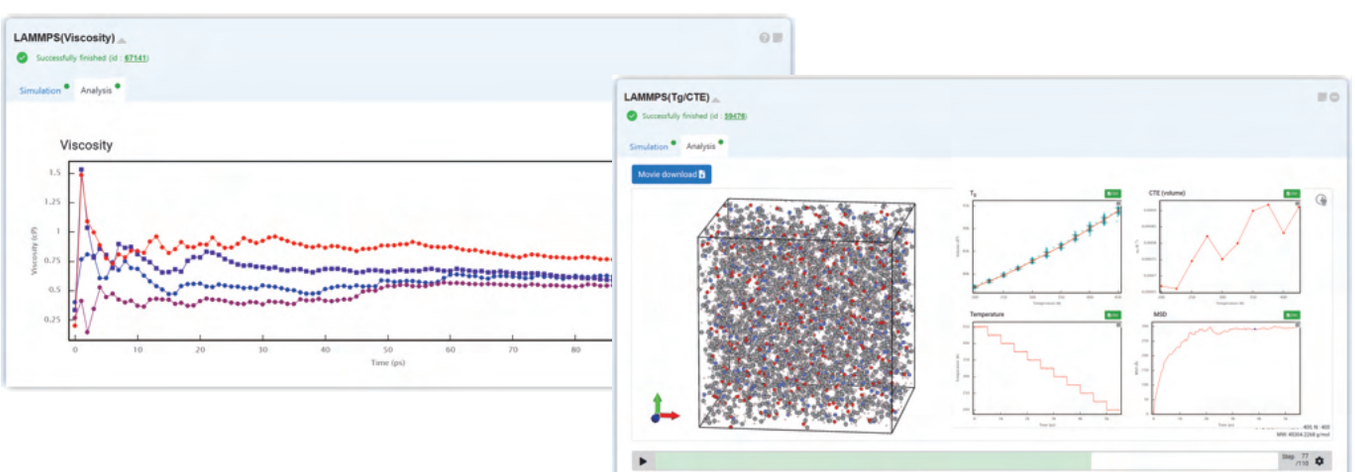
MatSQ Materials MD



GUI for LAMMPS

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

Calculation Examples



Available Properties

Structual 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

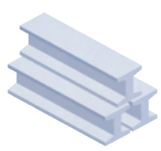
Dielectric Constant

Solubility Parameter

Melting/Boiling Point

Vapor Pressure

Applications of CALPHAD



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

CALPHAD

Database on the Cloud

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

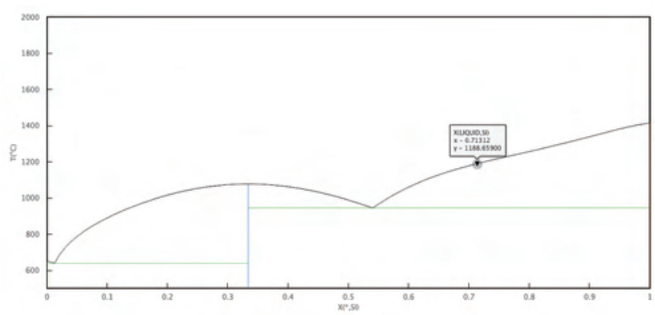
Pay per Phase Diagram

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

Calculation Examples of Chemistry

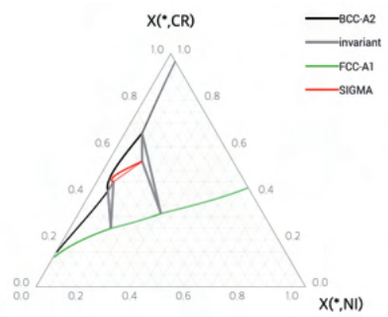
Binary Phase Diagram

You can calculate the phase diagram between two elements.



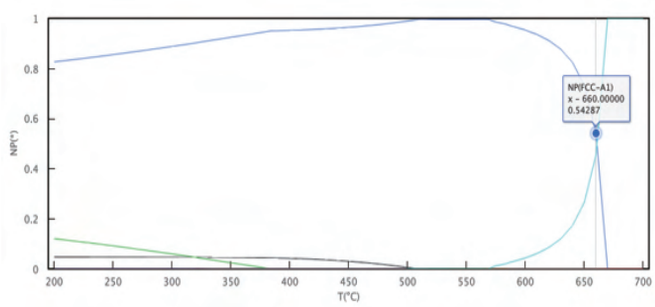
Ternary Phase Diagram

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.



Calculation Examples of Chemistry (Cont.)

List-Equilibrium

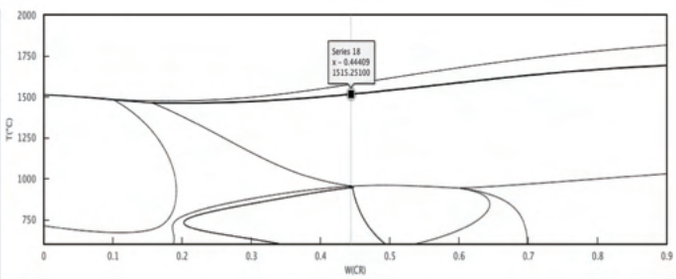
You can calculate the information of each phase according to the temperature condition.

```
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)
```

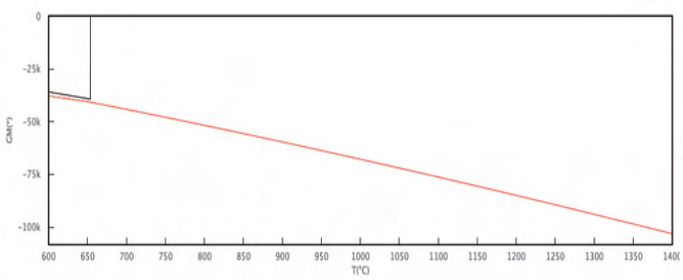
User-Defined Diagram

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



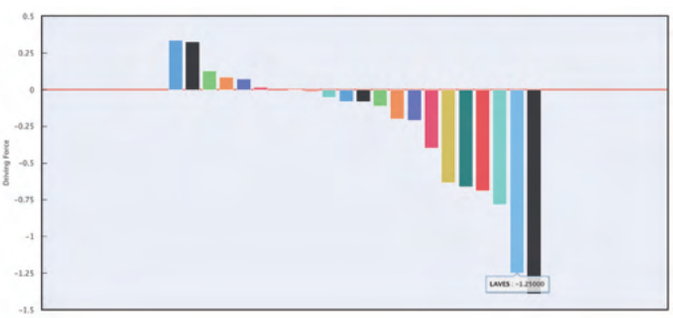
Function Diagram

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



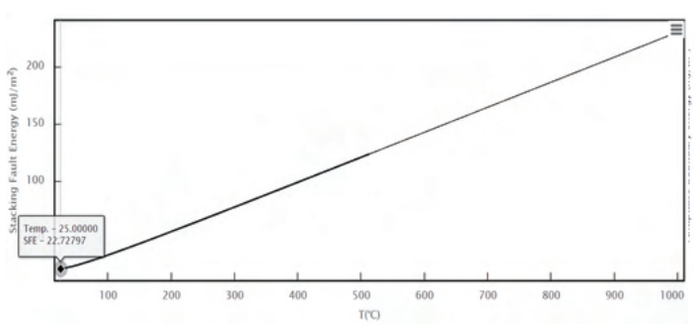
Driving Force

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



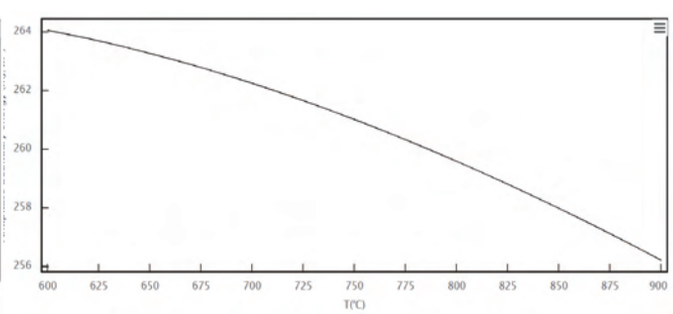
Stacking Fault Energy

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.



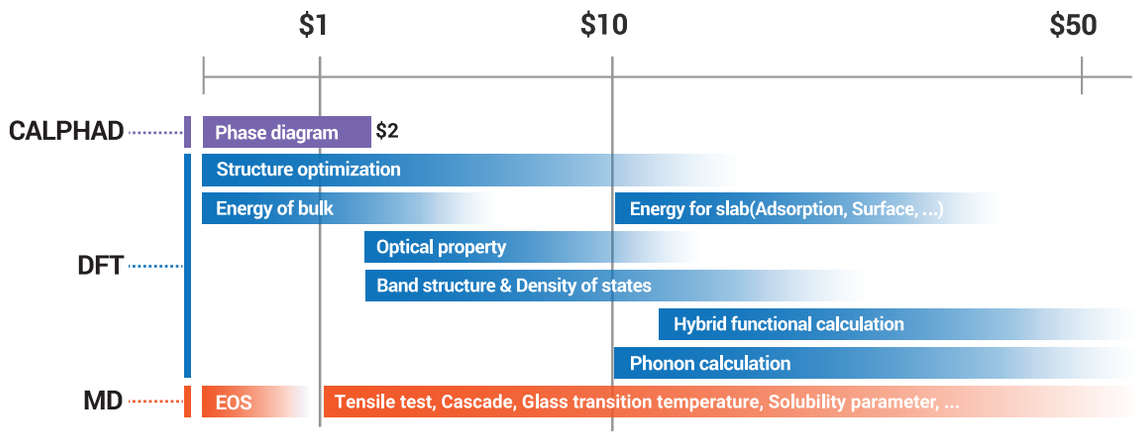
5 Pricing

Price (DFT/MD)

MatSQ Pricing

HPC : Pay-as-you-go

$0.25 per core hour



※ Bulk Purchasing Option : Atom Pack

Bundle Package - Atom Pack

Buy Atom Pack and get a discount up to 50%!

Atom Pack I	Atom Pack II	Atom Pack III	Atom Pack IV	Atom Pack V
$1,000	$2,000	$3,000	$4,000	$5,000
10% OFF	20% OFF	30% OFF	40% OFF	50% OFF
~~4,000~~ 4,430 cpu hour	~~8,000~~ 10,000 cpu hour	~~12,000~~ 17,142 cpu hour	~~16,000~~ 26,666 cpu hour	~~20,000~~ 40,000 cpu hour

If you are not sure about the HPC usage, subscription plan is ready

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

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

Database : Pay-per-use

MatSQ CALPHAD

Academy DB $0.01	Commercial DB $1.00	Commercial DB $2.00
Binary System Thermodynamics information for several binary sytems	**MatSQ AL 1.0** Commercial data for Al-base systems	**MatSQ Ni 2.0** Commercial database for Ni-base systems
Fe-Cr-Mo-Si-V-C System Thermodynamics information for steel systems (Fe-Cr-Mo-Si-V-C)	**MatSQ HEA 1.0** Commercial HEA database for Co-Cr-Fe-Mn-Ni-V systems	**MatSQ FE 2.0** Commercial database for Fe-base systems(Including Co, Cu, and W)

Storage : Amount/mo.

100GiB	500GiB	1TiB	2TiB	5TiB
Free	$ 20	$ 40	$ 72 ~~$ 80~~ 10% OFF	$ 170 ~~$ 200~~ 15% OFF

We provide the FREE Storage up to 100GiB.
Please subscribe to the Storage plan, if you desire to maintain data more than 100GiB.

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