AI Driven
Innovation & Quality

neotrident®

About Neotrident Technology

Neotrident Technology has been focusing on the field of material science research and development for more than 20 years. Through the innovative application of cloud computing, mobile Internet and scientific artificial intelligence technology,Neotrident Technology helps enterprises and innovative scientific research institutions to quickly carry out digital transformation of research and development and realize intelligent innovation.

Neotrident Technology possesses industry-leading comprehensive mobile Internet solutions, spanning from digital research and development to intelligent innovation. These include the iLabPower research and quality digitalization platform (covering the entire R&D process and quality testing), the SDH Scientific Data Genomics Platform, and the MaXFlow Scientific Artificial Intelligence Innovation Platform.

Neotrident Technology has over a thousand users and is currently serving tens of thousands of China's tech elites, renowned research institutions, and universities, as well as world-leading defense contractors, top-ranking petrochemical companies, and star enterprises in material innovation. These entities are all utilizing Neotrident Technology's digital R&D and intelligent innovation platforms to realize their core strategic plans for intelligent innovation.

Intelligent innovation drives excellent quality.
Based on cloud computing and artificial intelligence

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MaXFlow

CATALOGUE

Introduction of MaXFlow

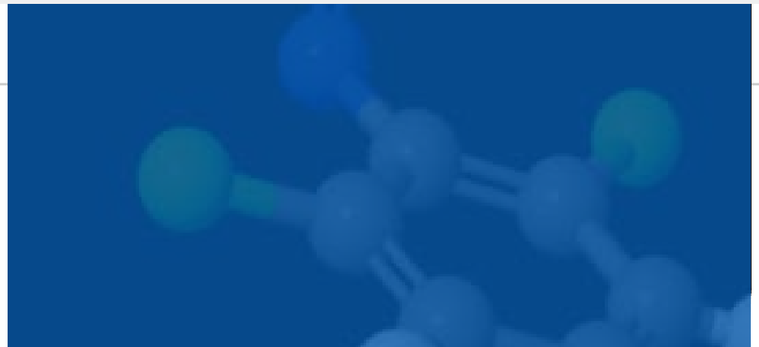
MaXFlow is a new generation of scientific molecular simulation and artificial intelligence innovation platform for new material design and research and development [1]. MaXFlow is independently developed by Changteng Technology, for all front-line innovative experimental scientists, molecular simulation and artificial intelligence experts, covering multiple research and development fields such as innovation discovery and process development.

MaXFlow platform is based on Browser-Server architecture, which integrates molecular simulation, artificial intelligence and new generation workflow technology. It can mine and visualize massive material data, extract and summarize the relationship between composition, process, structure and performance of materials, and realize knowledge sharing. Vigorously promote the development and design of new materials and new processes.

The MaXFlow platform enables AI experts to quickly build, optimize, and validate AI prediction models for different research scales for innovation needs. Artificial intelligence experts can also publish these prediction models as research results to MaXFlow's unique "APP resource square", so that front-line innovative experimental scientists can use these results to more accurately grasp the direction of innovation, more quickly improve innovation efficiency and ability, and highlight the core value of artificial intelligence experts in the innovation process.

The unique "APP release" function of MaXFlow platform can transform various complex and tedious processes of modeling , molecular simulation and multi-algorithm fusion into more easy to operate automated "applications" (APPs). It is convenient for experimental scientists to build the microstructure of various materials, establish a high-throughput virtual screening library, and quickly predict and analyze the physical and chemical properties of various materials without barriers. Realize the perfect combination of molecular simulation + artificial intelligence technology, experiment and production.

[1]MaXFlow has independent intellectual property rights and adopts two modes: Saas service and local deployment.



MaXFlow Function

一、MaXFlow workbench

The main screen of the entire platform and calls it the "workbench". It can realize the management of all kinds of files, such as preview and simple processing of data files. It can also realize the convenient call to the three main functions of model construction, workflow and APP.

■ Features of the workbench:

·My Workflow: View and manage workflows to create, edit, rename, clone, share, pre-publish, and delete workflows.

·My data: To view and manage all kinds of data, data types include: structure, table, image, sequence files and datasets; Management operations: Create new structure/table, edit, rename, clone, download, share, delete.

·My APPs: View and manage APPs published and downloaded by users, complete APP usage, editing workflow, pre-release editing, APP release, deletion and unrelease of published apps.

·Task list: View and manage the running information (task name, APP name, submission time, used resources, end time, running status), calculation files and calculation results of App calculation tasks.

·Shared data: The view and extraction of shared data within an organization, including data types: structures,tables, images, sequence files, and workflows.

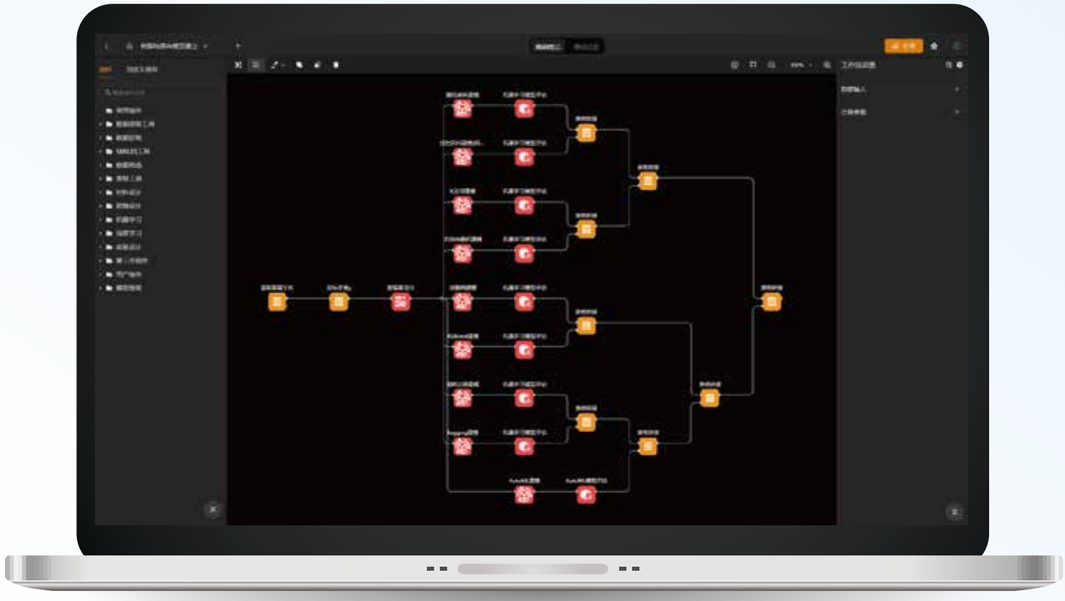
·Sample data: The data provided by Chuangteng for user reference and use, data types include: structure, table, picture, sequence file and workflow; 1200 different types of sample data are provided so far.

·Recycle Bin: Recycle bin holds files deleted within 7 days.

Workbench of MaXFlow

二、Workflow

Workflow is one of the core engines of MaXFlow platform. The advantage of running computing based on workflow is that it can automatically complete multi-step computing tasks, which can further help users to realize intelligent and integrated computing work. The MaXFlow platform encapsulates various algorithms as components, provides a component library with rich functions, and allows users to add custom functional components according to specific research needs. In the visual interface, users can drag and drop components on demand to build workflows, so as to flexibly and automatically execute various tasks from simple to complex molecular simulation, artificial intelligence, experimental design, and different algorithm mixing.



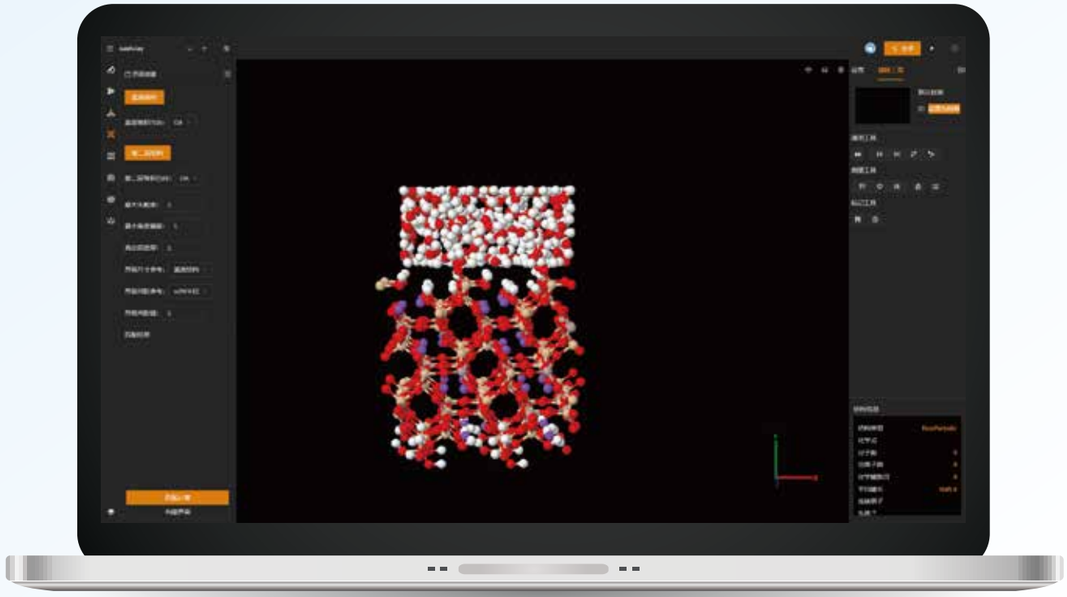
Edit workflow

三、Construction of Materials' microstructure

MaXFlow platform provides two ways of "crystal and molecule" visual interface and model building function components to build material microstructure.

■"Crystals and Molecules"visual interface

The "Crystal and Molecule" visual interface can be used for online material microstructure construction and visual editing, and the constructed structures can be used by various computing components of the MaXFlow platform.



MaXFlow platform "crystal and molecular" visual interface

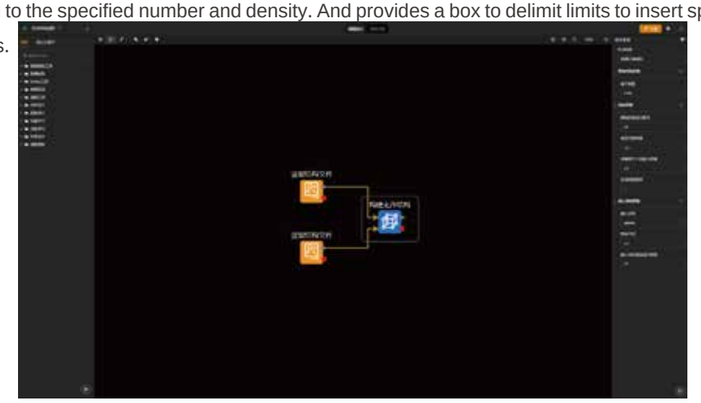
"Crystals and Molecules"visual interface function including:

Small molecule construction	·Add atoms, bonds ·Chemical bond editing ·Drawing ring structures ·Adding snippets ·Saturation of hydrogenation ·Preliminary optimization of the structure MMFF/ETDG
Polymer construction	·Construct homopolymer, block polymer and random polymer ·Custom repeat units ·Setting of components and proportions
Unordered structure construction	·System density setting ·Box type and size setting ·Set the number of generated structures
Crystal structure construction	·According to the space group, unit cell parameters and atomic coordinates, the crystal structure is built ·Construct the superunit cell ·Redefine the lattice ·Symmetry exploration ·Conversion of primitive cells ·Make P1
Surface / interface structure construction	·The surface is cut according to the face index, atomic layer thickness, and vacuum layer thickness ·Generate multiple possible surface structures ·Multiple possible interface structures satisfying the mismatch rate setting are output ·Construction of solid-liquid interface, liquid-liquid interface and other interface models
Nanotube construction	·The nanotube structure is generated
Model visualization	·Support dot line, stick, ball and stick, CPK, stick, cartoon display mode ·Support for color adjustment ·Supports the rotation and translation of the model ·Supports displaying various types of information about the current structure ·Support group definition, define atom, Angle, distance, dihedral Angle ·Support information tags, atom names, skeleton molecules ·Support bond length, bond Angle, dihedral Angle measurement
Structure file management	·File retrieval can be carried out according to structure type, structure label and modification time ·Preview structure files ·Global search for keywords is supported
Input and output file formats	·Supports the import of structure files in mol, mol2, cif, xsd, pdb, smiles and other formats ·Supports the export of structure files in cif, molV2000, molV3000, pdb, sdf and other formats

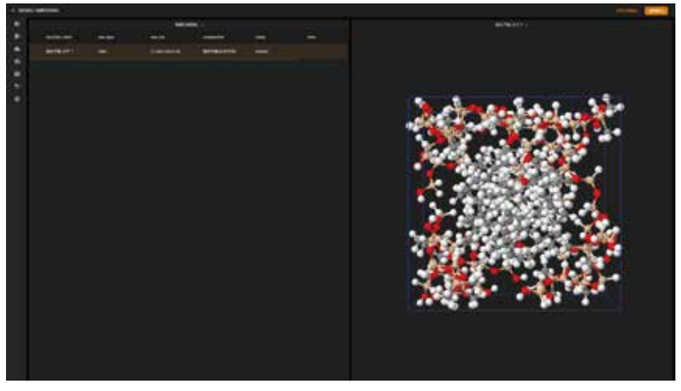
■ Models build functional components

Disorder Model

For the construction of complex and amorphous system model, MaXFlow can directly call the structure data read component, construct the disordered structure component, and pile all kinds of ions and molecules into the model according to the specified number and density. And provides a box to delimit limits to insert spheres, cylinders, and fill in molecules.



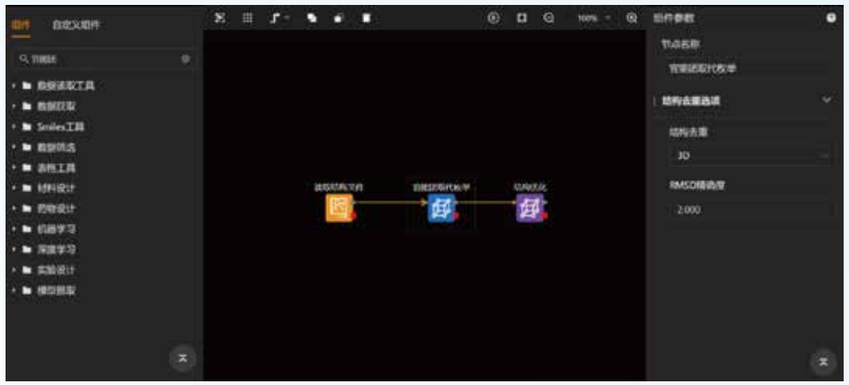
complex disorder build workflow model



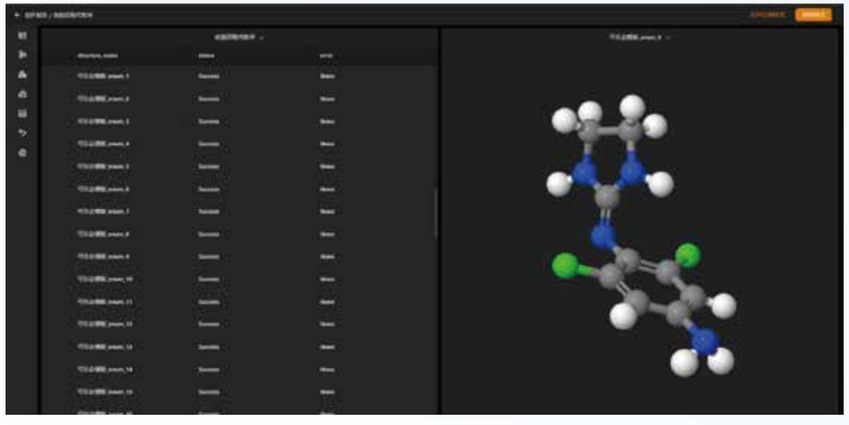
Results of complex disorder model

high-throughput Virtual molecular Enumeration

In order to discover potential active compounds, it is necessary to have a large compound structure database, and few databases are directly available at present. The MaXFlow platform provides a functional group substitution enumeration component, which can be called to perform functional group substitution enumeration based on the defined fragment molecules and their connection points, quickly generate a large number of compound structure models, and help users to efficiently complete the construction of high-throughput virtual library.



Functional group substitution enumeration workflow



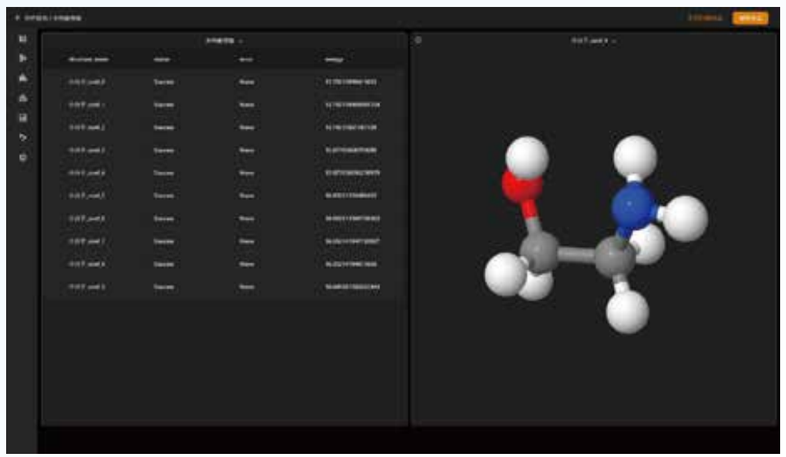
Functional group substitution enumeration results

MaXFlow

Multi-conformation search

According to the provided 3D structure, multiple spatial isomers are generated, and a certain number of reasonable structures are obtained by energy minimization optimization. The multi-conformation search component supports conformational optimization of molecules using MMFF and UFF force fields.

Multi-conformation Search workflow

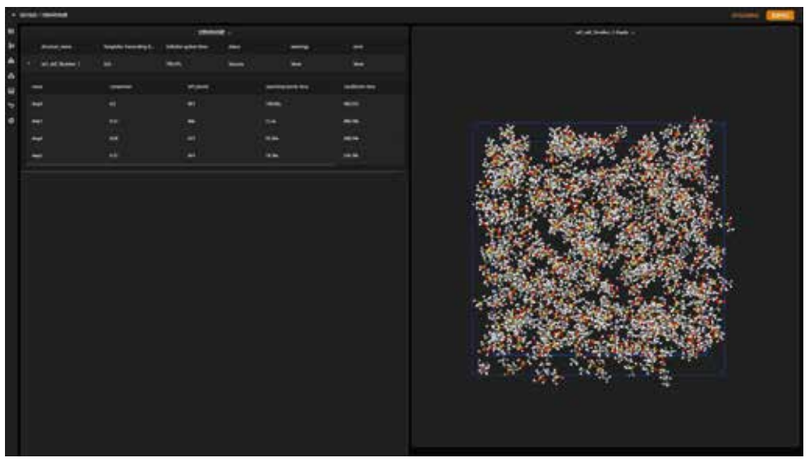


Display of multi-conformation search results

cross-linked structures

The excellent performance of thermosetting resin is attributed to its special wireless cross-linked 3D network structure and uncertain repeating units. However, its cross-linked molecular structure is very complex, and it is very challenging to quickly and reasonably construct cross-linked resin molecular models. The MaXFlow platform provides a cross-linking structure construction component, which can obtain cross-linking models under different cross-linking degrees according to the set cross-linking reaction mechanism based on molecules with specified reaction sites.

Cross-link structure building workflow



Cross-linked structure construction results

四、Molecular simulation

At present, the simulation engine of MaXFlow platform includes general simulation engine components based on quantum mechanics and molecular mechanics and molecular dynamics, which realizes the visualization of simulation parameters. Users do not need to prepare input files in advance, and can directly set parameters in the graphical interface, avoiding tedious operations. The simulation calculation function components of different methods can be seamlessly connected, combined with the visual interface and report interface of the MaXFlow platform, the process of model construction, calculation simulation and operation results output and view can be quickly realized, and the overall
scientific research efficiency of users can be greatly improved

Quantum mechanical method

Quantum Mechanics is a method that can study the electronic structure characteristics of materials. It has high accuracy and almost does not depend on any empirical parameters, so it is widely used in the simulation of various materials. Based on the stationary Schrodinger equation, the quantum mechanics method calculates the space and energy distribution of electrons outside the core when the nucleus meets a specific arrangement and packing, and further obtains the electrical, magnetic, optical, thermodynamic and mechanical properties of the system. The types of material systems that can be studied include: Various types of crystalline materials and possible defect structures, various dimensions of nanomaterials, various molecular and cluster materials.

♦ Structure optimization

It optimizes atomic coordinates, unit cell shape and size, supports GDIIS using quasi-Newton BFGS conditions, supports conjugate gradient, preconditioned conjugate gradient method PCG, BFGS quasi-Newton method, supports finite-memory BFGS, steepest descent method, FIRE, and projection velocity Verlet algorithm. Support to turn on or off space symmetry, time reversal symmetry.

♦ Single point energy calculation

Calculate the energy value of the system.

♦ Density of states analysis

Total density of states, sub-wave density of states, local density of states, Fermi level value.

♦ Band structure analysis

Band structure

♦ Phonon calculation

Infrared spectrum, Raman spectrum, phonon spectrum, phonon state density, eigenvector of each normal mode.

♦ Transition state search

Transition state search (Nudged Elastic Band-NEB method), reaction energy barrier, transition state structure

♦ Optical properties

Electron energy loss spectrum, virtual (real) part of dielectric function, solid permittivity, conductivity, refractive index, absorption coefficient, reflectance

♦ Mechanical properties

Elastic constant tensor, bulk modulus, shear modulus , Young's modulus, Poisson's ratio

♦ Electronic structure analysis

Orbital Occupancy, fatband band analysis

♦ Seebeck coefficient

Seebeck coefficient

♦ Electrostatic potential calculation

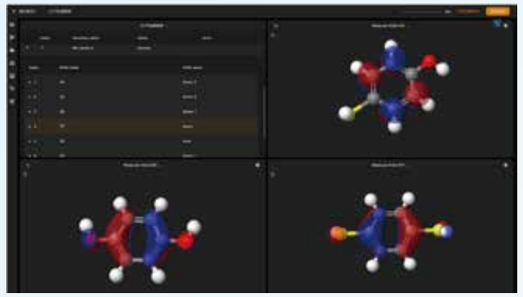
Calculate the electrostatic potential of the system.

♦ Frequency calculation

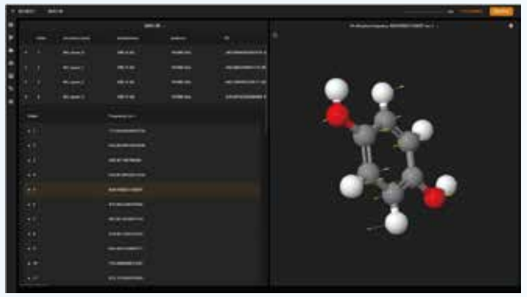
Thermodynamic properties calculation (entropy, enthalpy, Gibbs free energy, constant volume heat capacity, constant pressure heat capacity, zero point energy, etc.), simple harmonic vibration analysis, infrared spectroscopy (vibration frequency and intensity), Raman spectroscopy (vibration frequency and intensity).

♦ Molecular orbital view

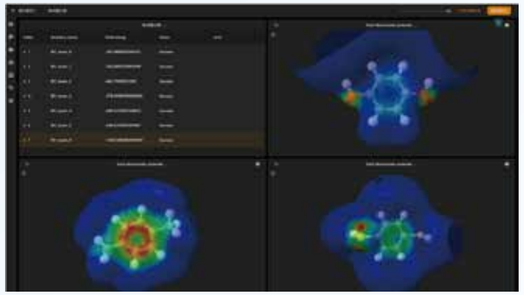
Calculation of electronic orbitals (e.g., HUMO, LUMO orbitals).



Molecular orbital calculation results



Frequency calculation results



electrostatic potential results

■ Classical simulation method

When the classical simulation method is only used to describe the various properties of a stationary state of the system, it is called Molecular Mechanics. When combined with Newton's equations of motion to describe the motion of nuclei under specific thermodynamic conditions, it is called Molecular Dynamics. The mixability, cohesive energy, wettability, mechanical properties, diffusion and barrier, surface and pore adsorption, various correlation functions and statistical averages of molecular properties can be obtained based on the results of molecular mechanics and dynamics. Of course , it is also possible to combine this description of microscopic particle interactions with Monte Carlo methods to build amorphous models, study molecular conformations, or search for possible adsorption sites.

■ TEAM Force field[1-6]

TEAM force field is the latest research results of Professor Sun Huai, a world-renowned force field expert from Shanghai Jiaotong University. The TEAM force field can be invoked by a variety of computational engines in the field of molecular simulation, such as GROMACS, LAMMPS, CHARMM or AMBER. Multiple force fields of the same group can be used jointly.. The valence parameters and charge parameters were obtained by fitting the energy data calculated by DFT (B3LYP/6-31G(d,p)), and the LJ parameters were obtained by fitting the experimental data of liquid state.

In MaXFlow, the TEAM force fields available to users are divided into two groups. The first group includes AMBER-General and AMBER-IonLiq, and the second group includes Team-Gen-eral, Team-Zeolite and Team-IonliQ. The former is based on AMber -like functions, At present, the two groups of force field support simulation systems are shown in the following table:

zeolit
ionic liquid
organic molecule, polymer
condensed nucleus, nitrile, nitro, positive ion, phosphate
hydrocarbon, aromatic hydrocarbon, alcohol, phenols, ehters, aldehydes, ketone, acides, esters
amide, anhydride, halogen(F, Cl, Br, I）,sulfate, sulfonate, mercaptan, sulfide, silane，siloxane

[1] Hierarchical atom type definitions and extensible all-atom force fields. Jin, Zhao; Yang, Chunwei; Cao, Fenglei; Li, Feng; Jing, Zhifeng; Chen, Long; Shen, Zhe; Xin, Liang; Tong, Sijia; Sun, Huai. J. Comput. Chem. 2016.

[2] On accuracy of predicting densities and solubility parameters of polymers using atomistic simulations. Wu, Liang; Chen, Long; Sun, Huai. Molecular Simulation 2017, 43, 510-518.

[3] Temperature Transferability of Force Field Parameters for Dispersion Interactions. Gong, Zheng; Sun, Huai; Eichinger, Bruce E. J. Chem. Theory Comput. 2018.

[4] Predicting Thermodynamic Properties of Alkanes by High-throughput Force Field Simulation and Machine Learning. Gong, Zheng; Wu, Yanze; Wu, Liang; Sun, Huai. J. Chem. Inf. Model. 2018

[5] Extension of TEAM Force-Field Database to Ionic Liquids. Zheng Gong and Huai Sun*. J. Chem. Eng. Data, 2019

[6] Pressure-viscosity relation of 2,2,4-trimethylhexane predicted using all-atom TEAM force field. Zheng Gong and Huai Sun*. Fluid Phase Equilibria 2019

The main functions of the implementation

♦ LMP_ Structure optimization

To optimize atomic coordinates and unit cell parameters, energy minimization algorithms include conjugate gradient (cg), steepest descent (steep), Newton-Larsen (nr), hftn (Hessian-free truncated Newton), quickmin, and fires.

♦ LMP_NVE、LMP_NVT、LMP_NPT、LMP_NPH

Based on Newton's equations of motion, the motion of nuclei under certain ensemble conditions is studied.

♦ LMP_Lannealing simulation

Based on the dynamic simulation of different temperature points, the repeated rising and cooling process of the system is realized, and the potential energy surface is scanned to find the optimal molecular conformation and interaction conformation.

♦ LMP_ Glass transition temperature prediction

The equilibrium molecular dynamics method was used to simulate the curve of the system density changing with temperature, and then the glass transition temperature was obtained. The density of the system at the same temperature is obtained by molecular dynamics calculations of first NVT and then NPT ensembles.

♦ LMP_Mechanical Property prediction

The mechanical property of the system: elastic modulus is calculated based on the dynamic trajectory file. Using equilibrium dynamics and non-equilibrium dynamics to calculate stress-strain curves, single multi-step stretching and cyclic multi-step stretching and compression processes can be completed. It supports custom XYZ different stretching directions and strain modes, and the strain mode supports global strain rate (scale), strain rate (erate and trate) and sinusoidal variation (wiggle).

♦ LMP_Reaction kinetics simulation

A simulation method combining the reactive force field ReaxFF with molecular dynamics to characterize dynamic chemical reaction processes.

♦ LMP_ Rheological property prediction

Based on the Green-Kubo (GK) formula, the equilibrium dynamics method (EDM) was used to calculate the viscosity of the system.

♦ LMP_thermal Conductivity Calculation (EMD)

Based on the Green-Kubo (GK) formula, the equilibrium dynamics method (EDM) was used to calculate the thermal conductivity of the system.

♦ LMP_Thermal Conductivity Calculation (NEMD)

The non-equilibrium dynamics method (NEMD) was used to calculate the thermal conductivity of the system.

♦ LMP_Analysis of structural properties

The changes of distance, Angle, dihedral Angle, density, volume, concentration, gyration radius, radial distribution function, structure factor/X-ray diffraction spectrum, cohesive energy density/solubility factor, interaction energy and other properties with time were analyzed.

♦ LMP_Analysis of thermodynamic properties

The Total Energy, Potential Energy, Kinectic Energy, Bond Energy, Angle Energy and Dihedral Energy were analyzed Energy), non-bonded interactions (Van der Waals Energy, Coulombic Energy), unit cell size and volume, temperature, pressure and its components, as a function of time.

♦ LMP_Kinetic properties analysis

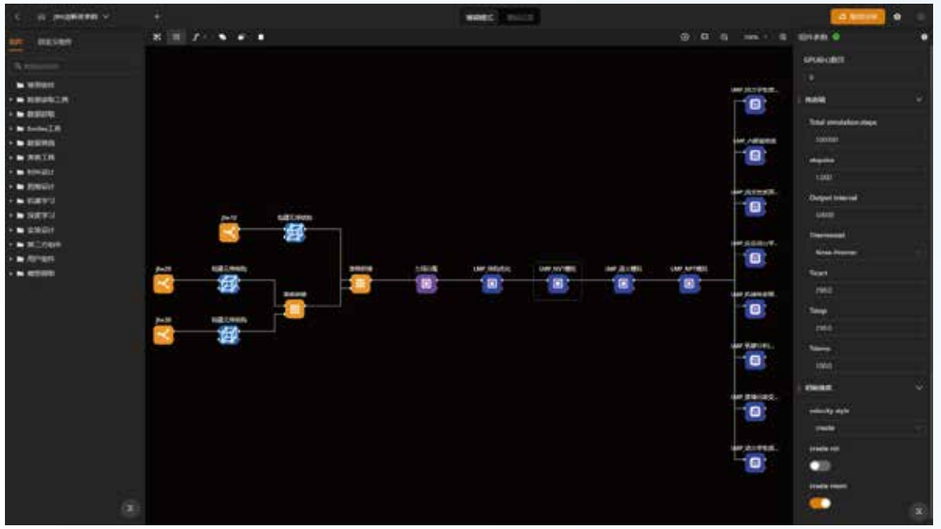
Dynamic autocorrelation functions, such as velocity autocorrelation functions and dipole autocorrelation functions, are analyzed.

♦ LMP_Hydrogen bond analysis

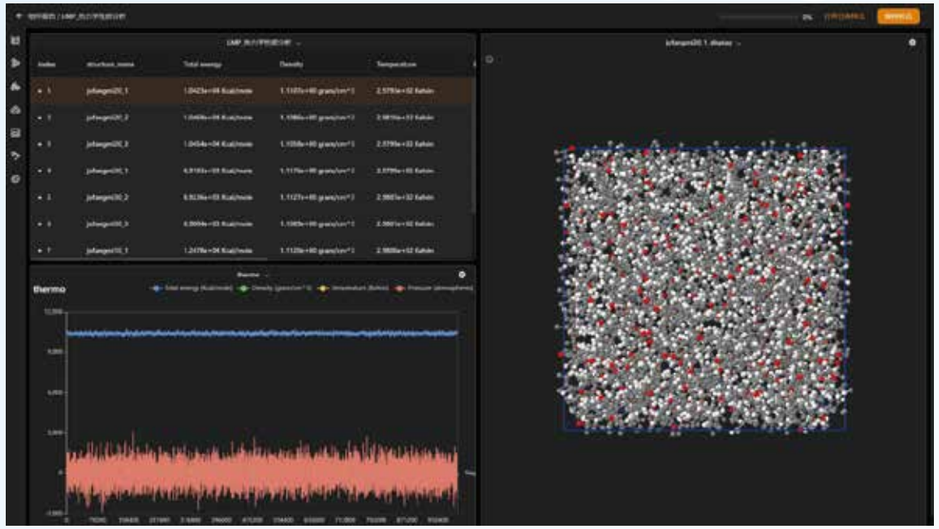
Analyze the hydrogen bonds in the structure and calculate the lifetime of each hydrogen bond

Features

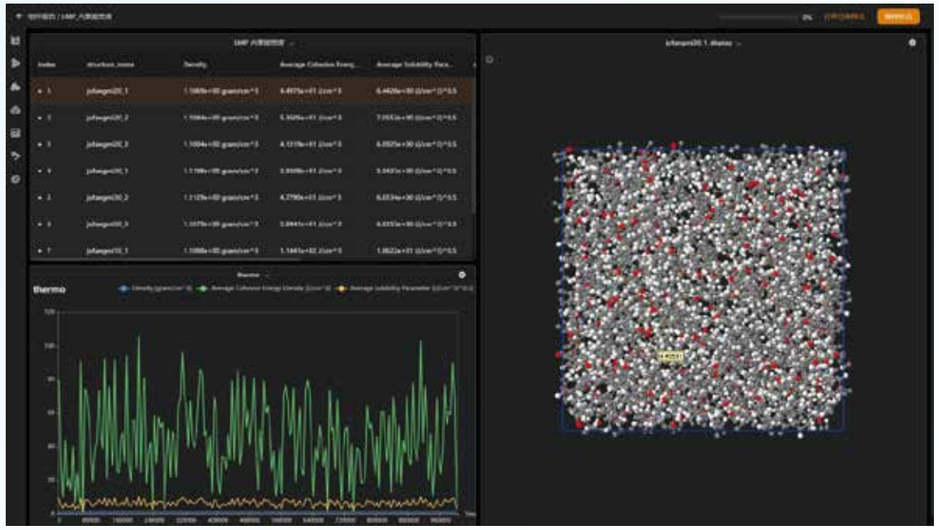
- Parallel computation is supported, using domain decomposition techniques with MPI parallelization to divide the simulation domain into small subdomains of equal computational cost, one of which is assigned to each processor to speed up the computation.
- Multiple augmented sampling algorithms are provided, including: parallel tempering, parallel replica dynamic, temperature accelerated dynamics, and simulated annealing.ture accelerated dynamics.
- Three polarizable models are supported, including: Drude dipole model, QEq, Core/shell model.



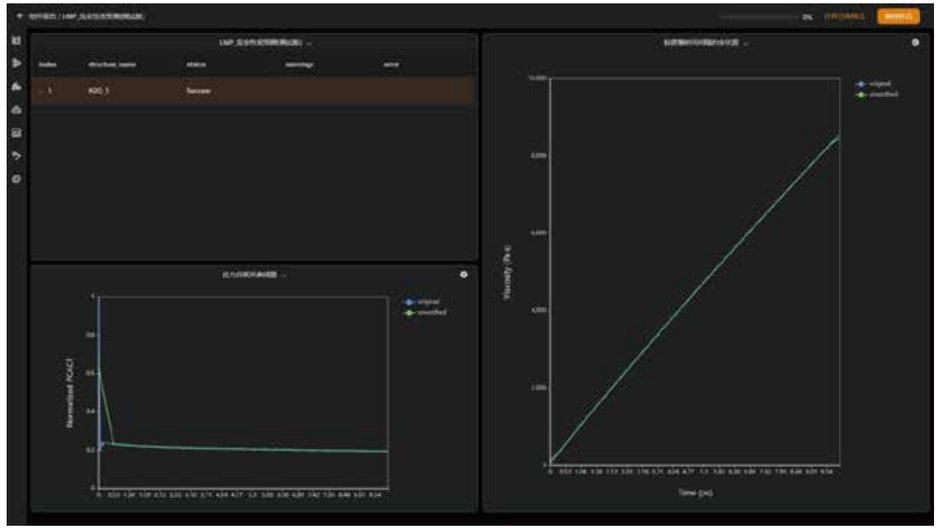
MaxFlow



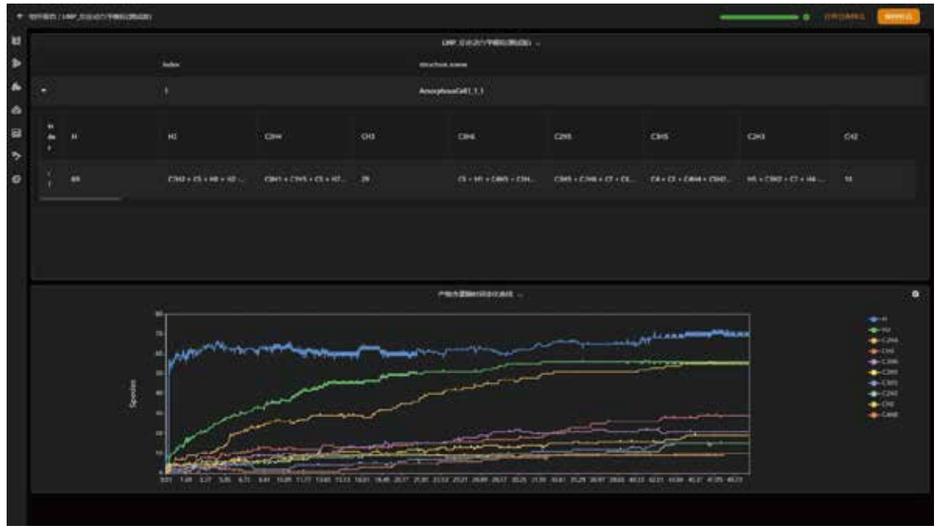
Thermodynamic properties calculation results



Calculation results of cohesive energy density and solubility parameters

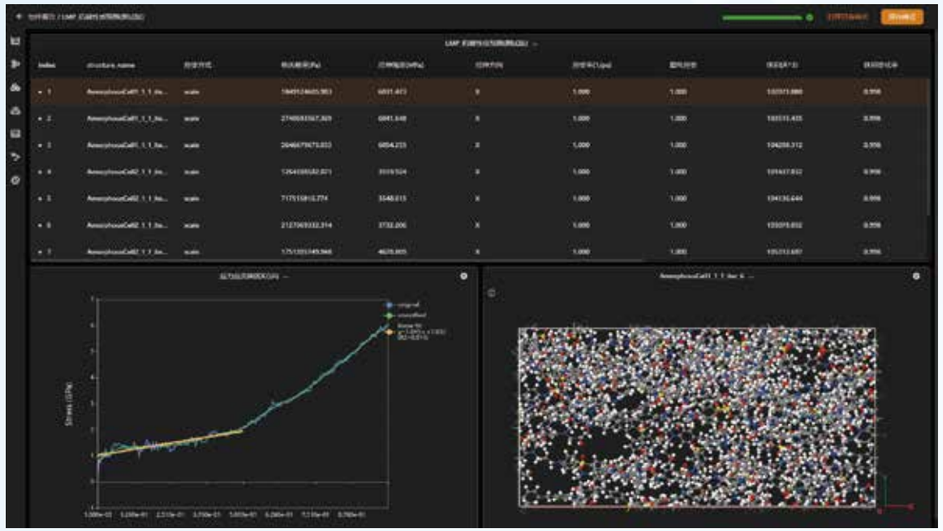


Viscosity calculation results



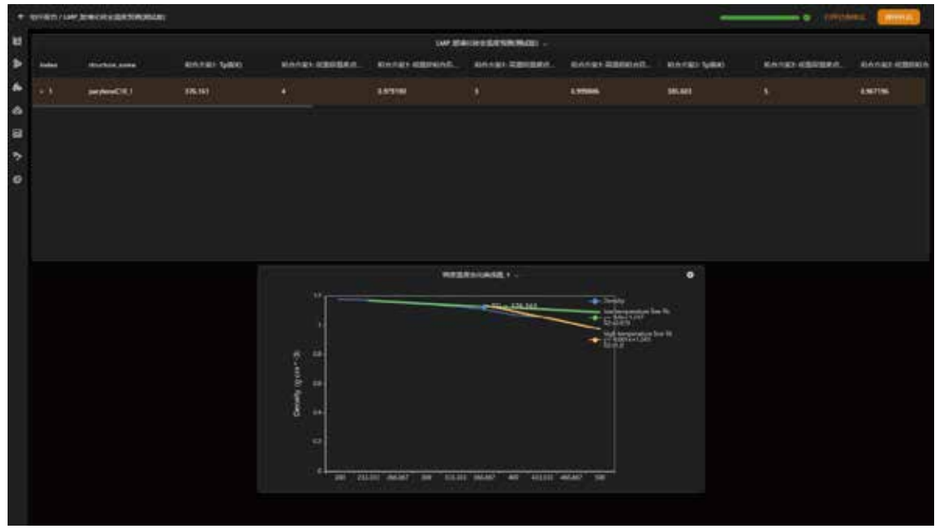
Reaction kinetics calculation results

MaxFlow

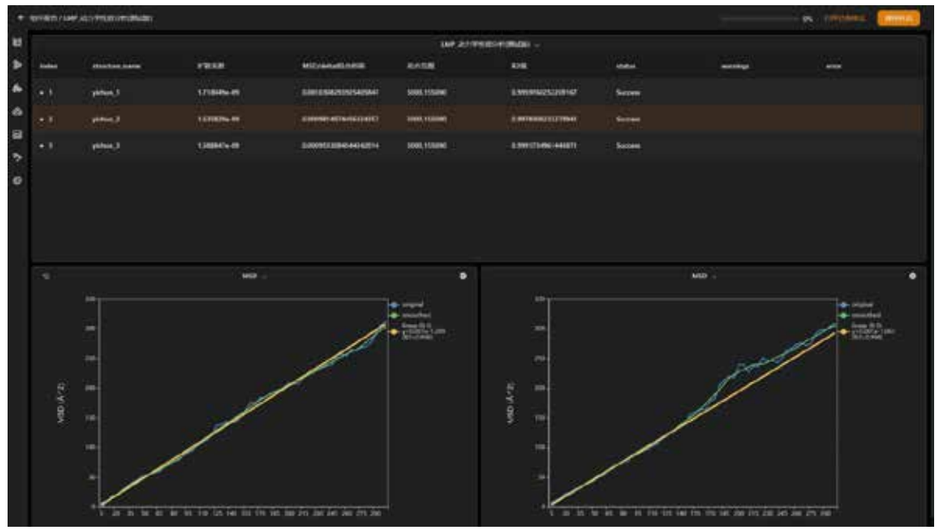


Mechanical properties calculation results

Hydrogen bond analysis calculation results



Glass transition temperature calculation results



Kinetic properties calculation results