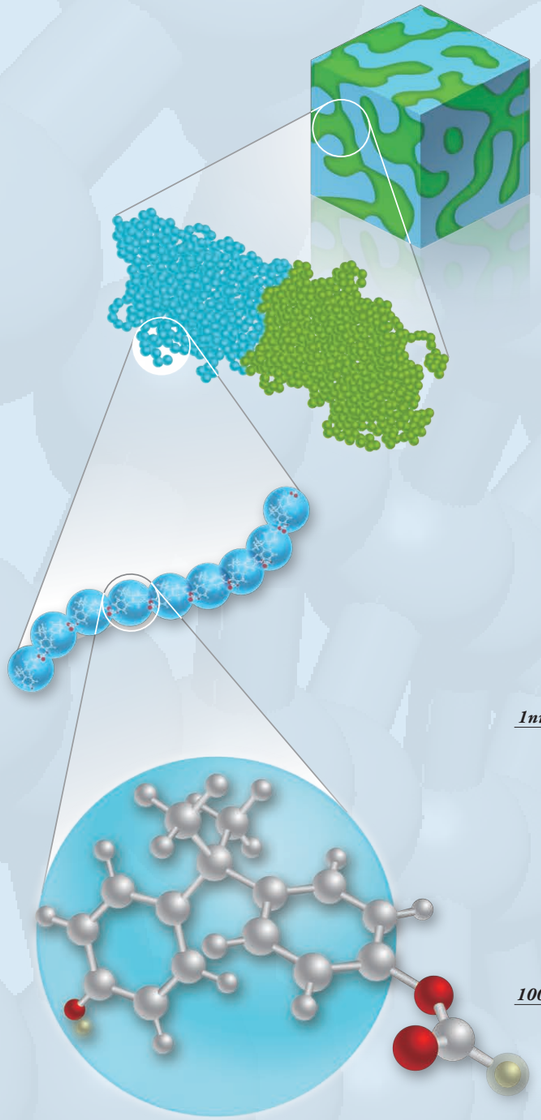
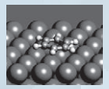
J-OCTA®

Integrated Simulation System for Soft Materials



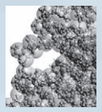
J-OCTA is multi-scale simulation software
which covers a wide range of scales,
from molecular simulation to continuum analysis.
In addition to various solvers according to each scale,
J-OCTA has molecular modeling tool,
various parameter estimation functions,
interface with external software, etc.
J-OCTA supports cutting-edge material design
and material development.

From molecular to macroscopic material properties



First-principles calculation SIESTA

The adsorption energy can be calculated by rotating / translating organic molecules placed on the surface (slab) structure of inorganic materials in any direction using the first principle calculation software "SIESTA". J-OCTA also includes the function to estimate potential parameters used in Molecular Dynamics simulation from the obtained energy curves.

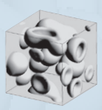


Molecular Dynamics COGNAC / VSOP

Evaluation of static and dynamic properties of materials based on atomistic and molecular levels is possible. All-atom and Coarse-Grained models (United-Atom, Beads-Spring and DPD, etc.) are supported. J-OCTA also includes Coarse-Grained potential estimation function and reverse mapping technology. A high speed MD solver VSOP is included, in addition, interfaces with LAMMPS, GROMACS and HOOMD-blue are also available.

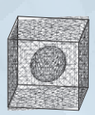
Rheology simulation VSOP / PASTA / NAPLES

Using Dissipative Particle Dynamics with entanglement effect, Slip-link model, and Primitive Chain Network model, rheological properties of polymer melts and solutions are evaluated, considering effects of molecular weight distribution and branch structures. Prediction of relaxation modulus, storage / loss modulus, elongational viscosity, etc. is possible.



Phase separation simulation COGNAC/VSOP/SUSHI/MUFFIN

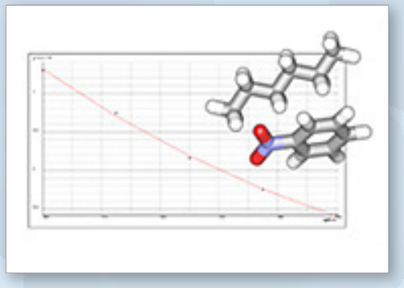
By using the mean field method like Self Consistent Field Theory and Dissipative Particle Dynamics, phase separation and interfacial structures of materials, including molecules of various structures and block copolymers, are predicted. Estimation of interaction parameter (χ parameter) and converting phase separation structure into Finite Element mesh are possible.



Multiphase simulation MUFFIN

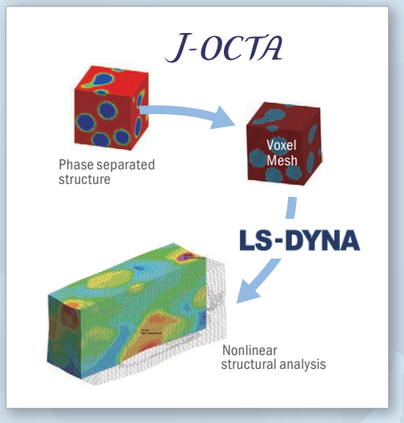
By using the phase separation structure obtained by the mean field method, etc., the Finite Element Analysis of the elastic material is possible. Mesh generation function is included. Evaluation of the relationship between the microstructure and material properties of composite materials is possible. In addition, interface with LS-DYNA for the nonlinear structure analysis is also available.

FMO helps to estimate χ(Chi) parameter.



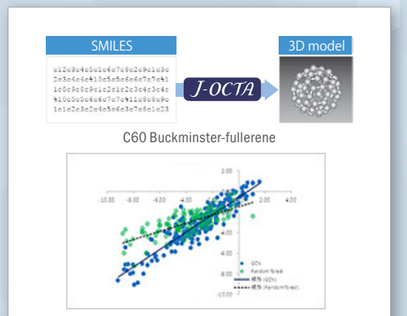
FCEWS (FMO-based Chi parameter Evaluation Workflow System) developed by Rikkyo University has been bundled in J-OCTA.
FCEWS is a new method to estimate the interaction parameter χ between segments that is necessary for the mean field method and for DPD. Users can perform χ estimation which uses FMO (Fragment Molecular Orbital) via J-OCTA interface directly.
This method is effective for the molecules that interact with other molecules through quantum chemical interaction, such as electronic polarization or delocalization, and for the cases where the molecular force field parameters are not sufficiently accurate.

Interface for LS-DYNA supports large-deformation simulation



It is in high demand to estimate and evaluate the behavior during large deformation of micro-structured composites which contain phase separation and filler, by performing simulations.
Existing FEM (Finite Element Method) engine of J-OCTA, "MUFFIN-Elastica" is for elastic simulation and is specialized for the behavior during a small deformation.
To extend its applicability to FEM simulation, J-OCTA has the interface for a multi-purpose nonlinear structural analysis engine "LS-DYNA".
The phase-separated structure computed by "COGNAC or "SUSHI" can be output as a mesh data for LS-DYNA simulation. After the user specifies the material properties for each component and deformation (boundary) condition, LS-DYNA simulation can be started from J-OCTA directly. As a material model being appropriate for nonlinear structural simulation, materials including elastoplastic, viscoelastic, and hyperplastic such as rubber are available for use.

Automatic MD calculation and QSPR using Deep Learning

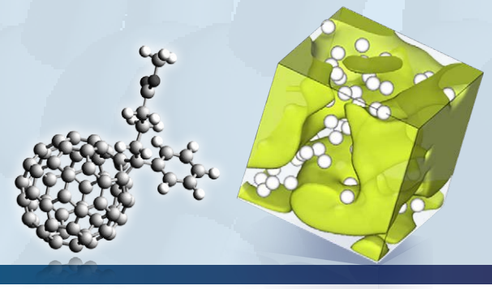


A comparison of two deep learning methods in solubility estimation. (Measured value and estimated value)

J-OCTA supports SMILES (Simplified Molecular Input Line Entry System) format.
J-OCTA reads molecular structures written in SMILES format and creates a 3D model. The obtained 3D model can be used to define and edit force field parameters for molecular dynamics application. Users can automate molecular dynamics calculation for a number of materials. Once the obtained material properties are compiled as a database, users can use it for machine learning and/or deep learning to evaluate Structure-Property Relationship (QSPR).

Please visit our website
for more information

http://www.j-octa.com/



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