■ Software Components

Functions	QMMM plus
MD Automatic Simulator	SOLUTION
MD Analysis	AMBINFO GMXINFO TRJ2GJF
QC Tools	GAUEDIT GAURUN GJOB
QC Analysis	GAUINFO GAUCUBE

SOLUTION	Automatic simulator of MD and QC for liquid solution
AMBINFO	Analyzer for MD outputs of AMBER
GMXINFO	Analyzer for MD outputs of GROMACS
GAUINFO	Analyzer for QC outputs of Gaussian
GAUCUBE	Analyzer for Gaussian Cube files
GAUEDIT	Editing tool for Gaussian input files
GAURUN/GJOB	Job controller for multiple Gaussian calculations
TRJ2GJF	AMBER trajectory to Gaussian input converter

*MD : Molecular Dynamics,　QC : Quantum Chemistry

■ System Requirements

Requirements ◎ : necessary ○ : recommended	QMMM plus
Python 2.6	◎
LSF, LAVA or Grid Engine	○
Gaussian09	○
AMBER14	○
AmberTools14	◎
GROMACS 4.6 or 5.0	◎
acpype.py	◎
Open Babel 2.x	◎
Gnuplot	○
Image Magick	○

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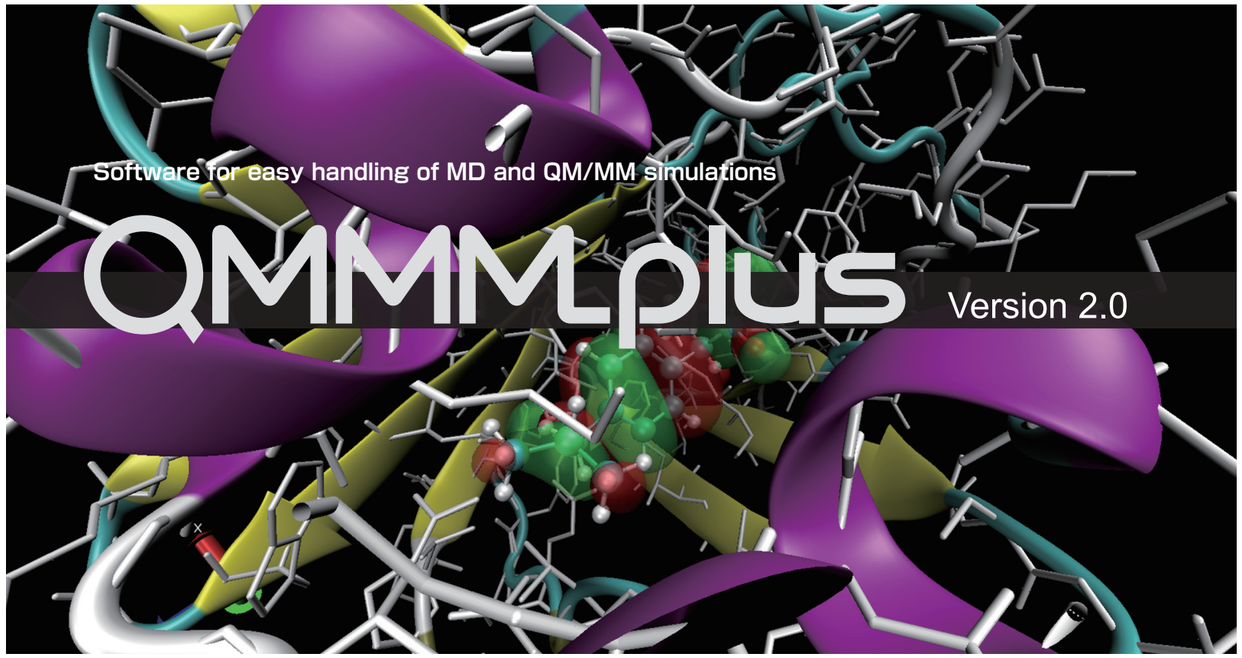
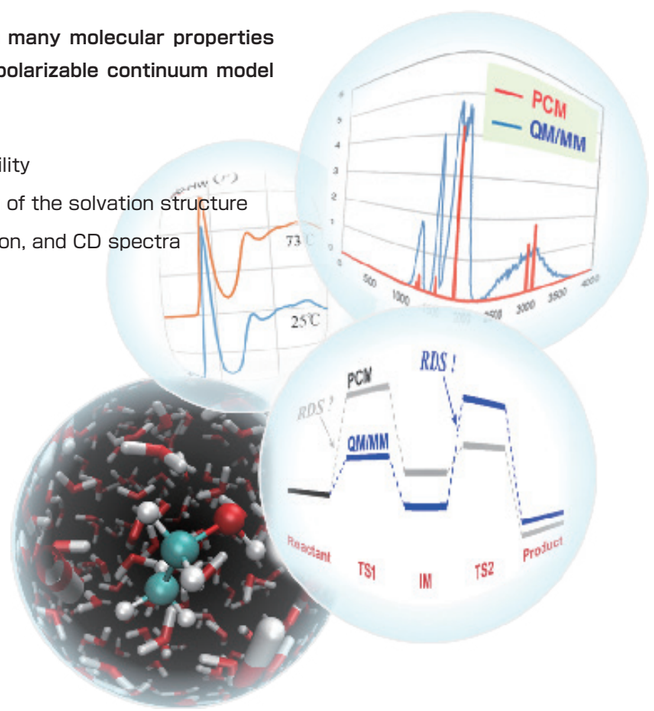
Software



You can easily and automatically obtain many molecular properties in mixed solvent beyond the traditional polarizable continuum model (PCM), for example,

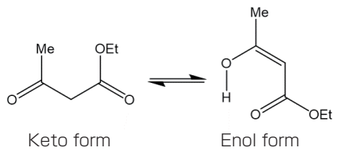
- Solvent dependence of the isomer stability
- Spectral band shape due to fluctuation of the solvation structure
- Solvatochromism for absorption, emission, and CD spectra
- Radial distribution functions
- Temperature effects

even if you know only Gaussian usage.



Overview

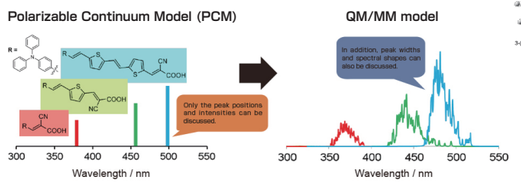
Tautomerism in Different Solvents



Prediction of stable isomer in solution

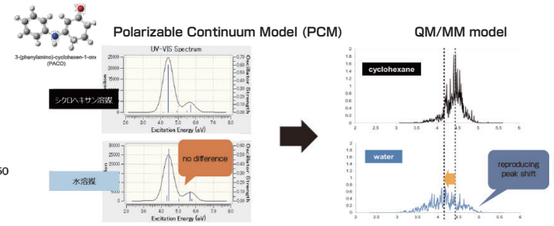
Solvents	Experiment population (keto:enol)	Calculation (PCM) relative energy (keto-enol)	Calculation (QM/MM) relative energy (keto-enol)
Cyclohexane	enol (38% : 62%)	○ enol (+4.3kcal/mol)	○ enol (+3.8kcal/mol)
Acetone	keto (99.9% : 0.13%)	× enol (+2.4kcal/mol)	○ keto (-3.2kcal/mol)
Water	keto (93.5% : 6.5%)	× enol (+0.9kcal/mol)	○ keto (-10.4kcal/mol)

Spectrum Width and Shift in Different Solvents



Only the peak positions and intensities can be discussed.

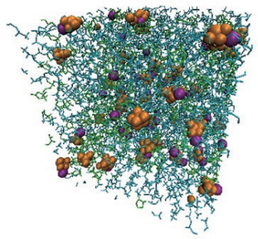
In addition, peak widths and spectral shapes can also be discussed.



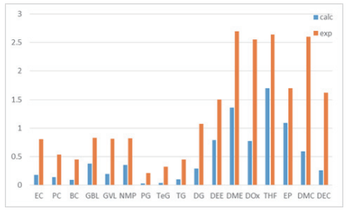
no difference

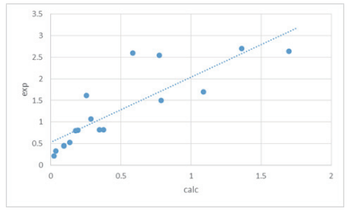
reproducing peak shift

Efficient Evaluation of Many Materials



Electrolyte consisting of four molecular (ionic) species.
Concentration can be set easily.





Diffusion coefficients for many electrolytes.
One material can be evaluated in only 30 minutes, hence 480 materials per a day using ten computers (16 core).

How to Use

① Create the input file

Set only molecule files, number of molecules, temperature and pressure conditions, and so on.
User also can modify details of MD calculation processes.

② Run

Just a single command. All simulation processes are automatically performed.

```
$ solution mer.input
```

```
[control]
n_core          = 16        parallel number and
style           = normal    calculation style

[molecule]
molecule01      = 1, BMC, input/merocyanine.gjf
molecule02      = 1000, AC, input/acetone.mol2
                  number of molecules and molecule files
                  (merocyanine : 1 molecule + acetone: 1000 molecules)

[md_default]
qmcondition     = PM6       conditions for QM/MM calculation
temperature     = 298.15    temperature
t               = 0.1       time
dt_output       = 0.001

[analysis]                  number of snapshots for quantum
n_data          = 64        chemistry analysis
gjf_template    = input/template-td.gjf
```

Input file

Functions

1. Molecular Dynamics Automatic Simulator

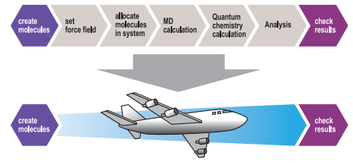
Automatic Calculation

Simulation for liquid solution have ever required many procedures such as creation of molecule, set of force field, allocation of molecules in system using many programs.

QMMM plus automates all these procedures. Only molecular structure files as well as conditions for temperature and pressure are required. No action required. Energy and spectra in liquid solution can be automatically calculated.

Restart

Available for restarting in middle of procedures.



Everyone can easily perform MD calculations even that experts have ever examined after a day.

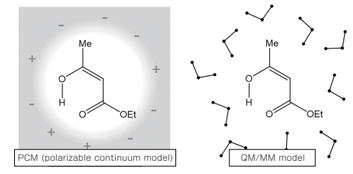
2. Molecular Dynamics Analysis

Time Evolution and Statistics of Energy and Temperature

Time evolution and statistics of energy, temperature, density, and interaction energy between a solute molecule and solvent molecules can be calculated.

Distribution and Diffusion of Molecules

RDF (radial distribution function) and diffusion behavior can be calculated.



Available also for QM/MM model.

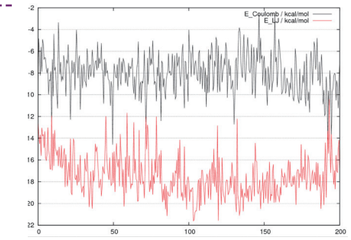
3. Quantum Chemistry Tools

Bulk Editor

Many Gaussian input files can be edited at once.

Bulk Execution

Many Gaussian jobs can be executed under limited number of CPU cores.



4. Quantum Chemistry Analysis

Statistics of Energy, Dipole, Atomic charges

Statistical analysis is available from many Gaussian output files. Energy, dipole moments and atomic charges are represented as values with standard deviations. Therefore, a new perspective such as softness of molecular structure as is proposed.

Spectrum in Liquid Solution (IR, Raman, UV-Vis, CD, NMR)

Since QMMM plus collects statistics from quantum chemistry calculations of many molecular structures in liquid solution, it provides continuous spectra with width and shape, whereas traditional quantum chemistry have ever provided line spectra.

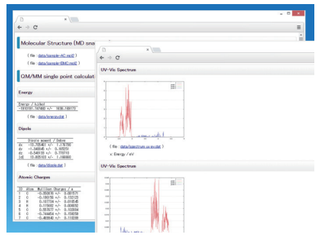
Property	Value
Total Energy / kcal/mol	15377.917692 +/- 382.471834
Kinetic Energy / kcal/mol	8030.652062 +/- 68.393689
Potential / kcal/mol	7347.265624 +/- 370.210350
Temperature / K	298.053425 +/- 2.538403
Pressure / bar	17.204695 +/- 1060.386258
Volume / Angstrom^3	106493.393877 +/- 3004.786944
Density / g/cm^3	1.370276 +/- 0.035797
E_Coulomb(VC_FIRST) / kcal/mol	-7.295341 +/- 1.887723
E_LJ(VC_FIRST) / kcal/mol	-16.714645 +/- 1.668658
E_Coulomb(EC_FIRST) / kcal/mol	-7.985196 +/- 1.821891
E_LJ(EC_FIRST) / kcal/mol	-17.422690 +/- 1.949266
E_Coulomb(Li+_FIRST) / kcal/mol	-115.599943 +/- 7.138112
E_LJ(Li+_FIRST) / kcal/mol	4.273472 +/- 2.159720
E_Coulomb(PF6_FIRST) / kcal/mol	-21.798688 +/- 2.892949
E_LJ(PF6_FIRST) / kcal/mol	-11.523351 +/- 1.801136

Time evolution and statistics of many properties.

5. Report

HTML-formatted Report

Calculation results are available in HTML format which can be viewed in a Internet browser. Tab-delimited output files are stored in “data” directory.



Calculation results are available from a browser.