

# Tutorial 05

QM/MM Calculation



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# MOMAP Tutorial 05

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# **MOMAP Tutorial 05**

# - QM/MM Calculation

The basic steps involved in the calculations are as follows:

- 1) Prepare QM/MM input files
- 2) Carry out QM/MM calculations
- 3) Do evc calculation etc.

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## Prepare QM/MM input files

**GaussView** would be the fastest option to prepare input files for QM/MM calculations. Before we can do QM/MM calculations, we have to first select which atoms are in which layer, by using **Tools->Select Layer**... option. For example, we first put everything into the Low layer (**Set Layer** -> **Low**, **Select All**, **Apply**), then choose the ligand + perhaps some nearby residues, and then move them to High layer.



The High Layer consists of the final three atoms (as QM atoms). The other atoms are placed into the Lower Layer (as MM atoms). A link atom is defined for the first carbon atom.

Once we have set up the layers, then we would have to decide which atoms should be set as **Freeze** (Yes, -1) and which atom should be set as **Freeze** (No, 0) during the optimization process, by operating from the GaussView menu **Tools** -> **Atom Groups** -> **Freeze** as follows:

G1:M1:V1 - Atom Gr	oup Editor	5.en					x
Atom Group Class: F	reeze	- V Exclusiv	e Cla	ss Actior	LS <b>T</b>	Group Actions	. •
Group ID	Highlight	Display			Atom Tags	Atom Count	
Freeze (No)		Show 🔻	+	_	1-95	95	
Freeze (Yes)		Show 🔻	+	_	96-1140	1045	
Freeze (-2)		Show 🔻	+	_		0	
Freeze (-3)		Show 🔻	+	_		0	
Persistent Visuals			Ok	He:	Lp	1	

GaussView would normally set this value to 0, that is, all atoms are set as **Freeze** (No), if we do not do anything. With GaussView 5 and 6, operation on freezing with Atom Group Class can be done from the GaussView menu **Tools** -> **Atom List** -> **Freeze** as show above.

Afterwards just choose Calculate->Gaussian calculation Setup..., in the Method tab select Multilayer Oniom Model and then define the Method separately for the Low Layer and High Layer (in the Method tab we will have Low Layer and High Layer tabs active if one selected the layers properly).

🕼 G2:M1:V1 - Gaussian Calculation Setup	×
Title:       2-layer OWION optimization         Keywords:       # opt onion(b3lyp/6-31g(d, p):uff)         Charge/Mult.:       0 1 0 1 0 1	
Job Type Method Title Link 0 General Guess Pop. PBC Solvation High Layer Medium Layer Low Layer Method: Ground State V DFT V Default Spin V B3LYP V Basis Set: 0-31G V V (d V, p V) Charge: 0 Spin: Singlet V Add. Keywords: Use sparse matrices	Add. Inp. Preview Multilayer ONIOM Model
	Help
Additional Keywords:	Update
Submit Quick Launch Cancel Edit Retain	Defaults

Click the **General** tab, and tick the **Write Connectivity**:

🔝 G2:M1:V1 - Gaussian Calculation Setup		×
Title:2-layer ONION optimizatKeywords:# opt onion (b3lyp/6-31gCharge/Mult.:0 1 0 1 0 1	ion (d,p):uff) geom=connectivity	
Job Type Method Title Link 0	General Guess Pop. PBC Sol	vation Add. Inp. Preview
Use Quadratically Convergent SCF	Ignore Symmetry	🗹 Write Cartesians
🖂 Use Modified Redundant Coordinates	Use Counterpoise	🗹 Write Connectivity
🖂 Write Gaussian Fragment Data	🗌 Additional Print	🗹 Write PDB Data
Compute Polarizabilities	Compute Optical Rotations	Read Incident Light Freqs Default 🔻
□ Use MaxDisk= 2 🗘 GB	Y	
Read Data From Checkpoint File		
Geometry: No	•	MO Guess
Optimization Force Constants: No	•	
		Help
Additional Keywords:		Update
Scheme: (Unnamed Scheme)		<ul> <li>Assign to Molecule Group</li> </ul>
Submit Quick L	aunch Cancel Edit Re	tain Defaults

**Note:** One should carefully check the correctness of atom connectivity which was generated by GaussView automatically if one would like to use MM method (UFF, AMBER *et al.*) to do the Low Layer calculation, especially the bond order in benzene ring.

The Gaussian input file may look like:

```
%chk=s0.chk
%nprocs=24
%mem=60GB
# opt oniom(b3lyp/6-31g(d,p):uff) geom=connectivity
2-layer ONIOM optimization
0 1 0 1 0 1
                      -1.04150621 0.0000000 -2.12610949 L
\mathbf{F} - \mathbf{F}
                 -1
F - F
                 -1
                      -2.03368194 -1.14289207 -0.41221877 L
                 -1 -2.03368194 1.14289207 -0.41221877 L
F-F_
                    -1.29903811 0.00000000 -0.75000000 L H-H_ 5
0.00000000 0.00000000 0.00000000 H
C-C_3
                 -1
                 0 0.0000000 0.0000000 0.0000000 H
0 0.0000000 0.0000000 1.10000000 H
C-C_2
Н-Н
0-0_2
                  0
                      1.12583302 0.00000000 -0.65000000 н
1 4 1.0
2 4 1.0
3 4 1.0
4 5 1.0
5 6 1.0 7 1.5
6
7
```

The  $6^{th}$  column is used to judge which atoms belong to the QM layer, normally the atoms marked with **H** are treated as QM (or free) atoms, which is later used in MOMAP to do the evc calculation.

In MOMAP, the 2<sup>nd</sup> column of data (in red box) can be omitted, that is, both 5 columns and 6 columns of data are supported.

## Carry out QM/MM calculations

Once the input files are prepared, we can use QM program to do the calculations. Here we use Gaussian g16 to do the calculations, and the Gaussian log output file (segment related to QM) may look like:

Title Car	d Required	
Symbolic	Z-matrix:	
Charge =	0 Multiplicity =	1 for low level calculation on real system.
Charge =	0 Multiplicity =	1 for high level calculation on model system.
Charge =	0 Multiplicity =	1 for low level calculation on model system.
C-C_R	- 1	0.7315 -9.7969 -7.57692 L
C-C_R	- 1	0.3898 -11.20542 -11.61389 L
C-C_R	- 1	0.49442 -12.11868 -10.58599 L
H-H_	- 1	0.47497 -13.05064 -10.76799 L
C-C_R	- 1	0.62992 -11.66088 -9.27435 L
H-H_	- 1	0.70805 -12.28647 -8.56401 L
C-C_R	- 1	0.64988 -10.29488 -8.99592 L
C-C_R	- 1	0.53102 -9.38892 -10.05365 L
H-H_	- 1	0.52456 -8.45499 -9.87672 L
C-C_R	- 1	0.42363 -9.83959 -11.35136 L
H-H	- 1	0.37178 -9.21709 -12.06743 L

However, there exist other cases where the output formats may differ, for example, if the **geom=check** is used in the Gaussian input file, the Gaussian input file may look like:

```
%chk=s1.chk
%nprocs=24
%mem=60GB
# oniom(b3lyp/6-31g(d) td(nstates=7):uff=qeq)=embed opt geom=check guess=read
2-layer ONIOM optimization
0 1 0 1 0 1
```

Then, the Gaussian log output file (segment related to QM) may look a bit different from those as shown above:

Title Card Required
Structure from the checkpoint file: "s1.chk"
Charge = 0 Multiplicity = 1 for low level calculation on real system.
Charge = 0 Multiplicity = 1 for high level calculation on model system.
Charge = 0 Multiplicity = 1 for low level calculation on model system.
Redundant internal coordinates found in file. (old form).
C,-1,-1.995,-7.384,-21.16
C,-1,-1.587,-7.947,-19.948
C,-1,-2.555,-8.168,-18.948
H,-1,-2.31,-8.584,-18.13
C,-1,-3.863,-7.774,-19.164
C,-1,-4.231,-7.199,-20.398
H,-1,-5.126,-6.916,-20.535
C,-1,-3.309,-7.042,-21.409
H,-1,-3.572,-6.707,-22.26
C,-1,0.429,-7.982,-21.156
C,-1,-0.186,-8.3,-19.939
C,-1,0.532,-8.93,-18.915
H,-1,0.128,-9.131,-18.078

Here, the data are separated by comma, rather than by empty spaces.

Note: The above three output data formats are supported by MOMAP.

### Do evc calculation etc.

Once the Gaussian log files are prepared, we can do the evc calculated as usual, for example, the momap.inp may look like:

```
do_evc = 1
&evc
ffreq(1) = "freq.log"
ffreq(2) = "freqes.log"
proj_reorg = t
```

Finally do the evc calculation:

```
momap -input momap.inp -np 1
Or
momap.py -i momap.in -n 1
```

Later on, we can use MOMAP to carry out other calculations.