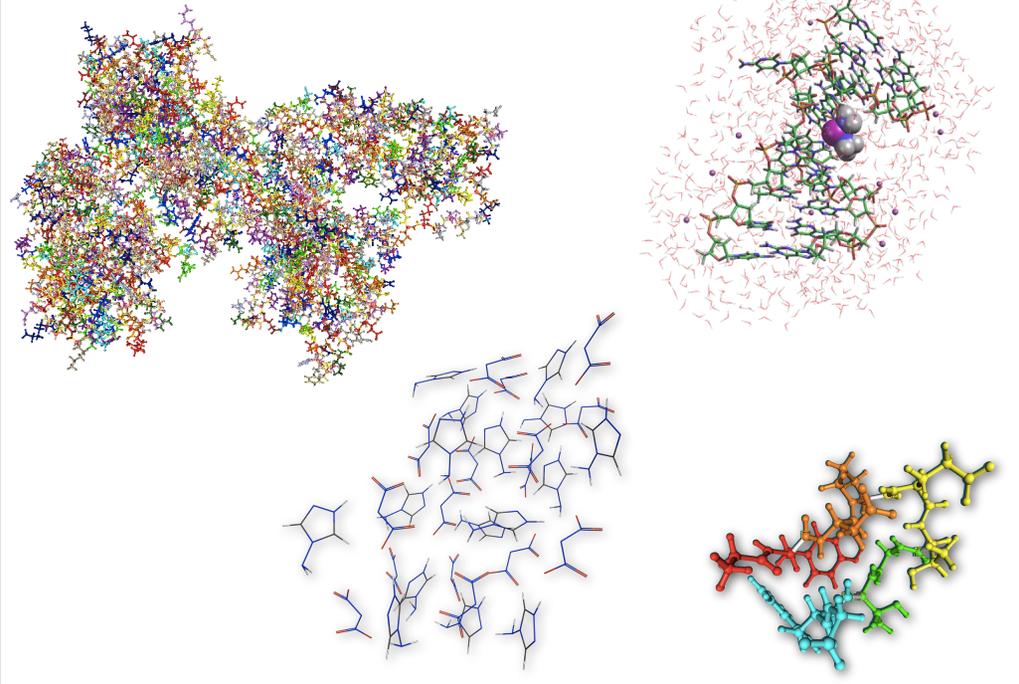


# Fragmentation methods



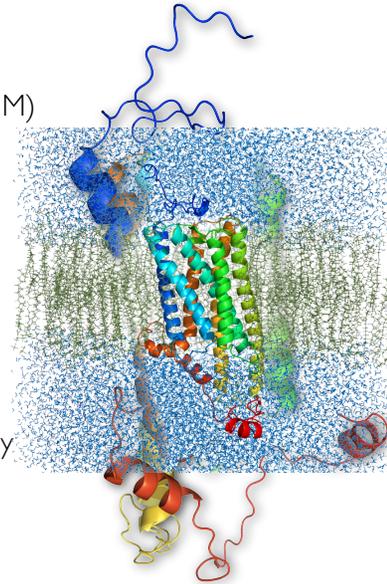
## Scaling of QM Methods

- HF, DFT scale as  $N^4$
- MP2 scales as  $N^5$
- CC methods scale as  $N^7$
- What if we could “freeze” the value of  $N$  regardless of the size of the system? Then each method would scale linearly with respect to the system size. This is the goal of fragmentation methods.

\*(where  $N$  is a measure of system size such as the number of basis functions)

## Fragmentation Methods

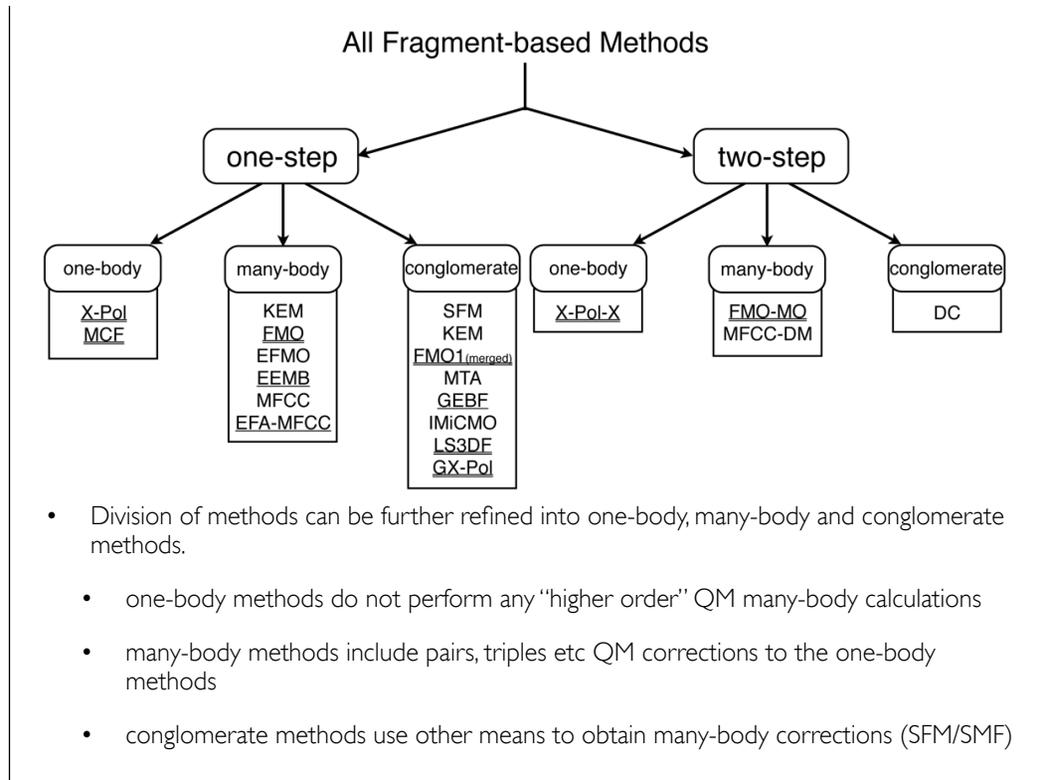
- Biomolecules contain hundreds or thousands of atoms, making accurate quantum calculations either very difficult or impossible
- Quantum Mechanics/Molecular Mechanics (QM/MM) methods have become popular in recent years, however;
  - As system size grows the QM region can get unwieldy
  - The energy contribution from the environment becomes too large to obtain reasonable accuracy from molecular mechanics



Fragmentation methods offer a unique solution to accurate calculations on large molecules

## Background & Motivations

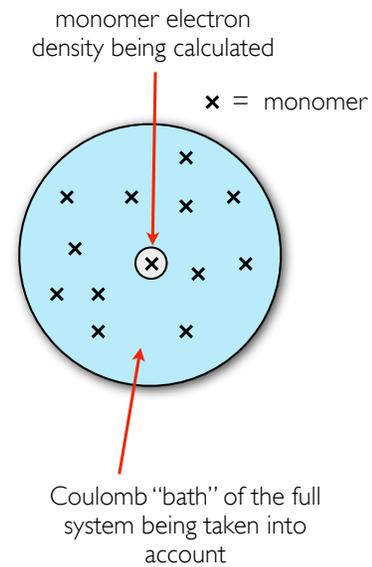
- Fragmentation methods can be divided into two groups, one-step and two-step
- One-step methods obtain the energy and properties directly from fragment calculations. Methods included are:
  - X-pol, FMO, KEM, MFCC, SFM (SMF) and MTA
- Two-step methods first compute some total property, for example the density, from fragment calculations. Other properties such as the total energy are then evaluated from the total property obtained in the first step. Examples of two-step methods are:
  - X-Pol-X, MFCC-DM and DC



## The Fragment Molecular Orbital (FMO) Method:

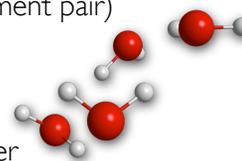
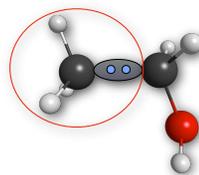
Kitaura et al.: CPL, [313](#), 701 (1999)

- Exchange and self-consistency are local in most molecules
- Treat non-local parts using just the Coulomb operator, thereby ignoring exchange
- Perform the molecular calculations individually in the rigorous Coulomb field of the whole system
- Improved by explicit many-body corrections for pairs and triples (dimers & trimers)
- The Coulomb bath allows for fragmentation without hydrogen capping

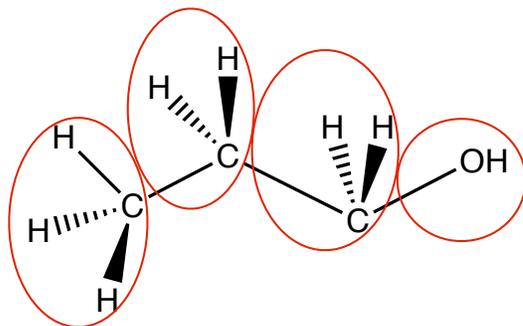


## The Fragment Molecular Orbital Method

- Bonds are fractioned electrostatically
- Electrons are assigned heterolytically
- FMO fragmentation should be conducted based upon chemical knowledge (not a formal “mathematical exercise”)
- Hydrogen bonding is accounted for by explicit dimer (fragment pair) calculations
- Dimer & trimer (fragment triple) calculations allow for other quantum effects to be taken into account



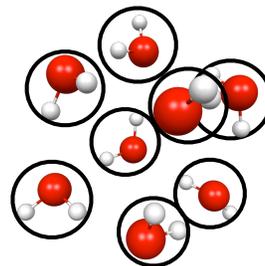
## The Fragment Molecular Orbital Method: Fragmentation Scheme



For covalently bonded molecules, we divide the fragment into pieces so as not to destroy bond electron pairs.

In molecular clusters, fragmentation is easier, requiring no covalent bond breaking.

We can have one molecule per fragment, two molecules per fragment etc



## The Fragment Molecular Orbital Method - Basic Methodology

The total energy of the system can be written as

$$\begin{aligned} E = & \sum_I^N E_I + \sum_{I>J}^N (E_{IJ} - E_I - E_J) \\ & + \sum_{I>J>K}^N \{ (E_{IJK} - E_I - E_J - E_K) - (E_{IJ} - E_I - E_J) \\ & - (E_{JK} - E_J - E_K) - (E_{KI} - E_K - E_I) \} + \dots, \end{aligned}$$

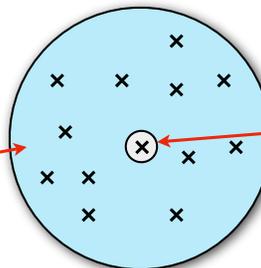
Where the monomer (I), dimer (IJ) and trimer (IJK) energies are obtained using the SCF method with modified Fock operators

## The Fragment Molecular Orbital Method

1. Divide molecule into fragments and assign electrons to these fragments
2. Calculate initial electron density distribution of the fragments in the Coulomb "bath" of the full system
3. Construct the individual fragment Fock operators using the densities calculated in 2 and solve for the fragment energies
4. Determine if the density has converged for all the fragments. If not, go back to step 3
5. Construct Hamiltonians for each dimer (trimer) calculation using the converged monomer densities from steps 3-4
6. Calculate total energy and electron density

### Steps 1-3:

Coulomb "bath" of the full system being taken into account



monomer electron density being calculated

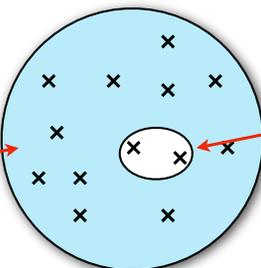
x = monomer

### Step 4:

Steps 1 through 3 are looped until the density of the full system converges to some predetermined threshold

### Steps 5-6:

converged Coulomb "bath" of the full system from monomer SCF



dimer (trimer) electron density being calculated in the presence of the converged ESP

each dimer (trimer) calculation is performed once

## The Fragment Molecular Orbital Method

The number of dimer calculations increases as "n choose 2" where n is the number of fragments.

7 fragments = 21 dimers

8 fragments = 28 dimers

16 fragments = 120 dimers

32 fragments = 496 dimers

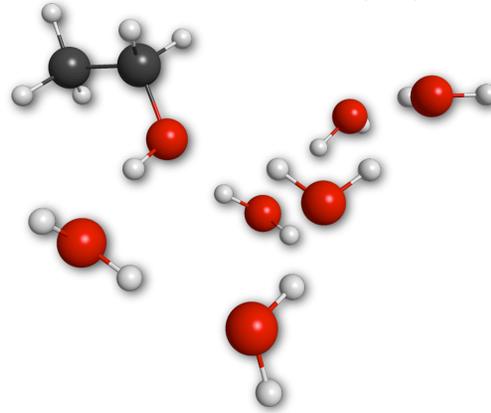
64 fragments = 2016 dimers

128 fragments = 8128 dimers

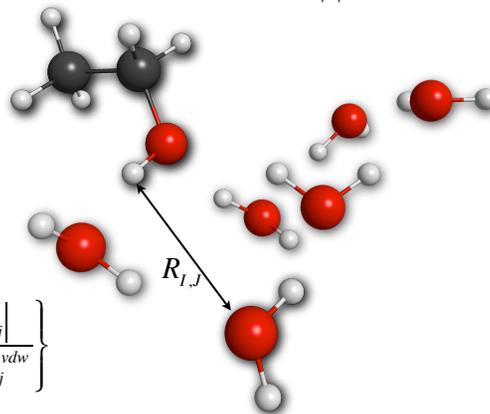
The total number of dimer calculations increases rapidly!

Two solutions: Approximations and parallelization

$$\# \text{ of dimers} = \frac{n!}{2!(n-2)!}$$



## The Fragment Molecular Orbital Method: Approximations

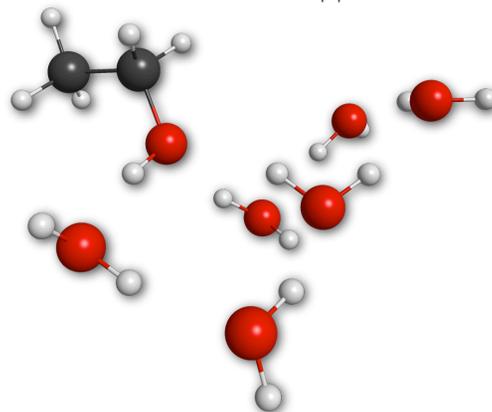


$$R_{I,J} = \min_{i \in I, j \in J} \left\{ \frac{|\vec{r}_i - \vec{r}_j|}{r_i^{vdw} + r_j^{vdw}} \right\}$$

User defined cut-off value  $R_{cut}$

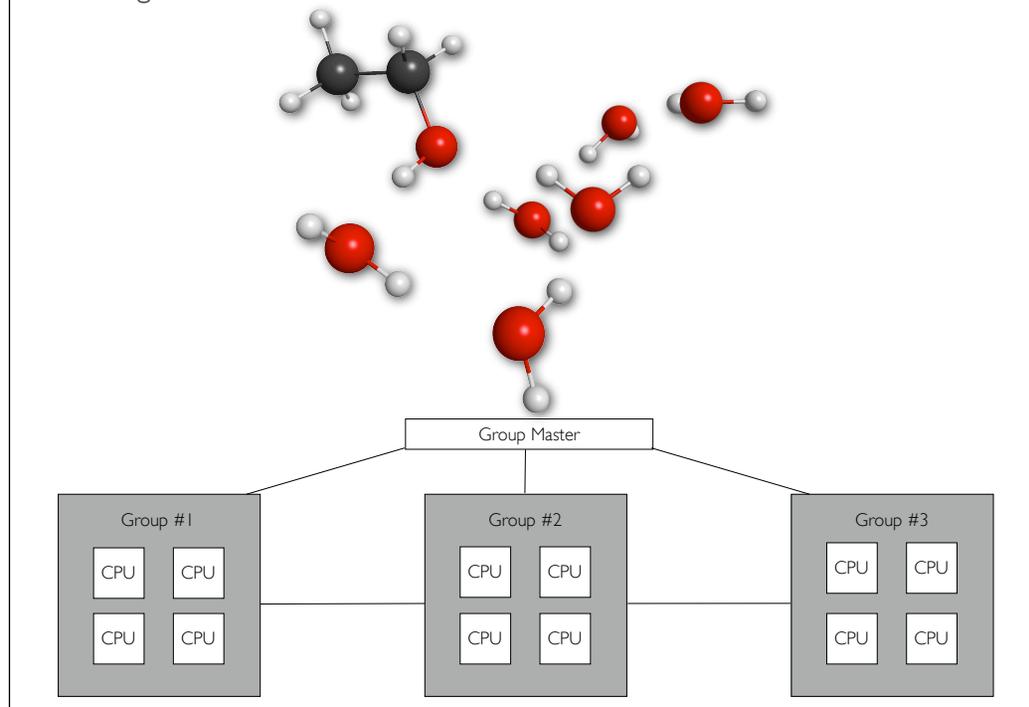
$$E^{FMO2} = \sum_I E_I + \sum_{I>J}^{R_{I,J} \leq R_{cut}} \Delta E_{IJ} + \sum_{I>J}^{R_{I,J} > R_{cut}} \Delta E_{IJ}^{sep}$$

## The Fragment Molecular Orbital Method: Applications



- The Generalized Distributed Data Interface (GDDI)
- GDDI allows for massively parallel calculations on clusters of computers or supercomputers
  - After the molecule is divided into fragments, each fragment is sent to a group which is composed of more than one processor or SMP enclosure
  - Each fragment is then run in parallel in each group
  - This provides two levels of parallelization, greatly speeding up the calculation

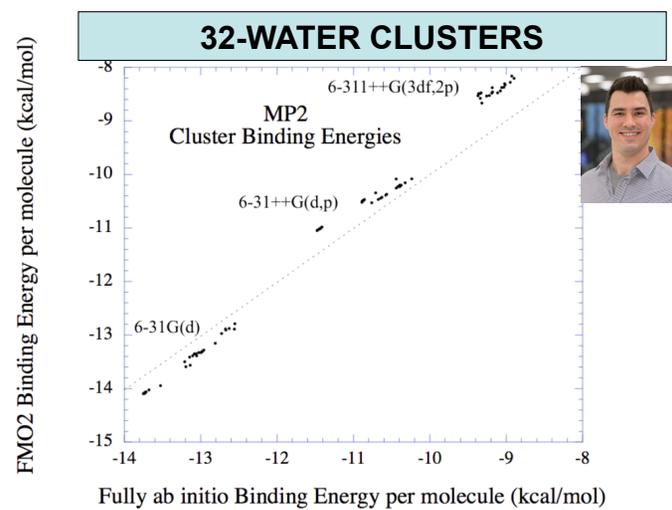
# The Fragment Molecular Orbital Method: Parallelization

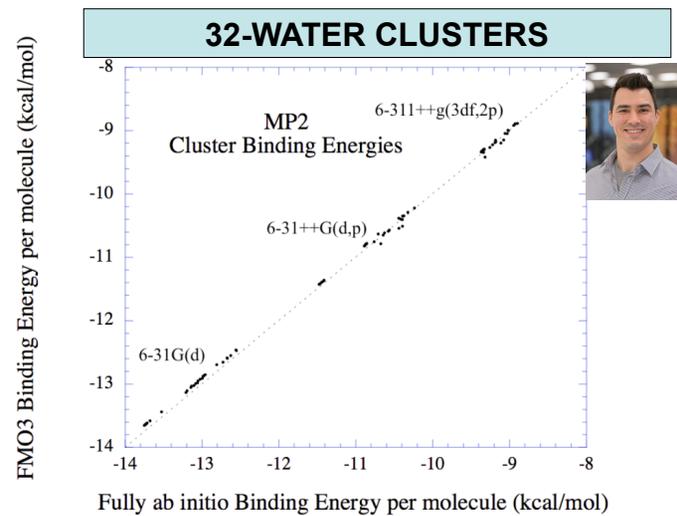


## The Fragment Molecular Orbital Method

- FMO has all of the following wavefunction types implemented
  - RHF, ROHF, DFT/TDDFT, MP2, CC, CIS and MCSCF (all of which support FMO3 except MCSCF)
- FMO also has a multilayer implementation allowing you to specify different levels of electron correlation or basis sets in different layers
- FMO is also interfaced with PCM and EFP for solvent effects
- RUNTYPs available are ENERGY, GRADIENT, OPTIMIZE and GLOBOP

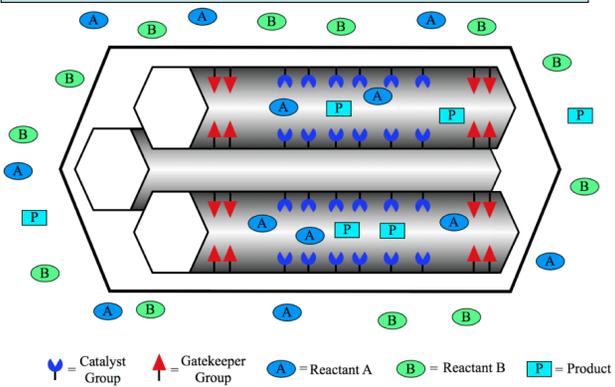
## The Fragment Molecular Orbital Method - Examples



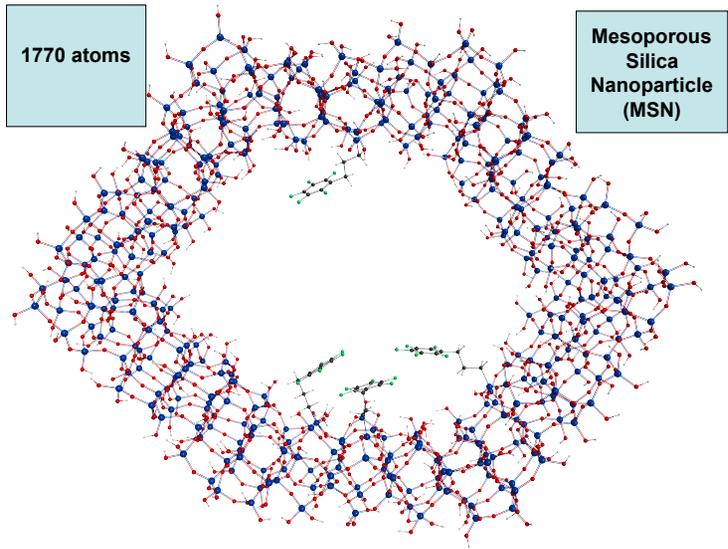


# The Fragment Molecular Orbital Method - Examples

## Heterogeneous Catalysis on MSN



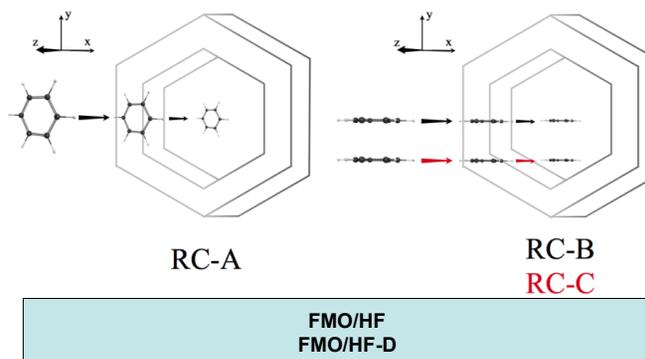
Gatekeeper groups selectively allow reactants "A" (not "B") to enter and form product "P"

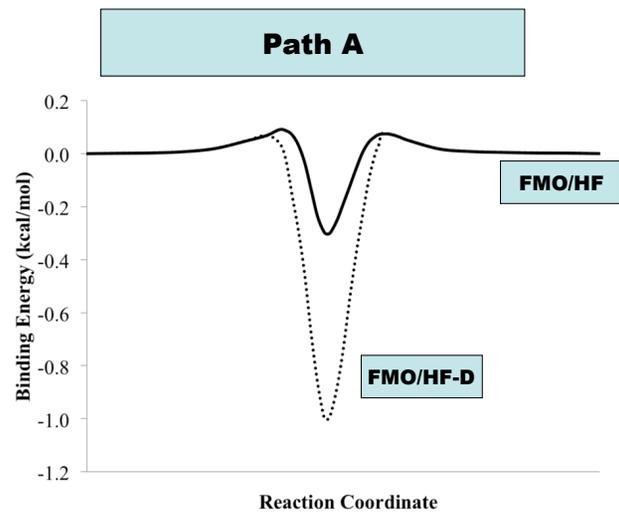


1770 atoms

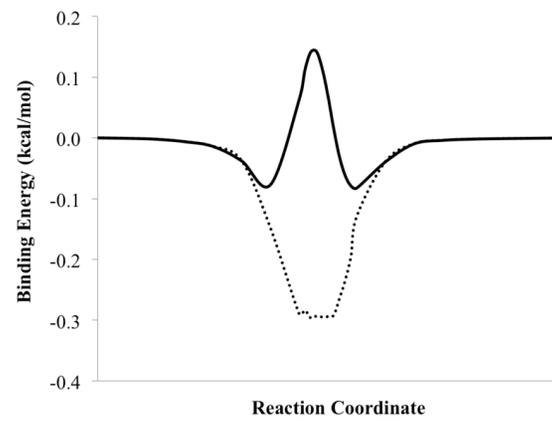
Mesoporous  
Silica  
Nanoparticle  
(MSN)

## Diffusion Through MSN Pore

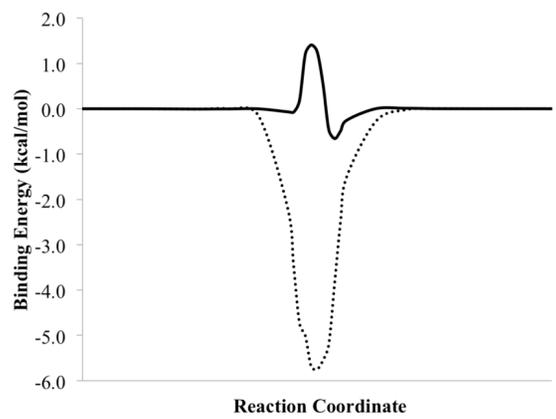




**Path B**



**Path C**



## The Fragment Molecular Orbital Method - Examples

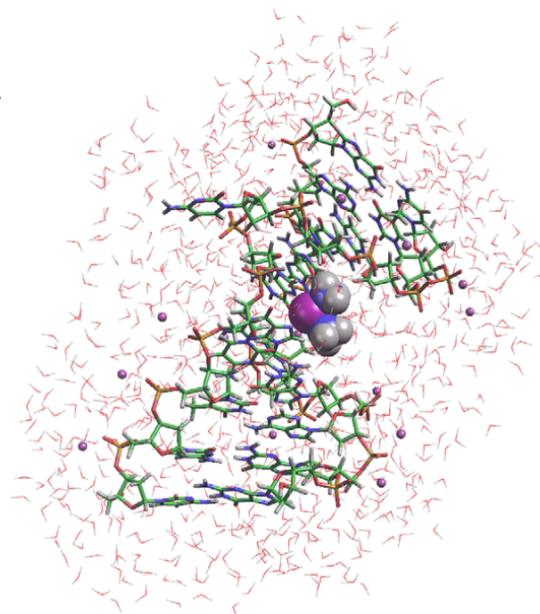
Hydrated cisplatin-DNA complex.  
FMO2-MP2 calculations were  
performed using the MCP model

Sodium ions and water molecules  
were relaxed with the Amber99  
force field

This calculation included:

3596 atoms

~997 fragments



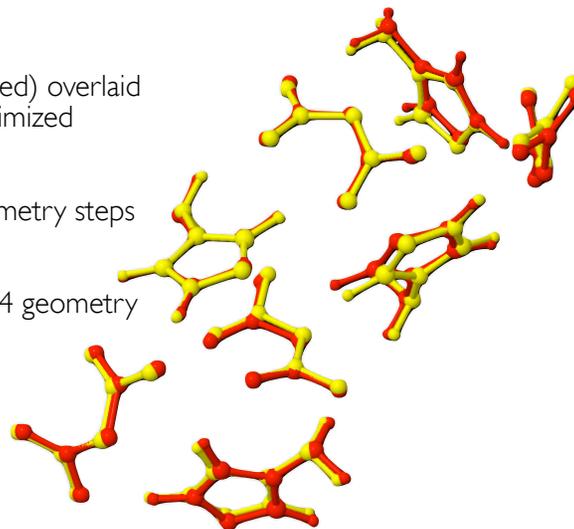
## The Fragment Molecular Orbital Method - Examples: Ionic Liquid

FMO2-MP2/6-31G(d)  
optimized\* octamer structure (red) overlaid  
with *ab initio* MP2/6-31G(d) optimized  
structure (yellow)

MP2 optimization took 105 geometry steps  
and ~63 hours

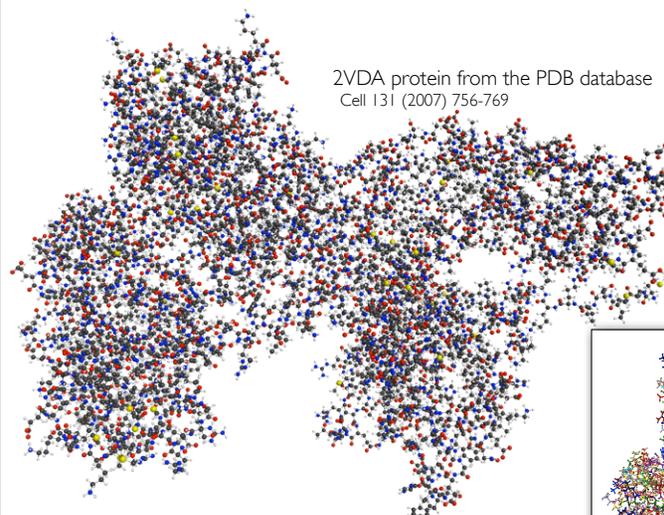
FMO2-MP2 optimization took 94 geometry  
steps and ~5.5 hours

\*Optimizations performed on 256  
CPUs of an IBM Power6 cluster with  
32 CPUs per node and 2 GB of  
RAM per CPU. GDDI was used for  
FMO2 calculation with one node  
per GDDI group.



Error = -2.23 kcal/mol  
RMSD = 0.04 angstroms

## The Fragment Molecular Orbital Method - Examples

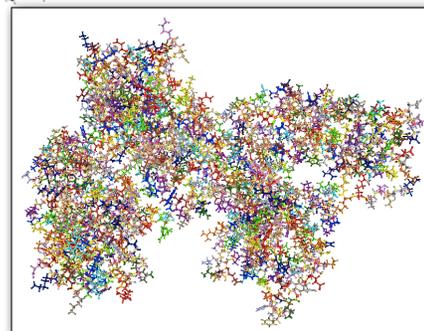


2VDA protein from the PDB database  
Cell 131 (2007) 756-769

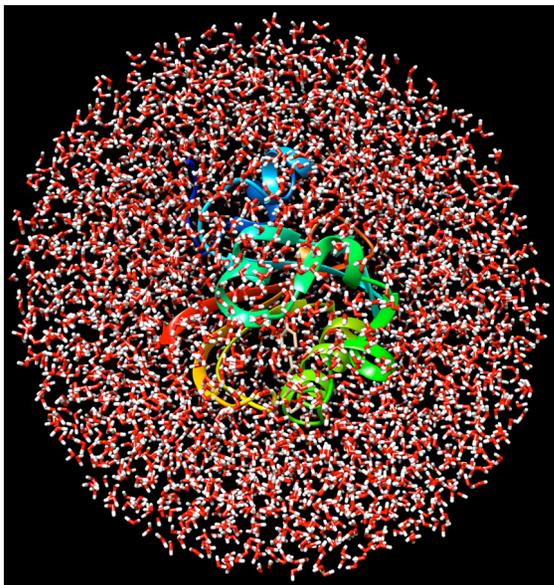
# Groups	# CPUs*	CPU time <sup>†</sup> (min)	Wall time (min)
8	256	1103	1533
16	512	566	775
32	1024	299	430
48	1536	210	415

\* 4.7 GHz IBM Power6 processors with 2GB of RAM per CPU and 32 CPUs per node

FMO2-MP2 single point energy calculation  
6-31G(d) basis set  
855 fragments (one residue per fragment)  
13625 atoms



## The Fragment Molecular Orbital Method - Examples



- 124 amino acid residues
- 3460 water molecules
- one residue or water per fragment
- FMO2-MP2/6-31 IG(d,p) energy calculation
- 131,432 basis functions
- 16,384 nodes (262,144 cores)
- ~10 hours
- ~72% of Blue Waters

# The Fragment Molecular Orbital Method

## Timings: Water Clusters

	6-31++G(d,p)				
	MP2	FMO2-MP2		FMO3-MP2	
Cluster Size	Wall Clock Time (seconds)	Wall Clock Time (seconds)	Error (kcal/mol)	Wall Clock Time (seconds)	Error (kcal/mol)
16	394	10	2.95	81	0.71
20	1119	11	4.66	141	0.17
32	9989	20	11.80	429	2.21

Each calculation was run on 6 nodes containing two 2.66 GHz Intel quad core Xeon processors (48 CPUs total) and 16 GB of RAM. For the FMO calculations, GDDI was used with each node specified as a group (6 groups total).

48 cores with 2 GB of RAM per core was the minimum computational requirement for the fully ab initio 32 water calculation.

## FMO2-MP2/aug-cc-pVDZ gradients:

### BG/P: ANL (Graham Fletcher)

		Racks: 1 2 4 8 16 32					
		Cores: 4096 8192 16,384 32,768 65,536 131,072					
Basis							
Waters	Atoms	Functions	Wall Time (minutes)				
128	384	5504	8.6	4.8	2.7	1.8	
256	768	11,008	19.8	10.5	5.8	3.4	2.2
512	1536	22,016		28.9	15.4	8.6	4.9
1024	3072	44,032			41.1	22.0	12.2

G.D. Fletcher, D.G. Fedorov, S.R. Pruitt, T.L. Windus and M.S. Gordon, J. Chem. Theor. Comp., **8**, 75 (2012).

# The Fragment Molecular Orbital Method

## Timings: Ionic Liquids

1-H,4-H-1,2,4-triazolium dinitramide octamer		
Timing* (minutes)		
6-31++G(d,p)		
#CPUs	FMO2-MP2	MP2
4	42.9	-
8	22.3	-
16	11.4	-
32	5.8	-
64	3.5	55.6

Full ab initio MP2 calculation requires ~77 GB of RAM  
FMO2-MP2 calculation requires less than 1 GB of RAM

Error = 0.67 kcal/mol

\* Timings for ionic liquid clusters performed on a computer cluster containing 2.66GHz Intel Xeon processors.

Each node contains two 4 core CPUs and 16 GB of RAM.

GDDI division was across individual nodes (1 group = 8 CPUs)

## The Fragment Molecular Orbital Method - Memory Requirements

CCSD(T)/aug-cc-pVQZ single point energy calculation on a cluster of six water molecules

	64 cores 8 cores/node	64 cores 1 core/node
CCSD(T)	80 GB RAM per node	32 GB RAM per node
FMO3-CC	12 GB RAM per node	4 GB RAM per node

\*One water molecule per FMO fragment

CCSD(T)/aug-cc-pVQZ single point energy calculation on a cluster of six argon atoms

	64 cores 8 cores/node	64 cores 1 core/node
CCSD(T)	36 GB RAM per node	19 GB RAM per node
FMO2-CC	9 GB RAM per node	4 GB RAM per node

\*Two argon atoms per FMO fragment (total of three fragments)

# The Fragment Molecular Orbital Method

## Memory Requirements

Memory requirements per node (in GB) for fully  
*ab initio* CCSD(T)/6-31++G(d,p) energy  
calculation on hexamer cluster

Total # of CPUs	Number of Cores per Node				
	1	2	4	8	16
1	643				
2	381	643			
4	250	381	644		
8	185	250	382	645	
16	152	185	251	384	648
32	136	152	186	253	386
64	127	136	153	187	255
128	123	128	137	154	190

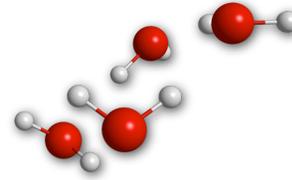
Memory requirements per node (in GB) for  
FMO2-CCSD(T)/6-31++G(d,p) energy  
calculation on any size cluster

Total # of CPUs	Number of Cores per Node				
	1	2	4	8	16
1	8				
2	5	9			
4	4	5	9		
8	3	4	5	9	
16	2	3	4	6	9
32	2	2	3	4	6
64	2	2	3	3	4
128	2	2	2	3	3

## The Effective Fragment Potential Method

Originally developed to describe aqueous solvent effects on molecules of biological interest.

The EFP method is an ab initio based model potential for the evaluation of intermolecular forces.



Each molecule is represented as a fragment of fixed geometry with a set of parameters derived from ab initio calculations.

In the original implementation (EFP1 - only water) the interaction energy between fragments consists of three terms: Coulomb, polarization and exchange repulsion.

$$E^{EFP1} = E^{Coul} + E^{pol} + E^{exrep}$$

$$E^{EFP2} = E^{Coul} + E^{pol} + E^{disp} + E^{exrep} + E^{ct}$$

## The Effective Fragment Molecular Orbital Method

The EFMO method was developed to integrate the FMO and EFP methods in an effort to provide a generally applicable, accurate and efficient approach to large molecular systems.

(FMO fragmentation) + (EFP interactions) + (other modifications) = EFMO

$$E^{FMO2} = \sum_I E_I + \sum_{I>J}^{R_{IJ} \leq R_{cut}} \Delta E_{IJ} + \sum_{I>J}^{R_{IJ} > R_{cut}} \Delta E_{IJ}^{sep}$$

$$E^{EFP2} = E^{Coul} + E^{pol} + E^{disp} + E^{exrep} + E^{ct}$$

$$E^{EFMO} = \sum_I E_I^0 + \sum_{I>J}^{R_{IJ} \leq R_{cut}} (\Delta E_{IJ}^0 - E_{IJ}^{pol}) + \sum_{I>J}^{R_{IJ} > R_{cut}} E_{IJ}^{Coul} + E_{tot}^{pol}$$

## The Effective Fragment Molecular Orbital Method

$$E^{EFMO} = \sum_I E_I^0 + \sum_{I>J}^{R_{I,J} \leq R_{cut}} (\Delta E_{IJ}^0 - E_{IJ}^{pol}) + \sum_{I>J}^{R_{I,J} > R_{cut}} E_{IJ}^{Coul} + E_{tot}^{pol}$$

The use of isolated fragment energies eliminates the need to calculate the ESP used in standard FMO method calculations.

The many-body interaction energy formerly computed using the ESP is replaced by the total EFP polarization energy.

However, the lack of dispersion limits the EFMO method to HF and DFT calculations.

Additional computational savings could be achieved by reducing the value of  $R_{cut}$

## The Effective Fragment Molecular Orbital Method: Fully Integrated

The original formulation of the total EFMO energy was fully integrated to include all five components of the EFP energy.

$$E^{EFMO} = \sum_I E_I^0 + \sum_{I>J}^{R_{I,J} \leq R_{cut}} (\Delta E_{IJ}^0 - E_{IJ}^{pol}) + \sum_{I>J}^{R_{I,J} > R_{cut}} E_{IJ}^{Coul} + E_{tot}^{pol}$$

$$E^{EFP2} = E^{Coul} + E^{pol} + E^{disp} + E^{exrep} + E^{ct}$$

$$E^{EFMO} = \sum_I E_I^0 + \sum_{I>J}^{R_{I,J} \leq R_{cut}} (\Delta E_{IJ}^0 - E_{IJ}^{pol}) + \sum_{I>J}^{R_{I,J} > R_{cut}} (E_{IJ}^{Coul} + E_{IJ}^{disp} + E_{IJ}^{exrep} + E_{IJ}^{ct}) + E_{tot}^{pol}$$

By including all intermolecular interactions, the user defined cut-off value  $R_{cut}$  can be reduced to neglect additional QM dimers.

The reduction in QM dimers lowers the computational requirements of FIEFMO calculations relative to standard FMO method calculations.

## The Effective Fragment Molecular Orbital Method

Average total number of separated and QM dimers

$R_{cut}$	8 waters		16 waters		32 waters		64 waters	
	separated	QM	separated	QM	separated	QM	separated	QM
0.6	28	0	120	0	496	0	2016	0
0.8	16	12	93	27	444	52	1904	112
1.4	5	23	65	55	363	133	1730	286
2.0	0	28	30	90	237	259	1418	598

## The Effective Fragment Molecular Orbital Method

Average Signed Errors  
(kcal/mol)

R <sub>cut</sub>	6-31++G(d,p)		6-311++G(3df,2p)	
	FMO2	FIEFMO	FMO2	FIEFMO
8 water molecules				
0.6	-104.1	18.6	-104.4	2.3
0.8	-7.2	-5.7	-8.5	-8.5
1.4	-12.5	-8.4	-20.8	-9.4
2.0	-14.1	-8.8	-22.9	-9.6
32 water molecules				
0.6	-642.2	122.3	-654.2	16.2
0.8	-40.3	-25.6	-61.0	-57.0
1.4	-79.9	-45.8	-153.3	-64.2
2.0	-111.9	-53.9	-204.5	-65.6

$$Error = \frac{\sum_{i=1}^n (E_i^X - E_i^{MP2})}{n}$$

## The Effective Fragment Molecular Orbital Method

Binding Energy per Water Molecule  
(kcal/mol)

R <sub>cut</sub>	6-31++G(d,p)			6-311++G(3df,2p)		
	FMO2	FIEFMO	MP2	FMO2	FIEFMO	MP2
8 water molecules						
0.6	-23.7	-8.4	-10.7	-22.3	-9.0	-9.3
0.8	-11.6	-11.4	-10.7	-10.3	-10.3	-9.3
1.4	-12.3	-11.7	-10.7	-11.9	-10.4	-9.3
2.0	-12.4	-11.8	-10.7	-12.1	-10.5	-9.3
32 water molecules						
0.6	-30.9	-7.0	-10.8	-29.7	-8.8	-9.3
0.8	-12.1	-11.6	-10.8	-11.2	-11.1	-9.3
1.4	-13.3	-12.2	-10.8	-14.1	-11.3	-9.3
2.0	-14.3	-12.5	-10.8	-15.7	-11.3	-9.3



## The Effective Fragment Molecular Orbital Method

Timings performed on 10 nodes containing six 2.67 GHz Xeon X5650 cores per node with 24 GB of RAM

MP2/6-311++G(3df,2p)							
	FIEFMO		FMO2		FMO3		MP2
R <sub>cut</sub>	wall time	error	wall time	error	wall time	error	wall time
	8 Water Molecules + 2 Benzene Molecules						
0.6	602	6.6	1414	-65.8			
2.0	2178	-4.9	2825	-17.9	6391	-3.2	3955
	8 Water Molecules + 8 Methanol Molecules						
0.6	15	8.1	70	-149.8			
2.0	151	-8.3	224	-40.2	2268	-22.1	6793

Times are in seconds, and errors are in kcal/mol

# The Fragment Molecular Orbital Method

## Important GAMESS modules

\$FMO

\$GDDI: Specifies parallel run

\$FMOPRP: Sets up convergers, properties

\$FMOXYZ: Similar to \$DATA

\$FMOBND: Bond detachment description

\$OPTFMO: Geometry optimization driver

\$FMOHYB (\$FMOLMO): Fragmentation

The Fragment Molecular Orbital Method  
Example Input

```

$CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE MLEVEL=2 NPRINT=-5 $END
$CONTRL ISPHER=1 $END
$SYSTEM MWORDS=50 MEMDDI=8000 $END
$BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 $END
$BASIS DIFFS=.T. DIFFSP=.T. $END
$GDDI NGROUP=4 $END
$SCF DIRSCF=.T. $END
$STATPT NSTEP=1000 $END
$FMO
  NFRAG=4 NBODY=2
  MLEVEL(1)=2
  INDAT(1)= 0, 1, -11,
            0, 12, -18,
            0, 19, -29,
            0, 30, -36,
            0
  ICHARG(1)= 1, -1, 1, -1
  RESPAP=0 RESPPC=-1 RESDIM=4 RCORS=4
$END
$FMOPRP NPRINT=9 $END
$DATA

C1
H 1
C 6
N 7
O 8
$END
$FMOXYZ
N      7      -1.6436481742      6.5598603693      4.0549010799
N      7      -.6017808482      5.7521648546      4.3580412698
C      6      -.8929974200      4.8890111712      5.3232025052
N      7      -2.1613988514      5.1484280856      5.6809101978
C      6      -2.6022957882      6.1640265300      4.8770830604
H      1      .2831062363      5.7552108350      3.7923507454

```

```
$CONTRL RUNTYP=ENERGY MPLEVL=2 ISPHER=1 $END
$SYSTEM MWORDS=25 MEMDDI=400 $END
$BASIS GBASIS=ACCT $END
$GDDI NGROUP=1 $END
$SCF DIRSCF=.T. $END
$FMO
      NFRAG=6 NBODY=2 NACUT=3
      RESPAP=0 RESPPC=-1 RESDIM=2 RCORSD=2 MODESP=0
$END
$FMOPRP NPRINT=9 $END
$DATA
```

C1

H 1

O 8

\$END

\$FMOXYZ

O	8	-1.84679782	2.23116016	-0.31192821
H	1	-2.23259687	2.50892782	-1.14672530
H	1	-2.22940755	1.34182882	-0.13609287
O	8	0.80815905	2.58311296	0.04697235
H	1	-0.15681353	2.44873357	-0.09081087
H	1	0.87301040	3.18262029	0.79480898
O	8	1.36333847	-2.01869607	0.46308863
H	1	1.74867976	-2.29597974	1.29825509
H	1	1.74594593	-1.12941432	0.28699148
O	8	2.42866755	0.42117196	0.00092104
H	1	1.83418584	1.20489240	0.02542342
H	1	2.96642685	0.53956872	-0.78626174
O	8	-1.29129207	-2.37041116	0.10248699
H	1	-1.35570943	-2.96969914	-0.64555788

```
$CONTRL RUNTYP=ENERGY MPEVL=2 ISPHER=1 $END
$SYSTEM MWORDS=25 MEMDDI=400 $END
$BASIS GBASIS=ACCT $END
$GDDI NGROUP=1 $END
$SCF DIRSCF=.T. $END
$FMO
      NFRAG=6 NBODY=3 NACUT=3
      RESPAP=0 RESPPC=-1 RESDIM=4.5 RCORS=4
      RITRIM(1)=2,-1,2.5,2 MODESP=0
$END
$FMOPRP NPRINT=9 $END
$DATA
```

C1

H 1

O 8

\$END

\$FMOXYZ

O	8	-1.84679782	2.23116016	-0.31192821
H	1	-2.23259687	2.50892782	-1.14672530
H	1	-2.22940755	1.34182882	-0.13609287
O	8	0.80815905	2.58311296	0.04697235
H	1	-0.15681353	2.44873357	-0.09081087
H	1	0.87301040	3.18262029	0.79480898
O	8	1.36333847	-2.01869607	0.46308863
H	1	1.74867976	-2.29597974	1.29825509
H	1	1.74594593	-1.12941432	0.28699148
O	8	2.42866755	0.42117196	0.00092104
H	1	1.83418584	1.20489240	0.02542342
H	1	2.96642685	0.53956872	-0.78626174

```
$fmo
nbody=2
scftyp(1)=rhf
modgrd=16 scffrg(1)=rhf,rhf,rhf,rhf,rhf
mult(1)=1,1,1,1,1
nfrag=5 nlayer=1
icharg(1)= 0, 0, 0, 0, 0
frgnam(1)= ala001, ala002, phe003, ala004, ala005
indat(1)= 0
      1   -6
      7  -10   13  -16    0
     11   12   17  -20   23  -26    0
     21   22   27  -30   33  -46    0
     31   32   47  -50   53  -56    0
     51   52   57  -60   63  -66
     61   62   67  -72    0

$end
$data
alpha /ACE-ALA/-ALA/-PHE/-ALA/-ALA-NME/
c1
h-1 1 1 0 0
c-1 6 2 0 0
n-1 7 3 0 0
o-1 8 4 0 0
$end
```

**\$FMOLMO**

6-31G\* 15 5  
1 0 -0.065034 0.288264 0.000000 0.000000 0.604413  
0.290129 0.000000 0.000000 0.319045 -0.017106  
-0.017106 0.057935 0.000000 0.000000 0.000000  
0 1 -0.065041 0.288294 0.569833 0.000000 -0.201457  
0.290147 0.300784 0.000000 -0.106342 0.049599  
-0.017106 -0.008771 0.000000 -0.027223 0.000000  
0 1 -0.065040 0.288293 -0.284917 -0.493490 -0.201456  
0.290146 -0.150393 -0.260487 -0.106341 -0.000428  
0.032923 -0.008771 0.033353 0.013612 0.023577  
0 1 -0.065040 0.288293 -0.284917 0.493490 -0.201456  
0.290146 -0.150393 0.260487 -0.106341 -0.000428  
0.032923 -0.008771 -0.033353 0.013612 -0.023577  
0 1 1.010938 -0.011976 0.000000 0.000000 0.000000  
-0.054085 0.000000 0.000000 -0.000001 -0.003175  
-0.003175 -0.003175 0.000000 0.000000 0.000000

MINI 5 5

1 0 -0.104883 0.308874 0.000000 0.000000 0.521806  
0 1 -0.104883 0.308874 0.491961 0.000000 -0.173934  
0 1 -0.104883 0.308876 -0.245980 -0.426050 -0.173933  
0 1 -0.104883 0.308876 -0.245980 0.426050 -0.173933  
0 1 0.988209 0.063992 0.000000 0.000000 0.000000

Send

**\$FMOBND**

-9 11 6-31G\* MINI  
-19 21 6-31G\* MINI  
-29 31 6-31G\* MINI  
-49 51 6-31G\* MINI

Send

**\$fmoxyz**

1 H 0.19300000 0.04100000 0.10200000  
2 C -0.41100001 0.93599999 -0.03500000  
3 H 0.14399999 1.65600002 -0.63499999