OpenMX Tutorial

- First trial
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- Recommended trials
- OpenMX Viewer

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First trial

- Login

  For the tutorial, we will use DeltaServer, please login the machine.

- A trial calculation

  As a first step, please try to perform a SCF calculation for a methane molecule.

DeltaServer

Intel(R) Xeon(R) CPU E5520 @ 2.27GHz

192 cores (4 cores×48 processers) are available in total.

Login

$ ssh –YC userid@10.105.17.42

As for your account name and password, please look at the word file you received.

How to compile OpenMX

(1) Go to http://www.openmx-square.org/download.html
(2) Download openmx3.8.tar.gz and the patch
(3) Follow the instruction at
http://www.openmx-square.org/tech_notes/OpenMX-Compile.pdf

See also the page 11 in the manual.

Environment setting

Once you login DeltaServer, please do first the following:

```
$ make work
$ cp -rf /home/soft/openmx3.8/work/* ./work/
$ cd work
$ rm –rf *_rst
$ rm *.cube *.md *.md2 *.ene *.cif *.out *.xyz
```

Then, modify a line in ‘job.pbs’ as

```
$mpirun -machinefile $PBS_NODEFILE -np $ncpu $openmx Methane.dat -nt 2 > met.std
```

And, add a line in ‘Methane.dat’ as

```
DATA.PATH           /home/soft/openmx3.8/DFT_DATA13
```

A test calculation: Methane.dat

As a first trial calculation, let's try to calculate a methane molecule by

$ qsub job.pbs

After finishing the calculations, you will obtain 11 files and 1 directory.

met.std	standard output of the SCF calculation
met.out	input file and standard output
met.xyz	final geometrical structure
met.ene	values computed at every MD step
met.md	geometrical structures at every MD step
met.md2	geometrical structure of the final MD step
met.cif	cif file of the initial structure for Material Studio
met.tden.cube	total electron density in the Gaussian cube format
met.v0.cube	Kohn-Sham potential in the Gaussian cube format
met.vhart.cube	Hartree potential in the Gaussian cube format
met.dden.cube	difference electron density measured from atomic density
met_rst/	directory storing restart files

See the 17 p in the manual.

Methane.dat

```
kterm
[ozaki@vtpcc01 work]$ more Methane.dat
#
#  SCF calculation of a methane molecule by the LDA
#  and the cluster method
#

#
# File Name
#

System.CurrrentDirectory         ./    # default=./
System.Name                      met
level.of.stdout                    1    # default=1 (1-3)
level.of.fileout                   1    # default=1 (0-2)

#
# Definition of Atomic Species
#

Species.Number       2
<Definition.of.Atomic.Species
 H    H4.0-s1          H_TM
 C    C4.5-s1p1        C_TM_PCC
Definition.of.Atomic.Species>

#
# Atoms
#

Atoms.Number         5
Atoms.SpeciesAndCoordinates.Unit   Ang # Ang|AU
<Atoms.SpeciesAndCoordinates
 1  C      0.000000    0.000000    0.000000     2.0  2.0
 2  H     -0.889981   -0.629312    0.000000     0.5  0.5
 3  H      0.000000    0.629312   -0.889981     0.5  0.5
 4  H      0.000000    0.629312    0.889981     0.5  0.5
 5  H      0.889981   -0.629312    0.000000     0.5  0.5
Atoms.SpeciesAndCoordinates>
```

(1) Value behind keyword
(2) The order is arbitrarily.
(3) Put # to the head of line for comment

Selected keywords:

The name of system

The number of atoms

Definition of species

Atomic coordinates

met.out

SCF history

```
************************************************************
************************************************************
                SCF history at MD= 1
************************************************************
************************************************************

  SCF=   1  NormRD=  1.000000000000  Uele= -3.523143659974
  SCF=   2  NormRD=  0.567253699744  Uele= -4.405605131921
  SCF=   3  NormRD=  0.103433490729  Uele= -3.982266241934
  SCF=   4  NormRD=  0.024234990593  Uele= -3.906896836134
  SCF=   5  NormRD=  0.011006215697  Uele= -3.893084558820
  SCF=   6  NormRD=  0.006494145332  Uele= -3.890357113476
  SCF=   7  NormRD=  0.002722267527  Uele= -3.891669816209
  SCF=   8  NormRD=  0.000000672350  Uele= -3.889285164733
  SCF=   9  NormRD=  0.000000402419  Uele= -3.889285102456
  SCF=  10  NormRD=  0.000000346348  Uele= -3.889285101128
  SCF=  11  NormRD=  0.000000515395  Uele= -3.889285101063
```

KS eigenvalues

```
************************************************************
************************************************************
          Eigenvalues (Hartree) for SCF KS-eq.
************************************************************
************************************************************

   Chemical Potential (Hartree) =   0.00000000000000
   Number of States             =   8.00000000000000
   HOMO =  4
   Eigenvalues
                Up-spin            Down-spin
         1  -0.69897190537228  -0.69897190537228
         2  -0.41522646150979  -0.41522646150979
         3  -0.41522645534084  -0.41522645534084
         4  -0.41521772830844  -0.41521772830844
         5   0.21218282298348   0.21218282298348
         6   0.21218282358344   0.21218282358344
         7   0.21227055734372   0.21227055734372
         8   0.24742493684297   0.24742493684297
```

Total energy

```
************************************************************
      Total energy (Hartree) at MD = 1
************************************************************

  Uele.          -3.889285101063

  Ukin.           5.533754016241
  UH0.          -14.855520072374
  UH1.            0.041395625260
  Una.           -5.040583803800
  Unl.           -0.134640939010
  Uxc0.          -1.564720823137
  Uxc1.          -1.564720823137
  Ucore.          9.551521413583
  Uhub.           0.000000000000
  Ucs.            0.000000000000
  Uzs.            0.000000000000
  Uzo.            0.000000000000
  Uef.            0.000000000000
  UvdW            0.000000000000
  Utot.          -8.033515406373
```

Mulliken population

```
************************************************************
************************************************************
                Mulliken populations
************************************************************
************************************************************

  Total spin S =  0.000000000000

                    Up spin      Down spin      Sum          Diff
     1    C      2.509755704  2.509755704  5.019511408  0.000000000
     2    H      0.372561098  0.372561098  0.745122197  0.000000000
     3    H      0.372561019  0.372561019  0.745122038  0.000000000
     4    H      0.372561127  0.372561127  0.745122254  0.000000000
     5    H      0.372561051  0.372561051  0.745122102  0.000000000

 Sum of MulP: up   =     4.00000 down         =     4.00000
              total=     8.00000 ideal(neutral)=     8.00000
```

Specification of the directory storing *.pao and *.vps

The directory *DFT_DATA* can be specified by the keyword in your input file as

DATA.PATH /home/soft/openmx3.8/DFT_DATA13

Database of PAO and VPS

http://www.jaist.ac.jp/~t-ozaki/vps_pao2013/

Database (2013) of optimized VPS and PAO

The database (2013) of fully relativistic pseudopotentials (VPS) and pseudo-atomic orbitals (PAO), generated by ADPACK, which could be an input data of program package, OpenMX. The data of elements with the underline are currently available. When you use these data, VPS and PAO, in the program package, OpenMX, then copy them to the directory, openmx*.*/DFT_DATA13/VPS/ and openmx*.*/DFT_DATA13/PAO/, respectively. The delta factor of OpenMX with the database (2013) is found at here.

Public release of optimized and well tested VPS and PAO so that users can easily start their calculations.

E																	
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	A															
	L	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
	A	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

Specification of PAO and VPS

PAO and VPS are specified by the following keyword:

```
<Definition.of.Atomic.Species
  O    O7.0-s2p2d1       O_PBE13
  H    H7.0-s2p1         H_PBE13
Definition.of.Atomic.Species>
```

- O7.0 means O7.0.pao.
- -s2p2d1 means 2, 2, and 1 radial functions are allocated to s-, p-, and d-orbitals.
- In this case, for oxygen atom, 2×1+2×3+1×5=13 basis functions are allocated.
- O_PBE13 meand O_PBE13.vps.

The path for O7.0.pao and O_PBE13.vps is specified by

DATA.PATH /home/soft/openmx3.8/DFT_DATA13

Default value is '../DFT_DATA13'.

How to choose basis functions: H_2O case

By clicking H7.0.pao and O7.0.pao in the database(2013), you may find the following

http://www.jaist.ac.jp/~t-ozaki/vps_pao2013/H/index.html

http://www.jaist.ac.jp/~t-ozaki/vps_pao2013/O/index.html

H7.0.pao

```
**************************************************
  Eigen values(Hartree) of pseudo atomic orbitals
**************************************************

Eigenvalues
Lmax= 3 Mul=15
  | mu    0  0     -0.23595211038442   <- 3
  | mu    0  1      0.14109389991827   <- 6
  | mu    0  2      0.61751730037441
  | mu    0  3      1.31890671598573
  | mu    0  4      2.24052765608302
  | mu    0  5      3.37954791544661
  | mu    0  6      4.73488369825610
  | mu    0  7      6.30608874470710
  | mu    0  8      8.09282718517299
  | mu    0  9     10.09464035732420
  | mu    0 10     12.31085267019158
  | mu    0 11     14.74057314485273
  | mu    0 12     17.38277845742691
  | mu    0 13     20.23645090753857
  | mu    0 14     23.30073926597344   <- 5
  | mu    1  0      0.10914684890465
  | mu    1  1      0.47776040452236
  | mu    1  2      1.06988680483686
  | mu    1  3      1.88261331124981
  | mu    1  4      2.91175885838084
  | mu    1  5      4.15601184789448
  | mu    1  6      5.61454131060210
  | mu    1  7      7.28681796296307
  | mu    1  8      9.17254361476158
  | mu    1  9     11.27156766390586
  | mu    1 10     13.58381334569800
  | mu    1 11     16.10921637499960
  | mu    1 12     18.84767560575107
  | mu    1 13     21.79902110024685
  | mu    1 14     24.96300480798286
  | mu    2  0      0.27851528500170
  | mu    2  1      0.76970400958463
  | mu    2  2      1.47576814497054
  | mu    2  3      2.39881523735167
  | mu    2  4      3.53713346447754
```

O7.0.pao

```
**************************************************
  Eigen values(Hartree) of pseudo atomic orbitals
**************************************************

Eigenvalues
Lmax= 3 Mul=15
  | mu    0  0     -0.87913976280231   <- 1
  | mu    0  1      0.06809061901229   <- 4
  | mu    0  2      0.52709275865941
  | mu    0  3      1.24995140722317
  | mu    0  4      2.21829552402723
  | mu    0  5      3.41945468859267
  | mu    0  6      4.84509607059749
  | mu    0  7      6.48825090142865
  | mu    0  8      8.34207134316001
  | mu    0  9     10.39973244132192
  | mu    0 10     12.65513764955926
  | mu    0 11     15.10428688136984
  | mu    0 12     17.74677530362947
  | mu    0 13     20.58633940582683
  | mu    0 14     23.62957122674031   <- 2
  | mu    1  0     -0.33075182895384
  | mu    1  1      0.16376499567753   <- 7
  | mu    1  2      0.64129274864838
  | mu    1  3      1.35995471521821
  | mu    1  4      2.31377697411480
  | mu    1  5      3.50052618379026
  | mu    1  6      4.91841590421346
  | mu    1  7      6.56499793348396
  | mu    1  8      8.43634105410091
  | mu    1  9     10.52733540479795
  | mu    1 10     12.83276989780839
  | mu    1 11     15.34880171573570
  | mu    1 12     18.07414632417004
  | mu    1 13     21.01013110934429
  | mu    1 14     24.15933607166566   <- 8
  | mu    2  0      0.26162948257116
  | mu    2  1      0.70705247436937
  | mu    2  2      1.34714706672243
  | mu    2  3      2.19799459356269
  | mu    2  4      3.26511989658328
```

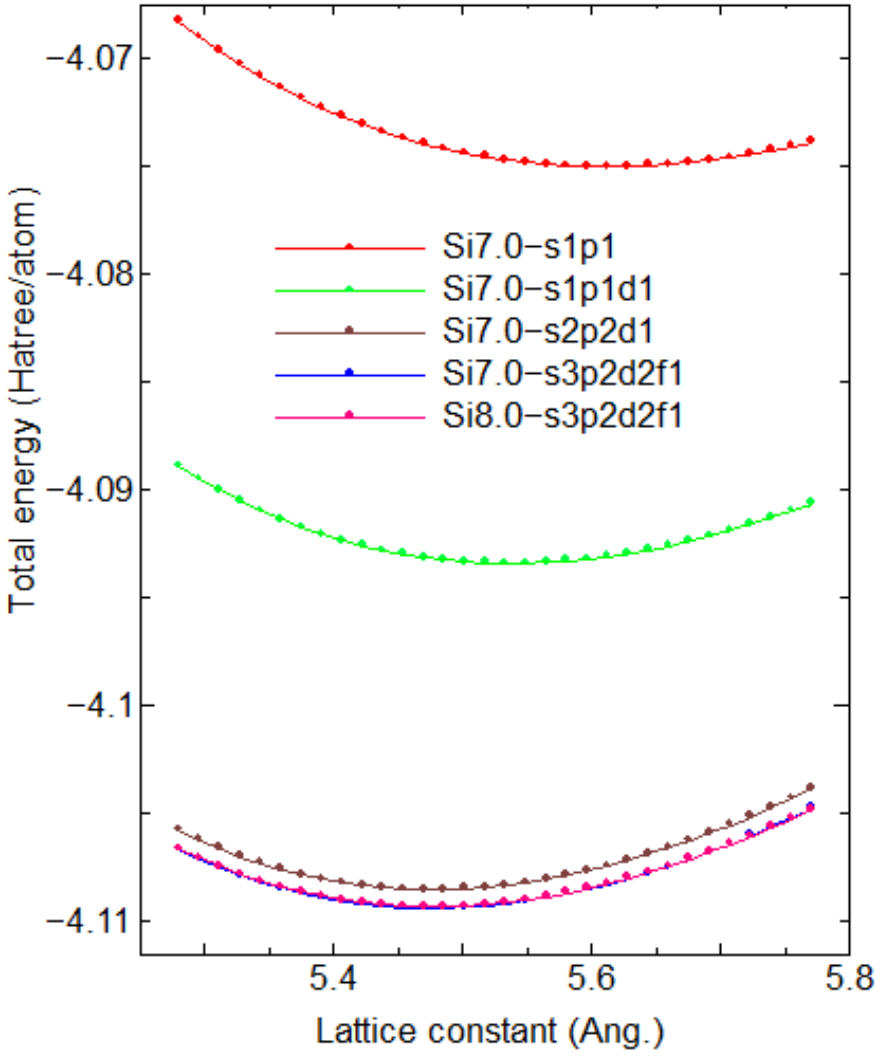
Choosing states with lower eigenvalues leads to H7.0-s2p1 and O7.0-s2p2d1.

How to choose basis functions: Si case(1)

Si7.0.pao

```
Eigenvalues
Lmax= 3 Mul=15
 | mu    0  0     -0.59320968623145 1
 | mu    0  1      0.01654247265872 4
 | mu    0  2      0.57915688461708 8
 | mu    0  3      1.39915528592998
 | mu    0  4      2.43106703909053
 | mu    0  5      3.63498884739274
 | mu    0  6      4.99885012002783
 | mu    0  7      6.55485759476897
 | mu    0  8      8.33541526908920
 | mu    0  9     10.34055461939939
 | mu    0 10     12.55818051232040
 | mu    0 11     14.98369777887096
 | mu    0 12     17.62014479571136
 | mu    0 13     20.47011746372617
 | mu    0 14     23.53245309073866
 | mu    1  0     -0.31460013133101 2
 | mu    1  1      0.12937640798489 5
 | mu    1  2      0.71637380083701
 | mu    1  3      1.54488697995006
 | mu    1  4      2.59211686526084
 | mu    1  5      3.84687324239366
 | mu    1  6      5.31246180826158
 | mu    1  7      6.99509799702661
 | mu    1  8      8.89454075291723
 | mu    1  9     11.00602102880752
 | mu    1 10     13.32692005826443
 | mu    1 11     15.85857455673626
 | mu    1 12     18.60272353142246
 | mu    1 13     21.55894843635971
 | mu    1 14     24.72602323954447
 | mu    2  0      0.01886411574821 3
 | mu    2  1      0.35893514996065 7
 | mu    2  2      0.94629918754692
 | mu    2  3      1.76201765644983
 | mu    2  4      2.81418723624388
 | mu    2  5      4.10656012645961
 | mu    2  6      5.63661971875011
 | mu    2  7      7.39522693820483
 | mu    2  8      9.37222098331867
 | mu    2  9     11.56227937764802
 | mu    2 10     13.96620568880690
 | mu    2 11     16.58651812641581
 | mu    2 12     19.42296574188659
 | mu    2 13     22.47308081363278
 | mu    2 14     25.73538272482773
 | mu    3  0      0.28356769151846 6
 | mu    3  1      0.79082836114569
 | mu    3  2      1.52992065308726
 | mu    3  3      2.52537261496132
```

Orbitals with lower eigenvalues in Si7.0.pao are taken into account step by step as the quality of basis set is improved.

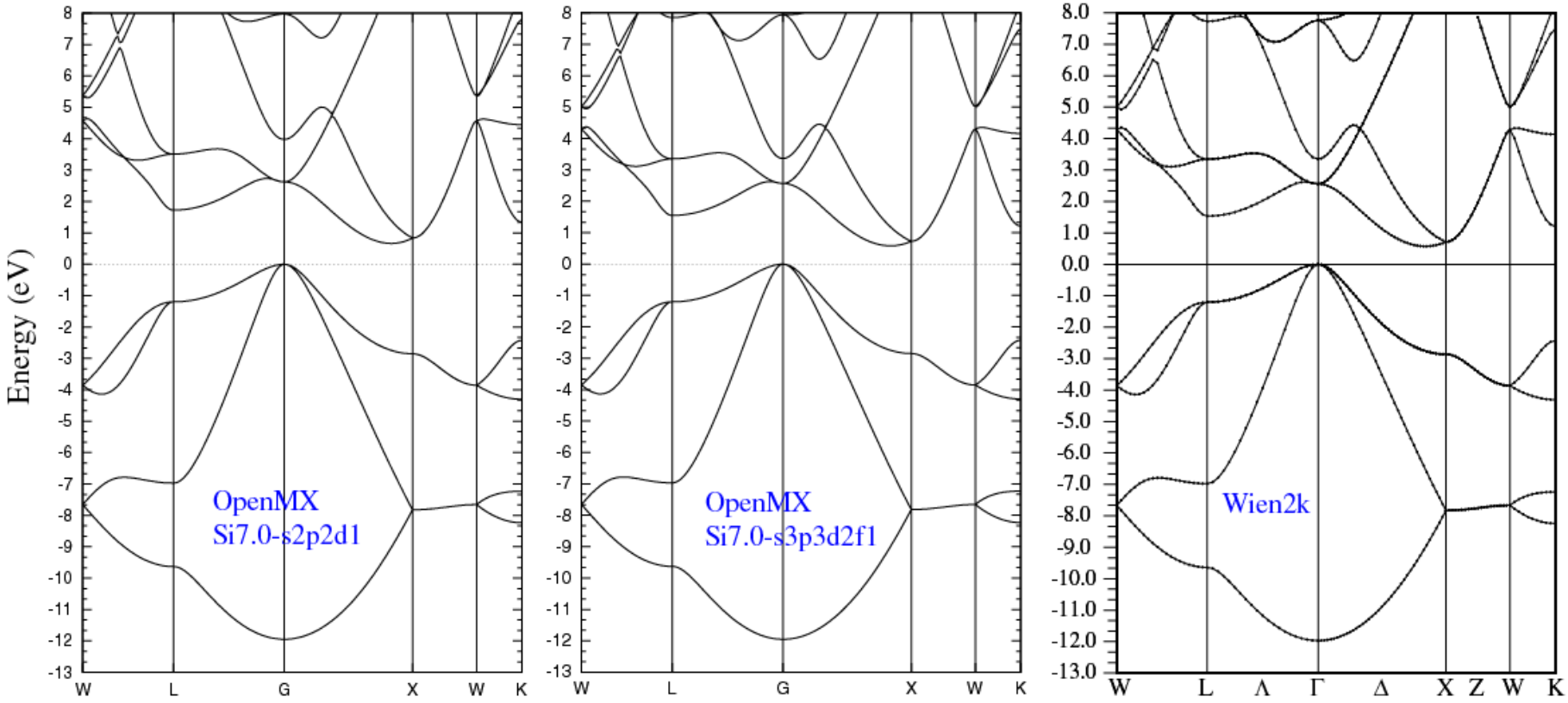


Si7.0-s2p2d1 is enough to discuss structural properties.

By comparing Si7.0-s3p2d2f1 with Si8.0-s3p2d2f1, it turns out that convergence is achieved at the cutoff of 7.0(a.u.).

How to choose basis functions: Si case(2)

With respect to band structure, one can confirm that Si7.0-s2p2d1 provides a nearly convent result.



While the convergent result is achieved by use of Si7.0-s3p2d2f1(Si7.0-s3p3d2f1), Si7.0-s2p2d1 is a balanced basis functions compromising accuracy and efficiency to perform a vast range of materials exploration.

Choice of cutoff energy

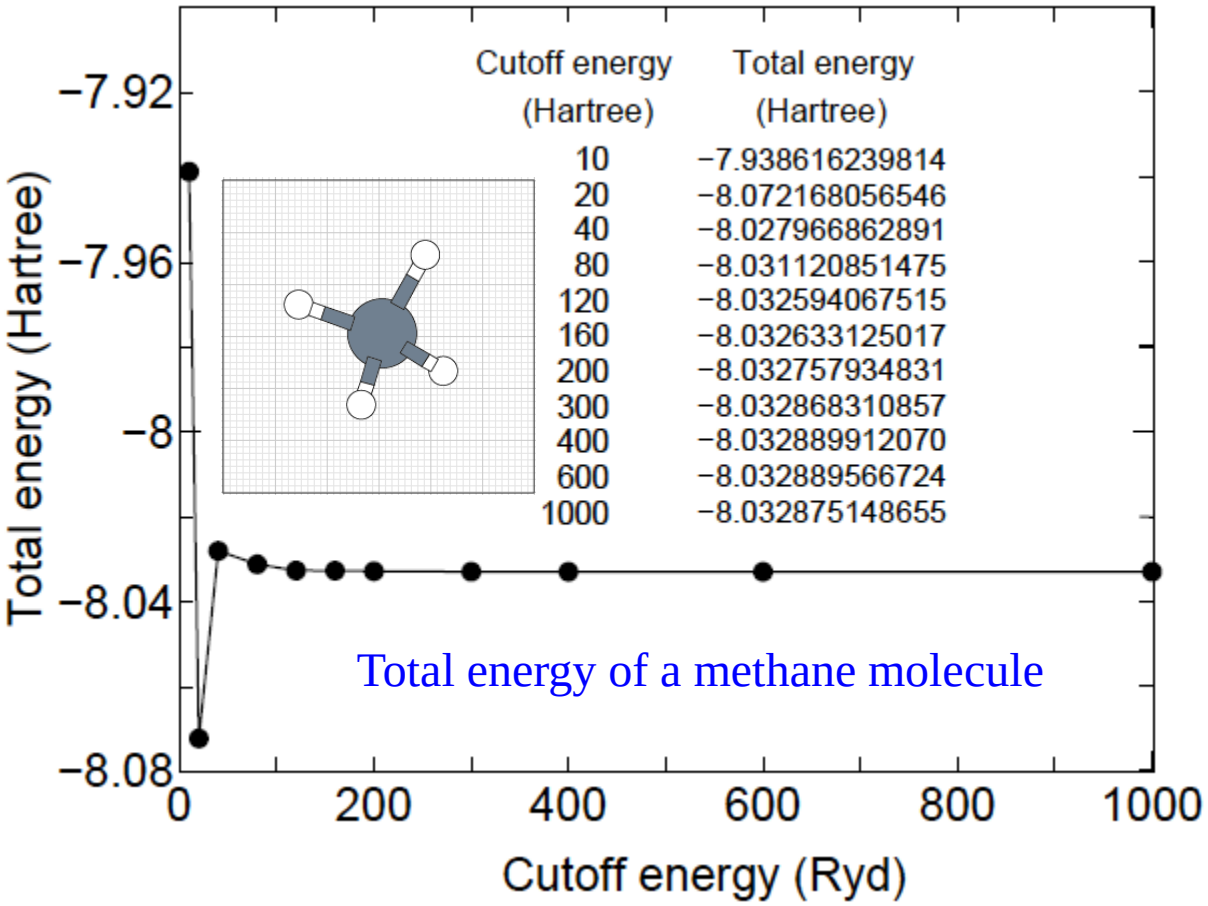
scf.energycutoff 200 # default=150 Ryd

The FFT grid is used to discretize real space and calculate $E_{\delta ee}$, E_{xc}, and can be specified by scf.energycutoff.

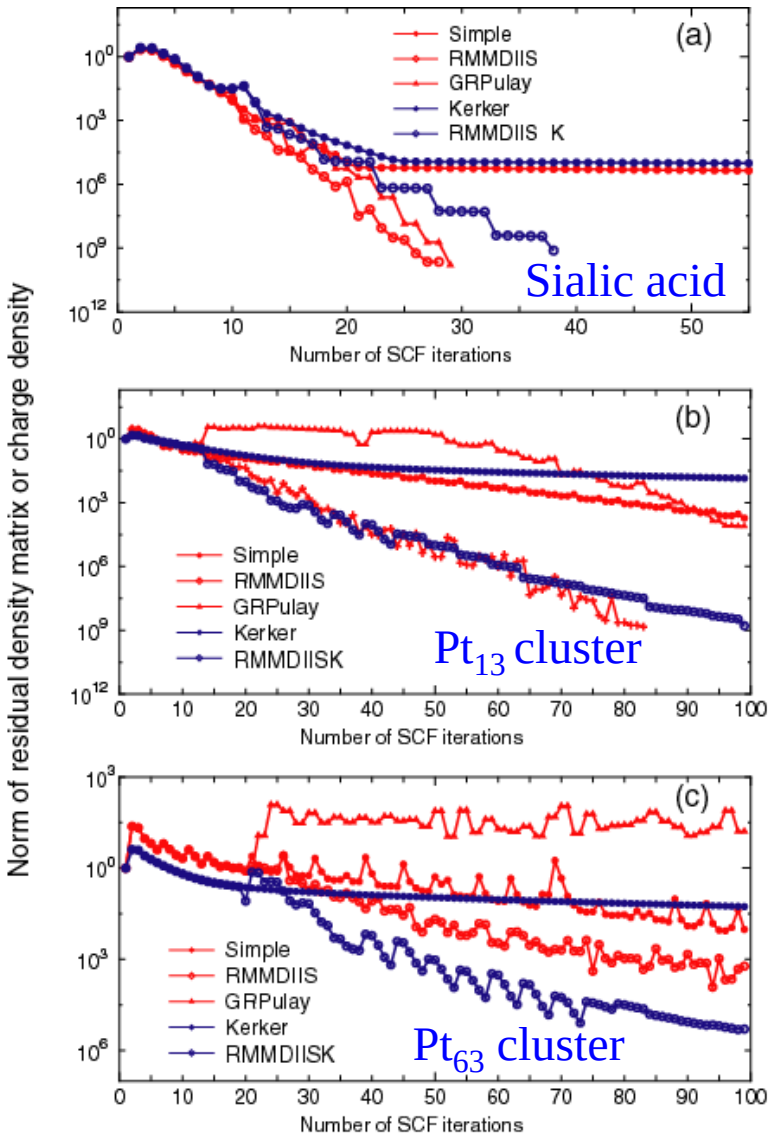
In most cases, 200 Ryd is enough to get convergence.

However, large cutoff energy (300-400 Ryd) has be used cases such as use of pseudopotentials with deep semi-core states.

Memory requiment
$O(E^{3/2})$



Mixing methods



Available mixing methods:

Simple mixing (Simple)

Residual minimization method in the direct inversion iterative subspace (RMM-DIIS)

Guaranteed reduction Pulay method (GR-Pulay)

Kerker mixing (Kerker)

RMM-DIIS with Kerker metric (RMM-DIISK)

RMM-DIIS for Hamiltonian (RMM-DIISH)

Recommendation:
RMM-DIISK or RMM-DIISH

See also the page 56 in the manual.

Visualization

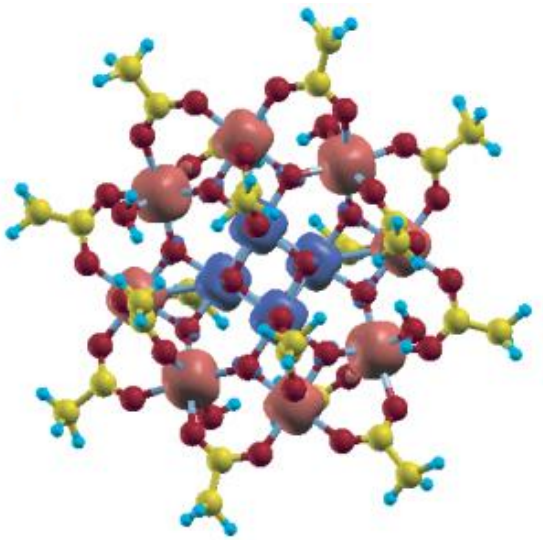
- Cube files such as *.tden.cube, *.sden.cube, *.dden.cube can be visualized by many software such as

  XCrySDen
  VESTA

- Also*.md file is stored in xyz format which can be visualized by XCrySDen and OpenMX Viewer.

  On phi, XCrSDen is available.

- Data on DOS and band dispersion can be visualized by gnuplot.



On the manual

Please download the manual at

http://www.openmx-square.org/openmx_man3.8/openmx3.8.pdf

The manual is self-contained, the most of calculations explained in the manual are traceable by using the input file stored in the directory ‘work’.

Please try to perform those calculations one by one depending on your interests.

Recommended trials

1. Geometry optimization

   Perform a geometry optimization using ‘Methane2.dat’.
   See the page 65 in the manual.

2. Density of states

   Calculate DOS using ‘Cdia.dat’
   See the page 79 in the manual.

All the input files can be found in the directory ‘work’.

3. Wannier functions

   Calculate Wannier functions for Si bulk using ‘work/wf_example/Si.dat’, and perform the band interpolation. See the page 159 in the manual.

4. Reaction barrier by the nudged elastic band (NEB) method

   Calculate a reaction barrier using ‘C2H4_NEB.dat’.
   See the page 182 in the manual.

5. Transmission of a carbon chain

   Calculate an electric transmission of a carbon chain using ‘Lead-Chain.dat’, ‘NEGF-Chain.dat’. See the page 136 in the manual.

6. Spin-orbit coupling

   Calculate a band structure by taking account of SOC using ‘GaAs.dat’.
   See the page 117 in the manual.

Geometry optimization (Methane2.dat)

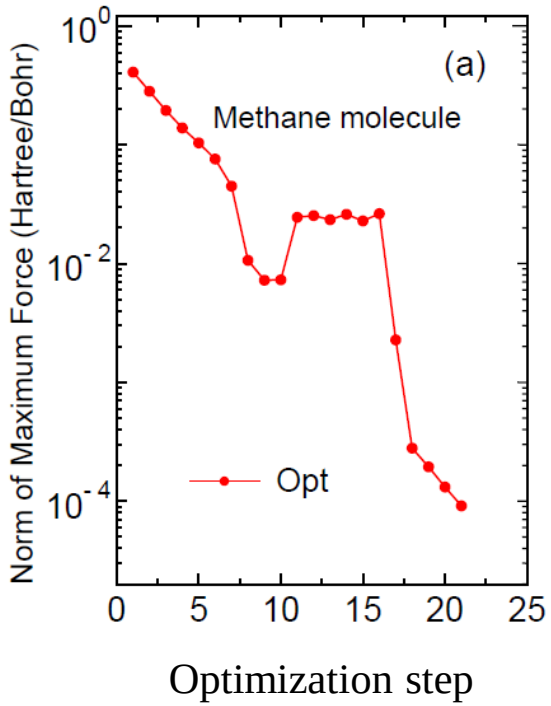
The x-coordinate of a methane molecule is displaced by 0.3 Å, and perform the geometry optimization.

```
<Atoms.SpeciesAndCoordinates
  1   C      0.300000     0.000000     0.000000     2.0   2.0
  2   H     -0.889981    -0.629312     0.000000     0.5   0.5
  3   H      0.000000     0.629312    -0.889981     0.5   0.5
  4   H      0.000000     0.629312     0.889981     0.5   0.5
  5   H      0.889981    -0.629312     0.000000     0.5   0.5
Atoms.SpeciesAndCoordinates>
```

Using the steepest decent (SD) method, the norm of maximum force converges as shown in the left figure:

met2.md can be visualized by OpenMX Viewer.

See also the page 65 in the manual.



Density of states (Cdia.dat)

Density of states (DOS) for Kohn-Sham eigenvalues can be calculated by the following two steps:

(1) SCF calculation

Perform the SCF calculation by ‘Cdia.dat’.

(2) DOS calculation

(2.a) In openmx/source, compile DosMain

$ make DosMain

(2.b) mv work, and perform the DOS calculation using ‘DosMain’.

$ ./DosMain cdia.Dos.Val cdia.Dos.Vec

See also the page 79 in the manual.

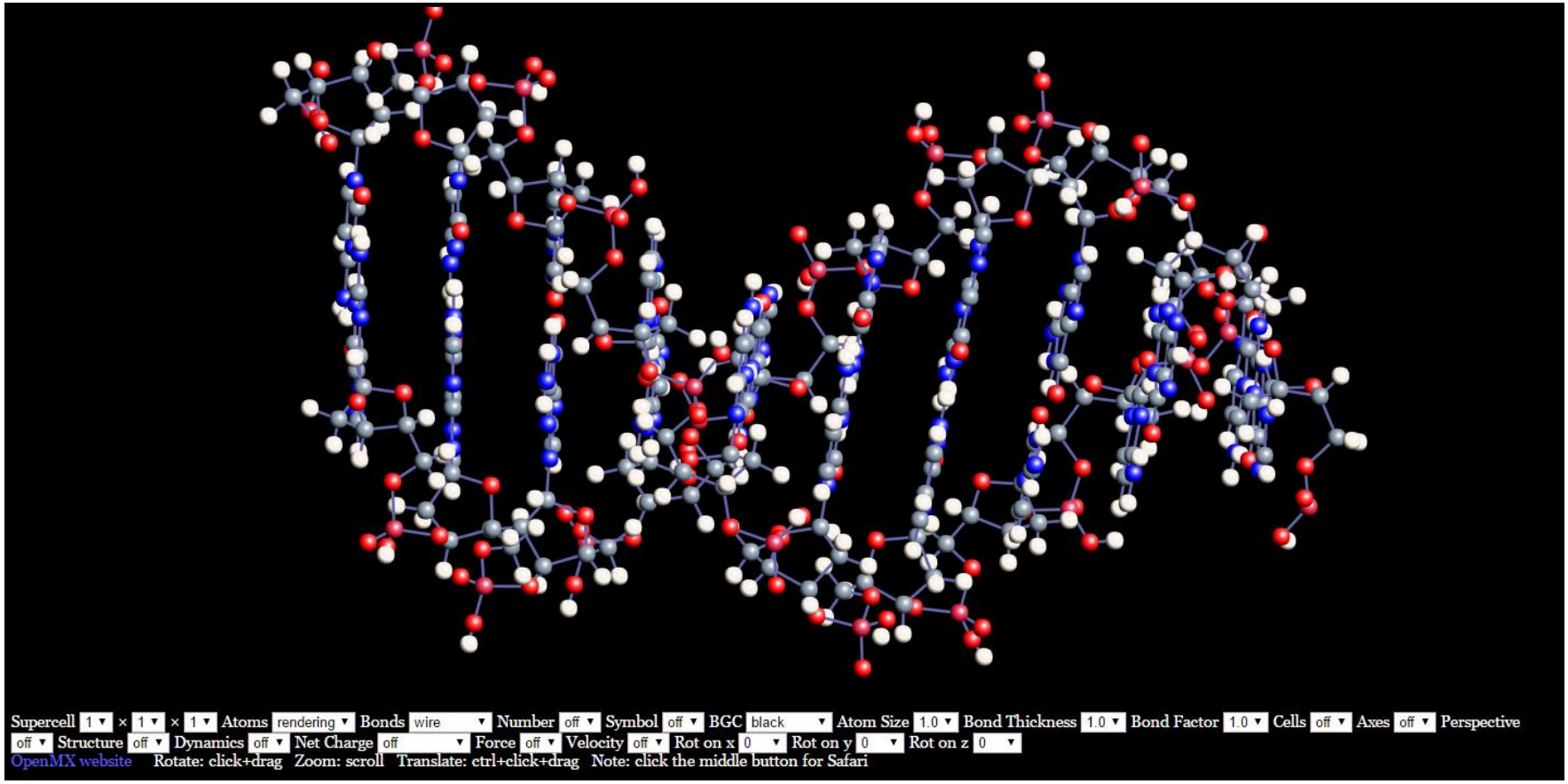
On OpenMX Viewer

http://www.openmx-square.org/viewer/

- 6611 lines written by html5, css3, js, and canvas2d
- dat, xyz, and md files are readable
- Rotation, zoom, and translation
- Easy change of atom size, bond thickness, and bond factor
- Atom index and atom symbol
- Supercell representation
- Structure analysis
- Analysis of geometry optimization
- Charge analysis
- Google Chrome recommended due to its performance

Easy check of a dat file

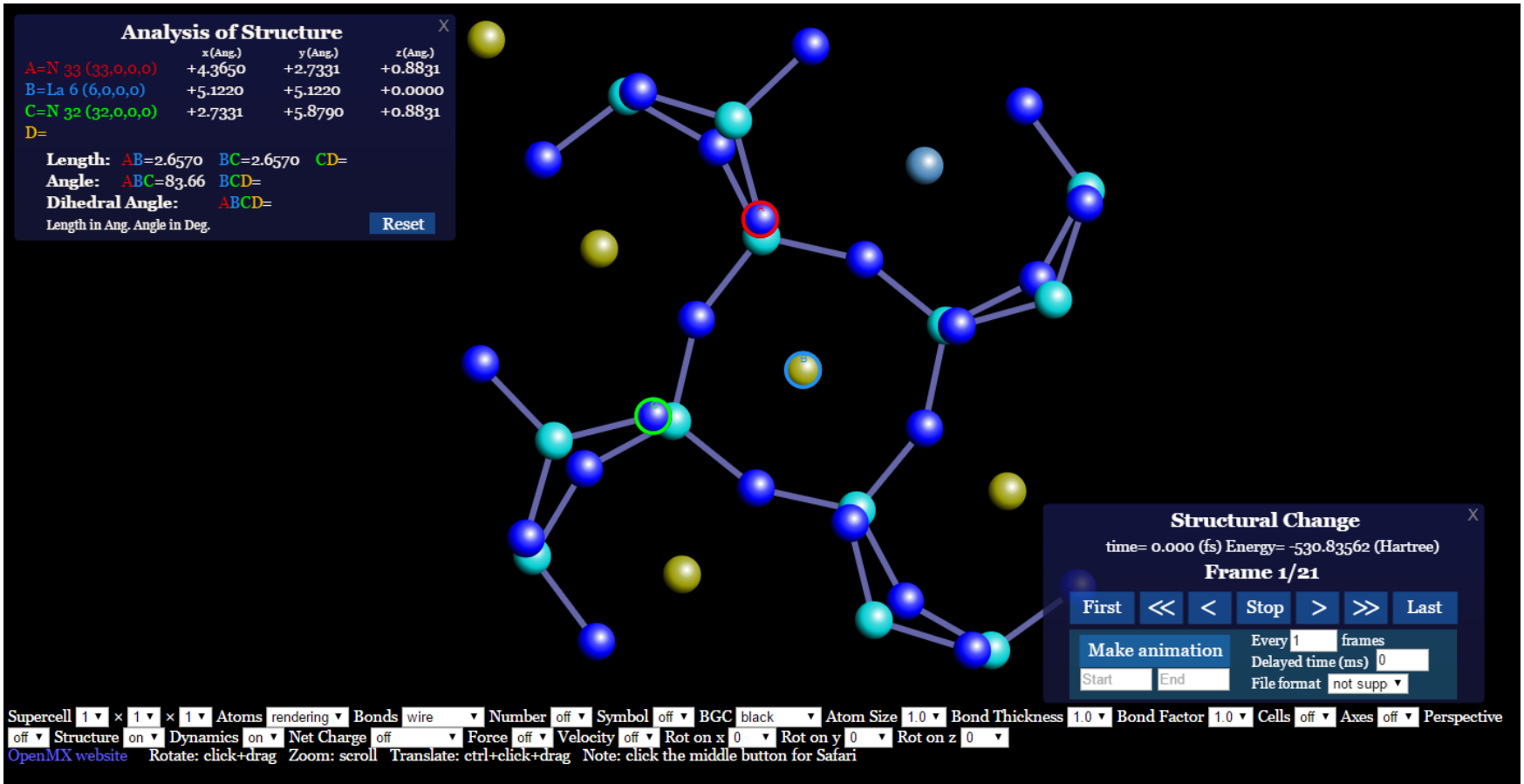
A dat file can be easily checked by drag and drop to any browser.



Analysis of structure optimization

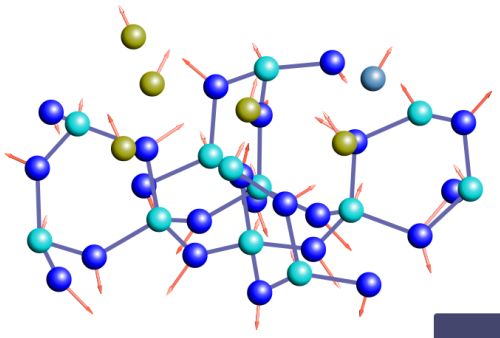
A md file can be easily analyzed by drag and drop to any browser.

- Trace of optimization process
- Analysis of structure
- Check residual forces

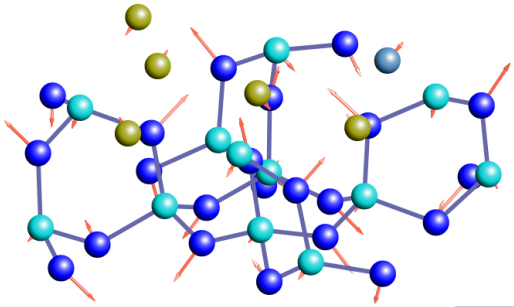


Analysis of structure optimization

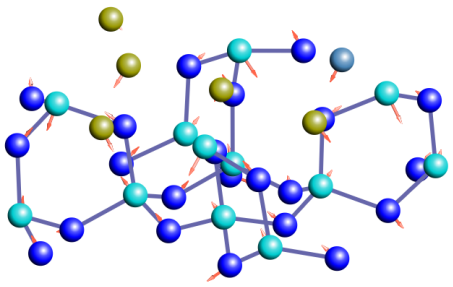
Residual forces can be visualized by vectors.



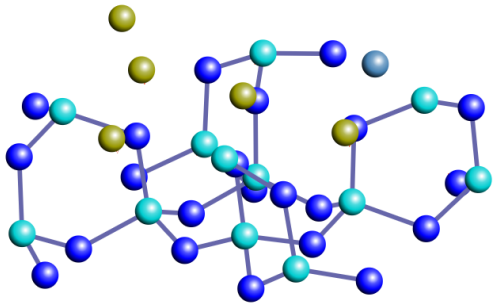
1 step



10 step



14 step



21 step

Analysis of structure optimization

Using a md file, one check easily check spatial charge distribution.