Densitizer

Electronic Structure Analysis Suite of Programs

User's Manual

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Overview

Densitizer is an electronic structure analysis suite of programs which processes Gaussian's formatted checkpoint as input and provide quantum chemical information about the intra/intermolecular electronic structure. *Densitizer* possesses no graphical interface; instead, results are provided as two popular formats .fch and .wfn which enables the user to plot and visualize orbitals and electron density counter maps via many other programs such as GaussView, Multiwfn, AIMAll, AIM2000, etc. *Densitizer* requires no other code/software/platform to be installed on the system and is provided as a standalone executable bundled with manual and sample files in a single extractable `.zip` archive.

On the initial execution of *Densitizer*, the program displays welcome screen including several information about the program and disappears on keyboard hit:

In the second screen, main analysis menu is displayed as below and user is required to input the number of analysis:

```
■ D:\test\dens\Densitize.exe                                          —   □   ×

Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) General Deformation
(11) Natural Deformation
(12) Natural KEP/RLX
(13) Natural Atom
(14) NBO/NLMO Toplogy
(15) Pi-Density Topology
(16) External Potential
(17) Bosonic Molecule
(18) Program's Manual

Enter analysis number: _
```

For more information of what each analysis does and what keywords are required, see Table 1 and the corresponding section in manual.

Preparation of input files and running *Densitizer*

Densitizer accepts absolutely single point jobs, if two or more formatted checkpoint `.fch` files are required as inputs. User must first have optimized the molecule with `opt nosym` keywords, then run required jobs with frozen geometries available in the optimization output; and user must be careful when preparing the single point jobs to make sure all `.fch/.out` files belongs to the same Cartesian coordinates. It can be simply verified by saving molecular geometry as Cartesian coordinate and make multiple copies of the same file with different names and keywords, then run Gaussian for each (see Appendix 4 for visual information). If the analysis require just one `.fch` file (regardless of other file types), *Densitizer* accepts optimization job as well and the required keywords can be applied in the optimization job, directly.

      Densitizer requires formatted checkpoint file (.fch or .fchk) of Gaussian program as input which can be made via `formchk` utility of Gaussian (see Appendix 5 for more information). In some cases, outputs (`.out`) files are also necessary, and Table 1 summarizes required files and keywords. There is no difference between Windows or Linux versions of Gaussian, and *Densitizer* supports formatted checkpoints and outputs of both in Windows platform.

> **All required files must be present in the same directory as *Densitizer* exists; otherwise, error messages appear prompting files not found.**

      If user intend to analyze NBO related analyses including natural KEP/RLX, natural atom, and, NBO/NLMO topology, additional keywords are required in both route and NBO sections, and also a filename in which NBO results are present (see Table 1). *Densitizer* accepts two types of NBO output. First way is direct use of NBO 3.0 program implemented in Gaussian. In this respect, the Gaussian input job looks like something like this:

```
%chk=water.chk
# nosym 6d 10f density pop=nboread iop(3/32=2)

watertest

0 1
O                    -0.04480287    0.50179211    0.00000000
H                     0.91519713    0.50179211    0.00000000
H                    -0.36525745    1.40672794    0.00000000

$NBO AONAO AONBO AONLMO $END
```

Once *Densitizer* prompts to enter NBO filename, user specifies the Gaussian's output filename. Second way is to use external NBO program (e.g., GenNBO) via .47 archive file. In this respect, the Gaussian input job looks like something like this:

```
%chk=water.chk
# nosym 6d 10f density pop=nboread

Watertest

0 1
O                    -0.04480287    0.50179211    0.00000000
H                     0.91519713    0.50179211    0.00000000
H                    -0.36525745    1.40672794    0.00000000

$NBO ARCHIVE FILE=water $END
```

After Gaussian calculation, user should include these keywords in the .47 file and run the external NBO program (see NBO manual for more information):

```
$NBO AONAO AONBO AONLMO $END
```

Once *Densitizer* prompts to enter NBO filename, user specifies the NBO output filename generated by the external NBO program.

If user include no file extension in the filename when *Densitizer* prompts to enter, *Densitizer* automatically searches for .fch and .fchk for formatted checkpoint, and .log, .out, .nbo for NBO results.

All examples of different analyses in the present manual are also located in the `samples` subdirectory of *Densitizer*'s installation directory

and the user is encouraged to run the one which is related to his interest before going ahead.

Once *Densitizer* is run, it asks some questions related to filenames, etc., and when all required information for initialization of program are collected, *Densitizer* read matrices and shows message

```
Computing…
```

at the bottom of main window. After calculation of all requested analyses, message

```
-- Clear --
```

will appears at the bottom which means *Densitizer*'s work is terminated (with or without error) and the user can now close the window, safely. Table 1 includes different analyses, required keywords, (minimum) number and type of input files, and the name of subdirectory in samples folder in which sample files are included.

Table 1. Summary of analyses, required keywords, number and type of required files, and the corresponding subdirectory foldername in the samples. Note that these are just quick samples and user must read the analysis section, carefully.

Analysis	Additional keywords	# Files	Samples
Intermolecular Interaction KEP/RLX/NOCV	nosym 6d 10f density	3 fch	inter
Intermolecular Cooperative Interaction	nosym 6d 10f density	7 fch	coop
Natural Transition Orbitals	nosym 6d 10f density td	2 fch	transition
Field Deformation	nosym 6d 10f density nosym 6d 10f density field=x+100	2 fch	field
Charge Deformation	nosym 6d 10f density	2 fch	charge
Doping Deformation	nosym 6d 10f density gen	2 fch	dope
Asymmetric Deformation	nosym 6d 10f density nosym 6d 10f density field=x+100 nosym 6d 10f density field=x-100	3 fch	asym
Correlation Deformation	nosym 6d 10f density mp2	1 fch	corr
Point-Charge Deformation	nosym 6d 10f density nosym 6d 10f density charge --- 1. 0. 0. 0.	2 fch	point
General Deformation	nosym 6d 10f density	2 fch	general
Natural Deformation	nosym 6d 10f density pop=nboread --- $NBO AONAO AONBO AONLMO $END $NBO ARCHIVE FILE=water $END	1 fch 1 out	naturaldef
Natural KEP/RLX	nosym 6d 10f density pop=nboread --- $NBO AONAO AONBO AONLMO $END $NBO ARCHIVE FILE=water $END	1 fch 1 out	naturalkep
Natural Atom	nosym 6d 10f density pop=nboread --- $NBO AONAO AONBO AONLMO $END $NBO ARCHIVE FILE=water $END	1 fch 1 out	naturalatom
NBO/NLMO Toplogy	nosym 6d 10f density pop=nboread --- $NBO AONAO AONBO AONLMO $END $NBO ARCHIVE FILE=water $END	1 fch 1 out	topo
Pi-Density Topology	nosym 6d 10f density	1 fch	pi
External Potential	nosym 6d 10f density iop(3/33=1,5/33=3)	1 fch 1 out	external
Bosonic Molecule	nosym 6d 10f density iop(3/33=1,5/33=3)	1 fch 1 out	boson

Densitizer output files and visualization

Densitizer creates three type of files `.fch`, `.wfn`, plus a single `.report.txt` file as outputs. While `.wfn` includes electron density, .fch includes both electron density and molecular orbitals; and depending on data, the output `.fch` files may include one or both. Those `.fch` files which are directly located on the results directory, includes both electron density and molecular orbitals data, whiles those located in the `num` subdirectory, includes just electron density data.

In the present manual, GaussView is used for visualization of `.fch`, and AIM2000 for `.wfn` files. Although Multiwfn and AIMAll are also able to open and visualize `.wfn` files, they have some inconsistencies with negative electron density as it is common in deformation electron density maps. On the other hand, for absolute electron densities, these two softwares work and well support `.wfn` files. Since the data included in `.fch` and `.wfn` files differ with their ordinary uses, instructions of how to open, use, and visualize these files are given in Appendices 1 to 3.

In most of cases, *Densitizer* creates a text file `report.txt` in which eigenvelues of deformation density (components) are stored. These eigenvalues also exist in the corresponding `.fch`, where orbital energies are replaced by these eigenvalues and appears if user opens by an appropriate software.

General structure of report file

The `.report.txt` file is a text file beginning with program's information and followed by molecular related parameters on which Gaussian calculations are performed, and is stored in the directory of output results:

```
                 >>>>>>>>>>>>>>>>>>>>>>>>><<<<<<<<<<<<<<<<<<<<<<
                 >>                                        <<
                 >>  D . e . n . s . i . t . i . z . e . r  <<
                 >>                                        <<
                 >>  Electronic Structure Analysis Program  <<
                 >>                                        <<
                 >>>>>>>>>>>>>>>>>>>>>>>>><<<<<<<<<<<<<<<<<<<<<<

Copyright (c) 2019,  Densitizer Ver. 1.1.36, All Rights Reserved.

Cite this program as:
S.M. Azami, Densitizer Ver. 1.1.36 (URL: http://densitizer.orbital.xyz)

Disclaimer:
This program is provided "as is" and comes with no warranty. Although
it is intended to develop effective and flawless code, in no event shall
Densitizer be held liable for any damage, incorrect data, or inaccurate
results arising from the use of the program.
=======================================================================

Molecular Formula          : H2C2
Charge                     : 0
Multiplicity               : 1
Number of Atoms            : 4
Number of basis elements   : 40
Number of Primitive Gaussians : 70
Number of Total Electrons  : 14
Number of Alpha Electrons  : 7
Number of Beta  Electrons  : 7
Number of Fragments        : 2
Number of Subcomplexes     : 0
SCF Type                   : RHF
Initial date and time      : 2019 Jun 11, 07:05:04
Final   date and time      : 2019 Jun 11, 07:05:28

Molecular Coordinates:
-------------------------------------------
1   C     0.700000     0.000000     0.000000
2   C    -0.700000     0.000000     0.000000
3   H     1.700000     0.000000     0.000000
4   H    -1.700000     0.000000     0.000000
-------------------------------------------
```

It follows by deformation density analysis of different phenomena as distinct sections, depending on the analysis requested by user. Each section is supplied by total concentration/depletion value, deformation orbital (DO) number, displaced charge, orbital occupancies, energies, and stabilization (Delta-E) of DOs in complex and fragments. Each section begins with total concentration and depletion of charge due to its title.

For example, below figure shows deformation density due to intermolecular kinetic energy pressure, where 0.248760 e is displaced. These values can be visualized with respect to the corresponding `.fch` which are different filenames for different analysis and will be discussed for each analysis, distinctly. As example, for intermolecular kinetic energy pressure, three files `DefKEPConc.fch`, `DefKEPDepl.fch`, `DefKEP.fch`, includes concentration, depletion, both concentration and depletion deformation densities, respectively:

`DefKEPConc.fch`   `DefKEPDepl.fch`   `DefKEP.fch`
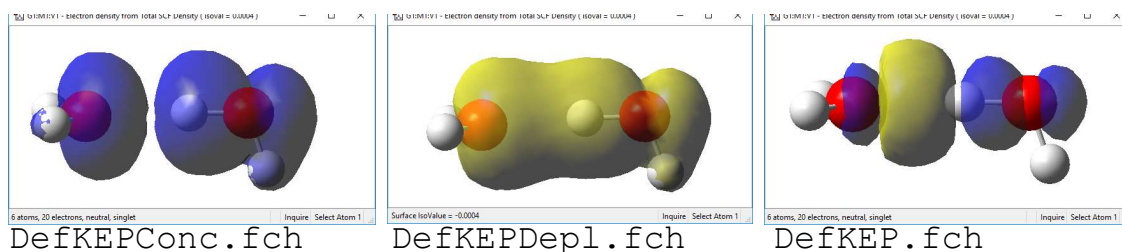
The first two columns, show the number of DO corresponding to depletion and concentration available in the other right columns and also to their number in GaussView orbital visualization window. Below figure shows these connections, clearly. Also, notice that the displaced charged values for each orbital is available in both report file, and right of the GaussView visualization window:
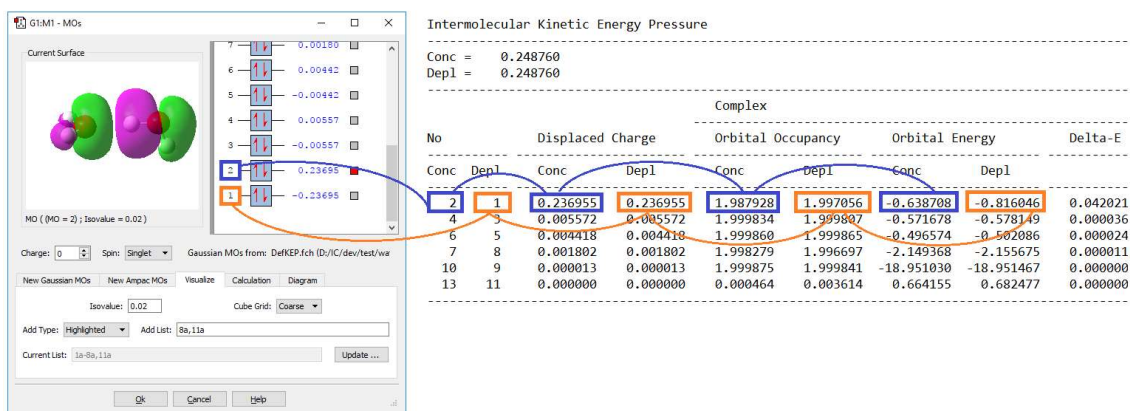
The rightest column is the stabilization energy (`Delta-E`) due to each DO with respect to its environment. In the above results, they are in the complex environment (see its subtitle).

Intermolecular Interaction Analysis

This analysis provides deformation density information of complex formation including kinetic energy pressure (KEP) due to Pauli repulsion (also known as steric effect), orbital relaxation (RLX), and natural orbitals for chemical valence (NOCV). In order to make Gaussian `.gjf` input jobs, fragments **must** be appeared continuously in the complex system and numbered as they exist in the complex. *Densitizer* supports both with and without BSSE correction. Below example shows correct Gaussian jobs of water dimer, where xyz coordinates of two fragments are highlighted as blue and green.

Complex

Frag2   Frag1
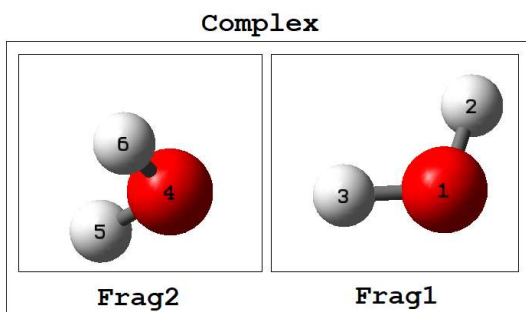
Note how atom numbers are ordered, i.e., atom numbers of fragment 1 precede those of fragment 2.

BSSE corrected jobs:
To take into account BSSE correction, complex and fragments single point job are something like these:

`comp.gjf`

```
%chk=D:\test\dens\comp.chk
# b3lyp/6-31G** nosym 6d 10f

complex

0 1
O          -0.94320488    -2.68762673     0.00000000
H           0.01679512    -2.68762673     0.00000000
H          -1.26365946    -1.78269090     0.00000000
O          -1.74543284    -0.19446361     0.13175638
H          -1.95483880     0.43845606    -0.55901265
H          -1.82777487     0.22850095     0.98961462
```

frag1.gjf

```
%chk=D:\test\dens\frag1.chk
# b3lyp/6-31G** nosym 6d 10f massage

complex

0 1
 O                -0.94320488    -2.68762673     0.00000000
 H                 0.01679512    -2.68762673     0.00000000
 H                -1.26365946    -1.78269090     0.00000000
 O                -1.74543284    -0.19446361     0.13175638
 H                -1.95483880     0.43845606    -0.55901265
 H                -1.82777487     0.22850095     0.98961462

4 nuc 0.
5 nuc 0.
6 nuc 0.
```

frag2.gjf

```
%chk=D:\test\dens\frag2.chk
# b3lyp/6-31G** nosym 6d 10f massage

complex

0 1
 O                -0.94320488    -2.68762673     0.00000000
 H                 0.01679512    -2.68762673     0.00000000
 H                -1.26365946    -1.78269090     0.00000000
 O                -1.74543284    -0.19446361     0.13175638
 H                -1.95483880     0.43845606    -0.55901265
 H                -1.82777487     0.22850095     0.98961462

1 nuc 0.
2 nuc 0.
3 nuc 0.
```

Note that fragments possess additional massage keyword, all atoms are present in fragments' xyz coordinates, and nuclei of the other fragment(s) are neutralized in three last lines of fragments.

Without BSSE correction:
In this case, complex job file is the same as previous, while fragments include no massage keyword and no xyz coordination of the other fragment.

`comp.gjf`

```
%chk=D:\test\dens\comp.chk
# b3lyp/6-31G** nosym 6d 10f

complex

0 1
 O              -0.94320488   -2.68762673    0.00000000
 H               0.01679512   -2.68762673    0.00000000
 H              -1.26365946   -1.78269090    0.00000000
 O              -1.74543284   -0.19446361    0.13175638
 H              -1.95483880    0.43845606   -0.55901265
 H              -1.82777487    0.22850095    0.98961462
```

`frag1.gjf`

```
%chk=D:\test\dens\frag1.chk
# b3lyp/6-31G** nosym 6d 10f

complex

0 1
 O              -0.94320488   -2.68762673    0.00000000
 H               0.01679512   -2.68762673    0.00000000
 H              -1.26365946   -1.78269090    0.00000000
```

`frag2.gjf`

```
%chk=D:\test\dens\frag2.chk
# b3lyp/6-31G** nosym 6d 10f

complex

0 1
 O              -1.74543284   -0.19446361    0.13175638
 H              -1.95483880    0.43845606   -0.55901265
 H              -1.82777487    0.22850095    0.98961462
```

If the `.fch` files due to water dimer available in the `samples` subdirectory are to be analyzed, the main screen and input files should be something like this:
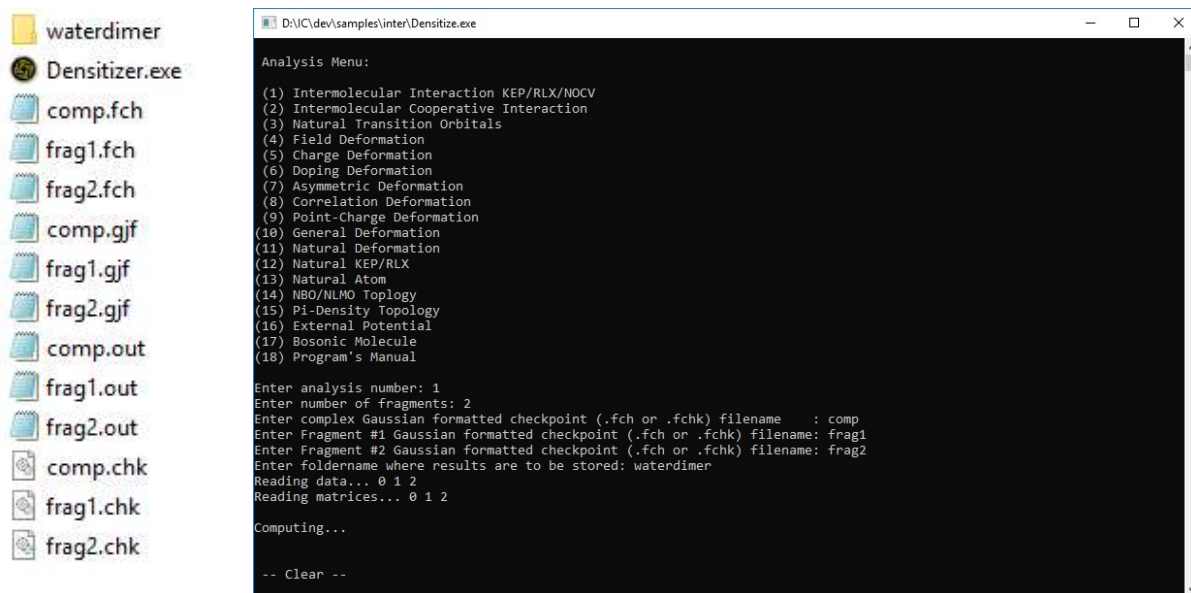
Densitizer creates the three types of output files directly in the same directory, and puts numbered .fch files in `num` subdirectory, which are density of deformation orbitals, and also pairs of densities of deformation orbitals with positive and negative eigenvalues (symmetrically distributed in common). Filenames, analyses and what they store are shown in below table:

Filename	Analysis	Includes
`DefKEP.fch`	Kinetic energy pressure (steric)	Density\Orbital
`DefKEP.wfn`	Kinetic energy pressure (steric)	Density
`DefKEPnnnn.fch`	Kinetic energy pressure (steric)	Density
`DefKEPPairnnnn.fch`	Kinetic energy pressure (steric)	Density
`DefRLX.fch`	Orbital relaxation (NOCV)	Density\Orbital
`DefRLX.wfn`	Orbital relaxation (NOCV)	Density
`DefRLXnnnn.fch`	Orbital relaxation (NOCV)	Density
`DefRLXPairnnnn.fch`	Orbital relaxation (NOCV)	Density
`DefTOT.fch`	Total deformation density	Density\Orbital
`DefTOT.wfn`	Total deformation density	Density
`DefTOTnnnn.fch`	Total deformation density	Density
`DefTOTPairnnnn.fch`	Total deformation density	Density

The report file includes three sections for Intermolecular Kinetic Energy Pressure, Intermolecular Relaxation (NOCV), and, Total deformation density analyses.

```
Intermolecular Kinetic Energy Pressure
------------------------------------------------------------------------------------
Conc =    0.248760
Depl =    0.248760
------------------------------------------------------------------------------------
                                    Complex
                        ----------------------------------------------------------
No          Displaced Charge        Orbital Occupancy      Orbital Energy      Delta-E
----------  ----------------------  ---------------------  --------------------  ----------
Conc  Depl  Conc        Depl        Conc        Depl       Conc        Depl
----------  ----------------------  ---------------------  --------------------  ----------
   2    1   0.236955    0.236955    1.987928    1.997056   -0.638708   -0.816046   0.042021
   4    3   0.005572    0.005572    1.999834    1.999807   -0.571678   -0.578149   0.000036
   6    5   0.004418    0.004418    1.999860    1.999865   -0.496574   -0.502086   0.000024
   7    8   0.001802    0.001802    1.998279    1.996697   -2.149368   -2.155675   0.000011
  10    9   0.000013    0.000013    1.999875    1.999841  -18.951030  -18.951467   0.000000
  13   11   0.000000    0.000000    0.000464    0.003614    0.664155    0.682477   0.000000
------------------------------------------------------------------------------------


Intermolecular Relaxation (NOCV)
------------------------------------------------------------------------------------
Conc =    0.277086
Depl =    0.277086
------------------------------------------------------------------------------------
                                    Complex
                        ----------------------------------------------------------
No          Displaced Charge        Orbital Occupancy      Orbital Energy      Delta-E
----------  ----------------------  ---------------------  --------------------  ----------
Conc  Depl  Conc        Depl        Conc        Depl       Conc        Depl
----------  ----------------------  ---------------------  --------------------  ----------
   1    2   0.199769    0.199769    1.099885    0.900115    0.094817    0.218551  -0.024718
   4    3   0.028553    0.028553    1.014277    0.985723    0.014049    0.030375  -0.000466
   5    6   0.025722    0.025722    1.012861    0.987139    0.073741    0.090843  -0.000440
   8    7   0.023041    0.023041    1.011520    0.988480    0.013157    0.028872  -0.000362
   9   10   0.000000    0.000000    2.000000    2.000000   -0.736755  -14.778280   0.000000
  11   12   0.000000    0.000000    2.000000    2.000000   -2.421961  -12.153795   0.000000
  13   14   0.000000    0.000000    2.000000    2.000000   -1.252247  -11.779755   0.000000
------------------------------------------------------------------------------------


Total
------------------------------------------------------------------------------------
Conc =    0.444501
Depl =    0.444501
------------------------------------------------------------------------------------
                                    Complex
                        ----------------------------------------------------------
No          Displaced Charge        Orbital Occupancy      Orbital Energy      Delta-E
----------  ----------------------  ---------------------  --------------------  ----------
Conc  Depl  Conc        Depl        Conc        Depl       Conc        Depl
----------  ----------------------  ---------------------  --------------------  ----------
   1    2   0.315207    0.270819    1.633414    1.672303   -0.294944   -0.499030   0.042178
   4    3   0.066125    0.109467    1.480093    1.118790   -0.781850   -0.268414  -0.022317
   6    5   0.026151    0.026661    1.052731    1.042357    0.054462    0.069419  -0.000427
   8    7   0.023549    0.023595    1.036960    1.025610    0.005274    0.016534  -0.000266
  10    9   0.012675    0.013898    1.133768    0.961496   -0.428145   -0.301279  -0.001240
  11   13   0.000578    0.000062    1.933373    1.989478   -2.171720  -17.602562  -0.000167
------------------------------------------------------------------------------------
```

These table continues horizontally to include the above information for fragments as well as complex.

Cooperative interaction analysis

Natural Transition Orbitals
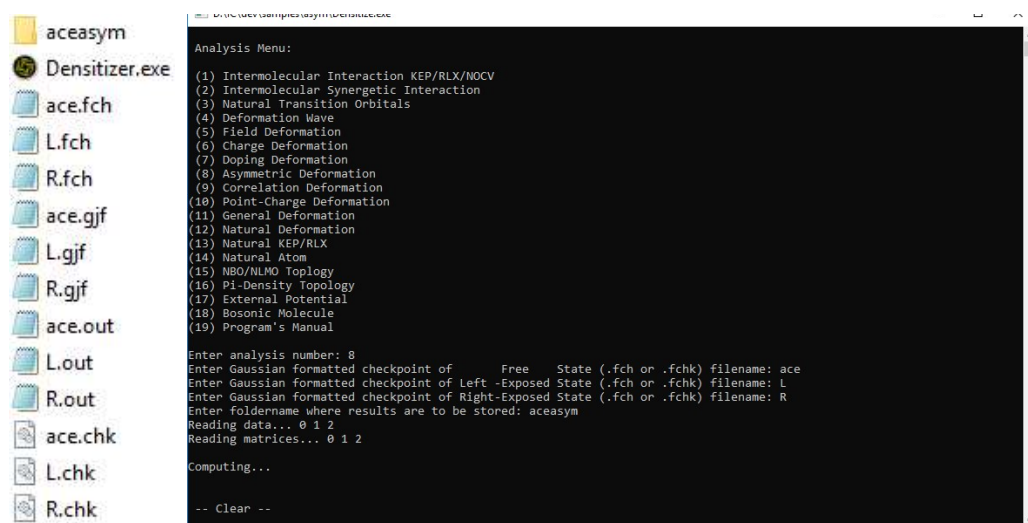
```
■ D:\test\dens\Densitize.exe                                          —   □   ×

Analysis Menu:

(1) Intermolecular Interaction KEP/RLX/NOCV
(2) Intermolecular Cooperative Interaction
(3) Natural Transition Orbitals
(4) Field Deformation
(5) Charge Deformation
(6) Doping Deformation
(7) Asymmetric Deformation
(8) Correlation Deformation
(9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 3
Enter excited state ("density" keyword included) Gaussian formatted checkpoint (.fch or .fchk) filename: form
(1) Absorption
(2) Fluorescence
Enter choice: 1
Enter foldername where results are to be stored: form
Reading data... 0 1
Reading matrices... 0 1        1 file(s) moved.


Computing...

 -- Clear --
```

Field electron deformation orbitals

Densitizer.exe	4/3/2019 8:51 AM	Application	3,317 KB
ace.fch	4/3/2019 9:09 AM	FCH File	53 KB
ace100.fch	4/3/2019 9:09 AM	FCH File	53 KB
ace.gjf	4/3/2019 9:08 AM	GJF File	1 KB
ace100.gjf	4/3/2019 9:08 AM	GJF File	1 KB
ace.out	4/3/2019 9:09 AM	OUT File	11 KB
ace100.out	4/3/2019 9:09 AM	OUT File	12 KB
ace.chk	4/3/2019 9:09 AM	Recovered File Fra...	524 KB
ace100.chk	4/3/2019 9:09 AM	Recovered File Fra...	524 KB

```
D:\test\dens\Densitize.exe                                    —    □    ×

Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 4
Enter field-free   Gaussian formatted checkpoint (.fch or .fchk) filename: ace
Enter field-dressed Gaussian formatted checkpoint (.fch or .fchk) filename: ace100
Enter foldername where results are to be stored: ace
Reading data... 0 1
Reading matrices... 0 1

Computing...


 -- Clear --
```

Charge deformation


```
Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 5
Enter neutral Gaussian formatted checkpoint (.fch or .fchk) filename: cyc
Enter charged Gaussian formatted checkpoint (.fch or .fchk) filename: cat
Enter foldername where results are to be stored: cyc
Reading data... 0 1
Reading matrices... 0 1

Computing...


 -- Clear --
```

Doping deformation

Asymmetric deformation


```
Analysis Menu:

(1) Intermolecular Interaction KEP/RLX/NOCV
(2) Intermolecular Synergetic Interaction
(3) Natural Transition Orbitals
(4) Deformation Wave
(5) Field Deformation
(6) Charge Deformation
(7) Doping Deformation
(8) Asymmetric Deformation
(9) Correlation Deformation
(10) Point-Charge Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Potential
(18) Bosonic Molecule
(19) Program's Manual

Enter analysis number: 8
Enter Gaussian formatted checkpoint of       Free    State (.fch or .fchk) filename: ace
Enter Gaussian formatted checkpoint of Left -Exposed State (.fch or .fchk) filename: L
Enter Gaussian formatted checkpoint of Right-Exposed State (.fch or .fchk) filename: R
Enter foldername where results are to be stored: aceasym
Reading data... 0 1 2
Reading matrices... 0 1 2

Computing...


-- Clear --
```

Correlation deformation

Densitizer.exe	4/3/2019 10:10 AM	Application	3,317 KB
cyc.fch	4/3/2019 10:13 AM	FCH File	82 KB
cyc.gjf	4/3/2019 10:12 AM	GJF File	1 KB
cyc.out	4/3/2019 10:13 AM	OUT File	25 KB
cyc.chk	4/3/2019 10:13 AM	Recovered File Fra...	524 KB

```
D:\test\dens\Densitize.exe                                                          —    □    ×

Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 8
Enter correlated-level Gaussian formatted checkpoint (.fch or .fchk) filename: cyc
Enter foldername where results are to be stored: cyccorr
Reading data... 0 1
Reading matrices... 0 1

Computing...

 -- Clear --
```

Point-Charge deformation

Fermion-Boson deformation

General deformation

Densitizer.exe	4/3/2019 10:10 AM	Application	3,317 KB
cycb3.fch	4/5/2019 11:47 PM	FCH File	175 KB
cychf.fch	4/5/2019 11:47 PM	FCH File	175 KB
cycb3.gjf	4/5/2019 11:44 PM	GJF File	1 KB
cychf.gjf	4/5/2019 11:45 PM	GJF File	1 KB
cycb3.out	4/5/2019 11:47 PM	OUT File	19 KB
cychf.out	4/5/2019 11:46 PM	OUT File	18 KB
cycb3.chk	4/5/2019 11:47 PM	Recovered File Fra...	592 KB
cychf.chk	4/5/2019 11:47 PM	Recovered File Fra...	592 KB

```
D:\test\dens\Densitize.exe                                    —   □   ×

Analysis Menu:

(1) Intermolecular Interaction KEP/RLX/NOCV
(2) Intermolecular Cooperative Interaction
(3) Natural Transition Orbitals
(4) Field Deformation
(5) Charge Deformation
(6) Doping Deformation
(7) Asymmetric Deformation
(8) Correlation Deformation
(9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 11
Enter initial-state Gaussian formatted checkpoint (.fch or .fchk) filename: cychf
Enter final-state   Gaussian formatted checkpoint (.fch or .fchk) filename: cycb3
Enter foldername where results are to be stored: cychfb3
Reading data... 0 1
Reading matrices... 0 1

Computing...


 -- Clear --
```

Natural Deformation

NBO 3.0 implemented in Gaussian:

Densitizer.exe	4/3/2019 10:10 AM	Application	3,317 KB
water.fch	4/6/2019 12:28 AM	FCH File	28 KB
water.gjf	4/6/2019 12:27 AM	GJF File	1 KB
water.out	4/6/2019 12:27 AM	OUT File	50 KB
water.chk	4/6/2019 12:28 AM	Recovered File Fra...	524 KB

```
D:\test\dens\Densitize.exe                                        —   □   ×

Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 12
Enter Gaussian formatted checkpoint (.fch or .fchk) filename: water
Enter filename where NBO results are present: water
Enter two atom numbers for interatomic analysis separated by spaces
and terminated by 0 as end:
1 2
2 3
0
Enter foldername where results are to be stored: water
Reading data... 0
Reading matrices... 0

Computing...


 -- Clear --
```

27

NBO 5.0 or higher as external source:


```
Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 12
Enter Gaussian formatted checkpoint (.fch or .fchk) filename: water
Enter filename where NBO results are present: waternbo5
Enter two atom numbers for interatomic analysis separated by spaces
and terminated by 0 as end:
1 2
2 3
0
Enter foldername where results are to be stored: waternbo5
Reading data... 0
Reading matrices... 0

Computing...

 -- Clear --
```

NBO/NLMO Topology


```
Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Perturbation
(18) Extract Data
(19) Program's Manual

Enter analysis number: 15
Enter Gaussian formatted checkpoint (.fch or .fchk) filename: eth
Enter filename where NBO results are present: eth
Enter NBO/NLMO numbers for topological analysis separated by spaces
and terminated by 0 as end (-1 for all NBOs/NLMOs with occ. > 0.1):
3 4 0
Enter foldername where results are to be stored: eth
Reading data... 0
Reading matrices... 0

Computing...


 -- Clear --
```

Analysis Menu:

(1) Intermolecular Interaction KEP/RLX/NOCV
(2) Intermolecular Cooperative Interaction
(3) Natural Transition Orbitals
(4) Field Deformation
(5) Charge Deformation
(6) Doping Deformation
(7) Asymmetric Deformation
(8) Correlation Deformation
(9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Toplogy
(17) External Potential
(18) Program's Manual

Enter analysis number: 16
Enter Gaussian formatted checkpoint (.fch or .fchk) filename: C20
Enter foldername where results are to be stored: C20
Reading data... 0 1
Reading matrices... 0 1

Computing...

-- Clear --

Analysis Menu:

(1) Intermolecular Interaction KEP/RLX/NOCV
(2) Intermolecular Cooperative Interaction
(3) Natural Transition Orbitals
(4) Field Deformation
(5) Charge Deformation
(6) Doping Deformation
(7) Asymmetric Deformation
(8) Correlation Deformation
(9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Potential
(18) Program's Manual

Enter analysis number: 13
Enter Gaussian formatted checkpoint (.fch or .fchk) filename: buta
Enter filename where NBO results are present: buta
Enter foldername where results are to be stored: buta
Reading data... 0
Reading matrices... 0

Computing...

-- Clear --

```
D:\test\dens\Densitize.exe                                    —  □  ×

Analysis Menu:

 (1) Intermolecular Interaction KEP/RLX/NOCV
 (2) Intermolecular Cooperative Interaction
 (3) Natural Transition Orbitals
 (4) Field Deformation
 (5) Charge Deformation
 (6) Doping Deformation
 (7) Asymmetric Deformation
 (8) Correlation Deformation
 (9) Point-Charge Deformation
(10) Fermion-Boson Deformation
(11) General Deformation
(12) Natural Deformation
(13) Natural KEP/RLX
(14) Natural Atom
(15) NBO/NLMO Toplogy
(16) Pi-Density Topology
(17) External Potential
(18) Program's Manual

Enter analysis number: 14
Enter Gaussian formatted checkpoint (.fch or .fchk) filename: form
Enter filename where NBO results are present: form
Enter atom numbers for topological analysis separated by spaces
and terminated by 0 as end (-1 for all atoms):
1 2 3 4 0
Enter foldername where results are to be stored: form
Reading data... 0
Reading matrices... 0

Computing...

-- Clear --
```

Natural Transition Orbitals / Charge Deformation / Field Deformation

This analyses provides deformation orbitals, where the required .fch input files are as below. Note that the molecular geometry of second .fch must be frozen to that in the first .fch file.

Natural Transition Orbitals: Excited state.

Charge Deformation: Neutral and charged species.

Field Deformation: Relaxed molecule, and that exposed to external electric field.

Filenames, analyses and what they store for these three analyses are shown in below table:

Filename	Analysis	Includes
NTO.fch	Natural Transition Orbitals	Density\Orbital
NTO.wfn	Natural Transition Orbitals	Density
NTOnnnn.fch	Natural Transition Orbitals	Density
NTOPairnnnn.fch	Natural Transition Orbitals	Density
CDO.fch	Charge Deformation	Density\Orbital
CDO.wfn	Charge Deformation	Density
CDOnnnn.fch	Charge Deformation	Density
CDOPairnnnn.fch	Charge Deformation	Density
EDO.fch	Field Deformation	Density\Orbital
EDO.wfn	Field Deformation	Density

`EDOnnnn.fch`	Field Deformation	Density
`EDOPairnnnn.fch`	Field Deformation	Density

Block Deformation Analysis

This analysis provides deformation density information of complex
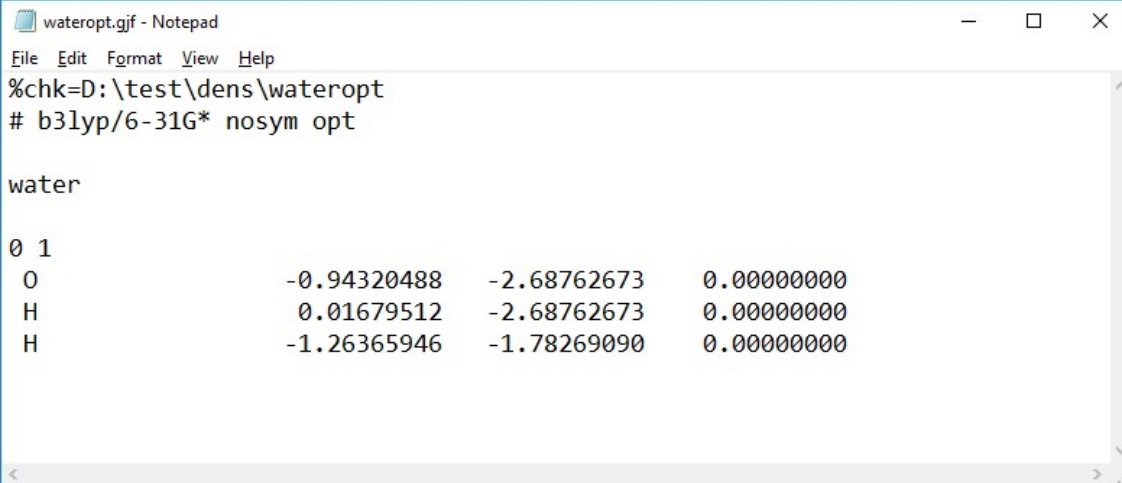
Natural KEP/RLX Analysis

This analysis provides deformation density information of complex

Natural Atom Analysis

This analysis provides deformation density information of complex

NBO/NLMO Topological Analysis

This analysis provides deformation density information of complex

Pi-Density Topology Analysis

This analysis provides deformation density information of complex

Extract Data

This analysis provides deformation density information of complex
% coeff mx my mz rx ry rz rr px py pz lx ly lz k
% coeff 1 2 3 4 5 6 7 8 9 10 11 12 13 14

Appendix A: Creation of single point jobs with frozen geometries

1- Create an input `.gjf` optimization job

2- Open the optimized output with GaussView and save as Cartesian:
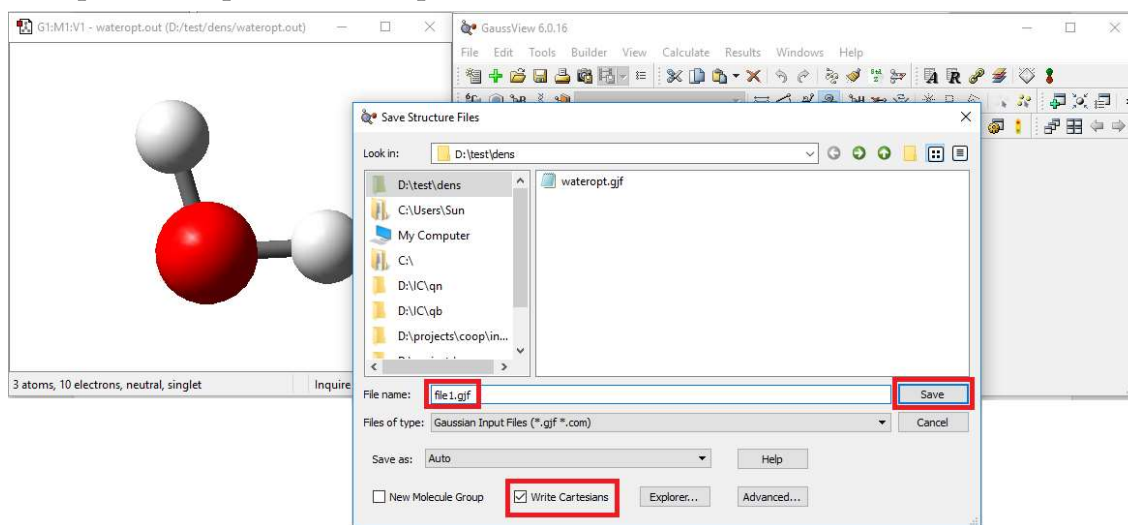
3- Create multiple copies of `file1.gjf` and modify their contents according to the analysis:

where green and red boxes show unmodified and modified contents, respectively:

file1.gjf - Notepad

%chk=D:\test\dens\file1.chk
b3lyp/6-31G* nosym 6d 10f

water

0 1
```
O                -0.96034100    -2.71187700     0.00000000
H                 0.00705500    -2.66256400     0.00000000
H                -1.23678300    -1.78350400     0.00000000
```

file2.gjf - Notepad

%chk=D:\test\dens\file2.chk
b3lyp/6-31G* nosym 6d 10f field=x+100

water

0 1
```
O                -0.96034100    -2.71187700     0.00000000
H                 0.00705500    -2.66256400     0.00000000
H                -1.23678300    -1.78350400     0.00000000
```

file3.gjf - Notepad

%chk=D:\test\dens\file3.chk
b3lyp/6-31G* nosym 6d 10f field=x-100

water

0 1
```
O                -0.96034100    -2.71187700     0.00000000
H                 0.00705500    -2.66256400     0.00000000
H                -1.23678300    -1.78350400     0.00000000
```

All these files are located in `single` subdirectory of samples.

Appendix B: Creation of formatted checkpoint files (`.fch`/`.fchk`)

Formatted checkpoint file must be created with the same version and same platform of Gaussian. For example, if Linux version of Gaussian is used to run jobs, its checkpoint `.chk` file cannot be converted in Windows platform. On the other hand, once `.fch` file is created, it can be used in any other platform, safely. It means Linux users must make `.fch` files in Linux, make a copy of them in Windows, in the same directory as *Densitizer* exists, and run *Densitizer*.

Linux users:

Run

```
formchk file.chk file.fch
```

Windows users:

Run Gaussian, point to `FormChk` utility, and open the checkpoint `.chk` file. It automatically creates a `.fch` file in the same directory.
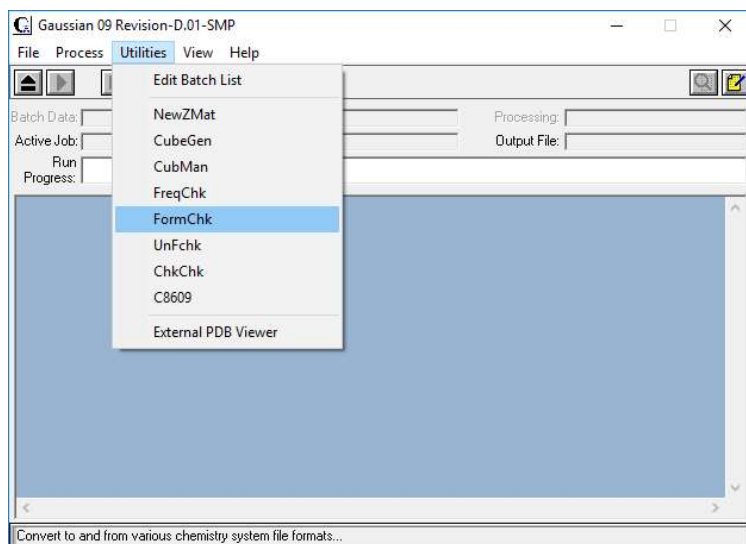
Appendix C: Visualization of Deformation Density by GaussView
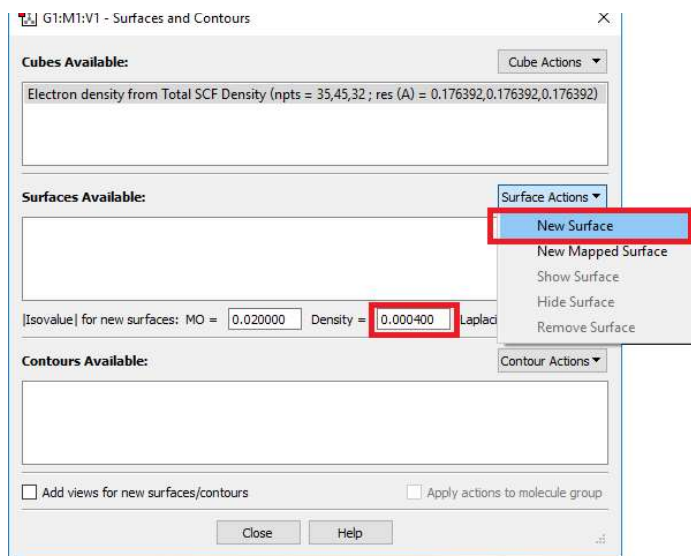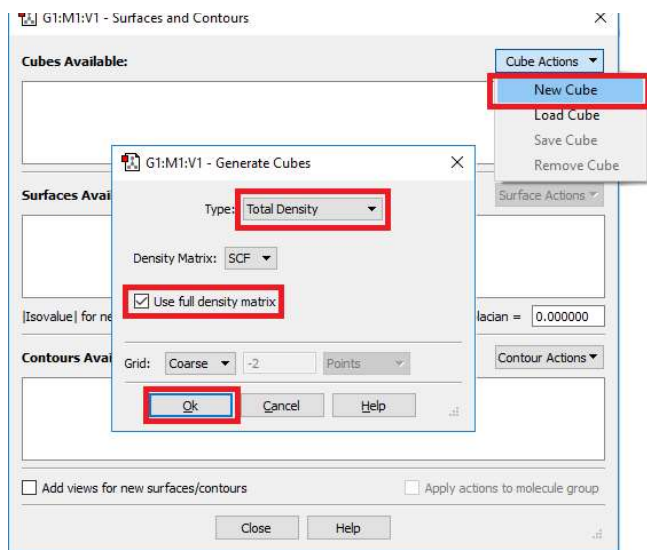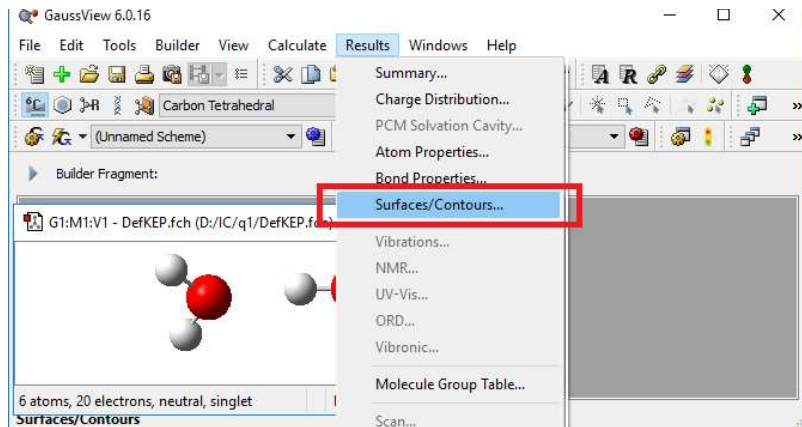
Appendix D: Visualization of Orbitals by GaussView
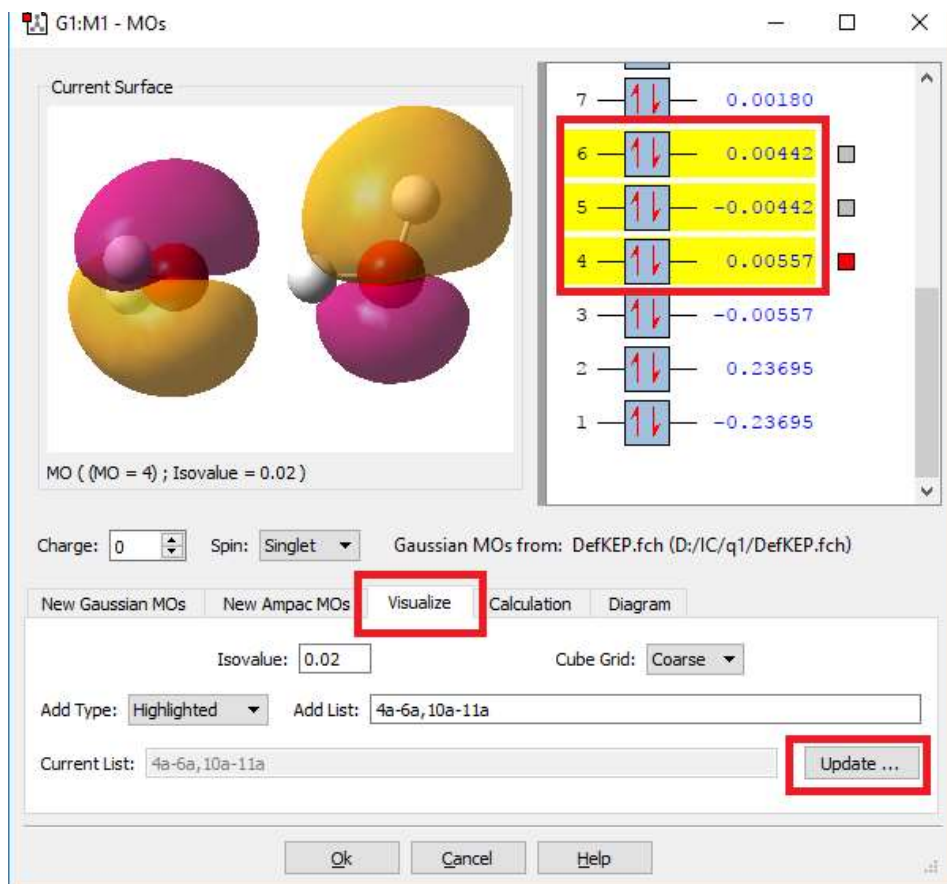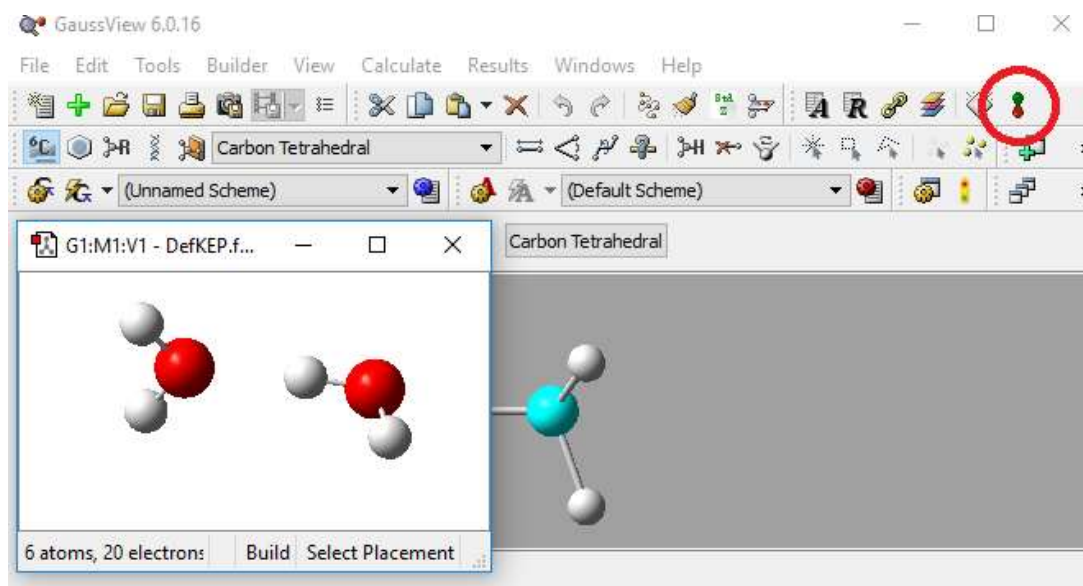
Appendix E: Topological Analysis by AIM2000

Appendix F: Contents of `num` folder