Tutorial of using *sobEDA.sh* to perform sobEDA and sobEDAw analyses

Last update: 2023-Sep-18

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1 Prerequisite

Original paper of sobEDA/sobEDAw is *J. Phys. Chem. A*, **127**, 7023 (2023) https://doi.org/10.1021/acs.jpca.3c04374. It is strongly suggested to read through it first to gain necessary knowledge on how to properly use these methods.

To use *sobEDA.sh* to perform sobEDA or sobEDAw analysis, your machine should satisfy the following requirements:

(1) Bash shell: Commonly, a Linux system with Bash shell should be used, such as Rocky Linux. You may also use virtual machine or WSL under Windows.

(2) Multiwfn: Multiwfn (no older than the version updated on 2023-Jun-25) should have been installed. You can either install standard or noGUI version, the latter is easier to be installed in Linux environment because graphical libraries are not needed. Multiwfn can be downloaded freely at http://sobereva.com/multiwfn. Please check Section 2.1.2 of Multiwfn manual on how to install it under Linux.

(3) Gaussian: Gaussian program (no older than G16 A.03) should be installed.

(4) dos2unix command should be available in Linux. Which can be easily installed (for example, using *yum install dos2unix* in CentOS and Rocky Linux)

2 Use of sobEDA.sh

2.1 Running sobEDA.sh

After preparing the following files in current folder, and properly setting *sobEDA.sh*, then you can input path of *sobEDA.sh* script to start sobEDA/sobEDAw analysis

- **system.xyz**: Standard .xyz format file containing coordinate of the entire system. See Section 2.3 for details.
- **fragment.txt**: Definition of net charge, spin multiplicity, atom indices in each fragment. See Section 2.4 for details.
- **template.gjf**: Template input file of Gaussian, determining calculation level, net charge, and spin multiplicity of the entire system. See Section 2.5 for details.

After running of *sobEDA.sh*, Gaussian and Multiwfn will be automatically invoked. Details of calculation procedure will be shown on screen so that you can monitor the progress, finally sobEDA and sobEDAw terms are shown.

2.2 Setting *sobEDA.sh*

Before running *sobEDA.sh*, you should edit beginning part of this script to properly set some options:

- **gau**: Command of running Gaussian program. Assume that Gaussian 16 has been properly installed, just set it to *g16*.
- **mwfn**: Command of running Multiwfn program. Assume that Multiwfn has been properly installed, just set it to *Multiwfn*.
- **iCP**: If set to 0, then monomer basis functions will be used during fragment calculations.

If set to 1, then complex basis functions will be used during fragment calculations. The latter is more expensive, but highly recommended for sobEDAw analysis to yield better result. *When iCP=1, it is equivalent to employing Counterpoise correction to account for basis set superposition error (BSSE) problem.*

- **sobEDAw**: If set to 0, only sobEDA result will be finally given. If set to 1, both sobEDA and sobEDAw results will be finally shown. In the latter case, you should also define fitted parameters *c*, *a*, *r* involved in sobEDAw method by *parm_c*, *parm_a* and *parm_r* variables, respectively. In *sobEDA.sh* you can find that many *c*, *a*, *r* parameters for commonly used calculation levels have already been given as comments, so you can just uncomment corresponding line to use them. Parameters for more levels can be found in Tables 1 and 2 of original paper of sobEDA method.

- **irun**: This is for debug use. Commonly it should be set to 1. If set to 0, then script will only process existing files generated by previous calculation, no additional calculations by Gaussian will be actually conducted.

- **idetail**: Commonly it should be set to 0. If set to 1, full energy variation details will be finally printed, and additional cost is needed.

2.3 system.xyz

This file contains geometry of entire system in .xyz format used for sobEDA/sobEDAw analysis. The first line is number of atoms, the second line is comment and does not affect analysis, the rest of this file contains element name and X, Y, Z coordinates in Å for each atom, For example:

```
7
optimized
O           -0.03836200    1.54613400    0.00000000
H            0.06356500    0.57566500    0.00000000
H            0.85354600    1.90026300    0.00000000
N           -0.03836200   -1.37627100    0.00000000
H           -1.03728700   -1.54652400    0.00000000
H            0.34780000   -1.83229000    0.81779500
H            0.34780000   -1.83229000   -0.81779500
```

Note that you can easily generate the .xyz file via Multiwfn. Multiwfn can load wide variety of files and export the structure and wavefunction to rich formats. See Section 2.5 of Multiwfn manual on the formats that can be loaded. For example, Multiwfn can directly load output file of "opt" or "opt freq" task of Gaussian; after loading it, in the main menu if you input command *xyz*, you will enter the interface of exporting .xyz file. After inputting the file path to be exported (for example, */sob/system.xyz*), the system.xyz file will be generated. You can also visualize the loaded structure in Multiwfn by main function 0 (noGUI version of Multiwfn does not support this).

2.4 fragment.txt

The first line of this file is number of fragments. The rest part defines net charge, spin multiplicity and atom indices in each fragment. The following example defines two fragments, the first fragment has net charge of 0 and spin multiplicity of 1, corresponding to atoms 1-3,7,10-12; the second fragment has net charge of 1 and spin multiplicity of 2, corresponding to atoms 4-6,8,9. Evidently, union of all fragments must equal to the entire system.

```
2
0 1
1-3,7,10-12
1 2
4-6,8,9
```

You can use negative spin multiplicity to request Multiwfn to flip spin of the fragment when constructing promolecule wavefunction from corresponding fragment wavefunctions. In the following example, fragment 1 and fragment 2 will be viewed as doublet radical with α and β unpaired electron during this process, respectively.

```
2
0 2
1-4
0 -2
5-8
```

Note that spin flip should be properly set, so that the sum of α (β) electrons of all fragments is equal to α (β) electrons of the entire system.

2.5 template.gjf

This is template input file of Gaussian, a typical example is shown below. Note that there are two blank lines at the end of the file.

```
#p b3lyp/6-311+G(2d,p) em=gd3bj ExtraLinks=L608 nosymm

title line

0 1
[geometry]

-5 5

```

With the template file shown above, *sobEDA.sh* will invoke Gaussian to perform calculation for fragments and the entire system at B3LYP-D3(BJ)/6-311+G(2d,p) level. The net charge and spin multiplicity for the entire system is specified in this file, name 0 and 1, respectively. DO NOT change "#P", "ExtraLinks=L608" and "nosymm" keywords, all of them are needed in the analysis. The [geometry] part will be automatically replaced with the actual coordinate of fragments and entire system by *sobEDA.sh* when invoking Gaussian to calculate them.

The "ExtraLinks=L608" keyword is used to ask Gaussian to print detailed components of energy by link 608 module, while the *-5* at the last line tells link 608 that the current DFT functional is B3LYP. If you use other DFT functional, you should correspondingly change this index. See IOp(3/74) in Gaussian IOps reference for details, the index for commonly used functionals is given here: **-73 (MN15), -55 (M06-2X), -54 (M06), -53 (M06L), -35 (TPSSh), -13 (PBE0), -5 (B3LYP), -6 (B3PW91), -3 (BHandHLYP), 402 (BLYP), 1009 (PBE), 2523 (TPSS)**. Notice that because Gaussian (at least as of G16 C.02) is unable to print energy components for range-separated

functionals, functionals such as CAM-B3LYP, ωB97X, and HSE06 cannot be used in sobEDA/sobEDAw analysis.

The *5* at last line in above example requests link 608 module to use ultrafine integration grid, which is used by Gaussian 16 by default during SCF process.

Only DFT-D3(BJ) parameters of limited DFT functionals are built-in in Gaussian code. As of G16 C.02, to use such as TPSSh-D3(BJ) and BHandHLYP-D3(BJ), you have to manually define DFT-D3(BJ) parameters. Since G16 C.01, the parameters should be defined using IOps; for example, adding **IOp(3/174=1000000,3/175=1035400,3/177=279300,3/178=4961500) for BHandHLYP-D3(BJ), adding IOp(3/174=1000000,3/175=2238200,3/177=452900,3/178=4655000) for TPSSh-D3(BJ)**. These parameters come from supplemental information of GMTKN55 benchmark paper *Phys. Chem. Chem. Phys.*, **19**, 32184 (2017). If you are using Gaussian older than G16 C.01, you need to use environment variables to define the DFT-D3(BJ) parameters, see http://sobereva.com/210 for details.

Template files for some popular DFT functionals have been provided in "templates" folder in this package, you can directly use them after modifying file name.

Although sobEDA/sobEDAw is defined based on dispersion-corrected DFT, it is also possible to ignore the dispersion correction, namely just removing the "em=gd3bj" keyword. In this case, the dispersion correction term reported by *sobEDA.sh* will be exactly zero.

It is important to note that solvation effect is not directly taken into account in sobEDA method, and **implicit solvation model ("scrf" keyword) should not be directly specified in the template file**. Please search "solvation" in original paper of sobEDA on how to correctly consider the solvation effect. Briefly speaking, contribution of solvation effect to interaction energy should be manually calculated via Gaussian, it is never difficult.

2.6 Files produced by *sobEDA.sh*

After this script finishes running, you will find following files in current folder:

- fragment[index].gjf, out, fch: They are input file, output file and .fch file of corresponding fragment.
- promol.gjf, out, chk, fch: They are input file, output file, .chk and .fch file of calculation of promolecule state. Note that *promol.fch* is generated by combining all fragment .fch files via Multiwfn.
- final.gjf, out, chk: They are input file, output file and .chk file of calculation of final state.

You can manually check input and output files to examine if the calculations were conducted in a correct way. Also, you can use Multiwfn to load .fch file (*final.chk* can be manually converted to .fch via formchk utility) to visualize orbitals via main function 0 or check real space functions such as spin density to check if reasonable wavefunctions have been obtained.
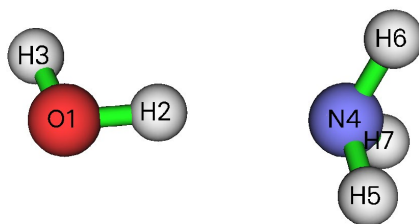
4 Examples

In this section some examples of using *sobEDA.sh* are given. All files for each example can be found from the file package of this tutorial, only some key points will be described below. Gaussian 16 C.02 and Multiwfn 3.8(dev) updated on 2023-Jun-24 are used in this example.

4.1 sobEDAw analysis for $H_2O \cdots NH_3$ dimer at B3LYP-D3(BJ)/6-311+G(2d,p)

w.CB level

Structure of this system:

All files of this example have been provided in "HOH-NH3" folder, please check them to understand how to set up this sobEDAw analysis. As you can see from the *sobEDA.sh* in this example folder, "iCP" is set to 1 to use complex basis functions for fragment calculations, "sobEDAw" is set to 1 to perform sobEDAw analysis after sobEDA analysis, and the line defining *c*, *a*, *r* parameters for the present level, namely "parm_c=0.550;parm_a=0.037;parm_r=2.750", has been uncommented to make them take effect.

Make sure that Gaussian and Multiwfn have been properly installed, then copy *sobEDA.sh*, *system.xyz*, *fragment.txt* and *template.gjf* from the example folder to current folder, then run *chmod +x ./sobEDA.sh* to add executable permission to the shell script, and then run *./sobEDA.sh |tee result.txt* to execute it, the information will be printed on both screen and *result.txt* in current folder. The result is

```
************************
***** Final results *****
************************


Total interaction energy:     -7.18 kcal/mol


Physical components of interaction energy derived by sobEDA:
Electrostatic (E_els):    -12.15 kcal/mol
Exchange (E_x):     -6.40 kcal/mol
Pauli repulsion (E_rep):     20.28 kcal/mol
Exchange-repulsion (E_xrep = E_x + E_rep):     13.88 kcal/mol
Orbital (E_orb):     -5.38 kcal/mol
DFT correlation (E_DFTc):     -2.70 kcal/mol
Dispersion correction (E_dc):     -0.83 kcal/mol
Coulomb correlation (E_c = E_DFTc + E_dc):     -3.53 kcal/mol


Variant of sobEDA for weak interaction (sobEDAw):
Note:    96.26% DFT correlation is combined with dispersion correction to yield a
SAPT-like dispersion term
Electrostatic (E_els):    -12.15 kcal/mol
Exchange-repulsion (including scaled DFT correlation):    13.78 kcal/mol
Orbital (E_orb):     -5.38 kcal/mol
Dispersion (E_disp):     -3.43 kcal/mol
```

As you can see, both sobEDA and sobEDAw results are shown. ΔE_{int} is -7.18 kcal/mol, the sobEDAw terms ΔE_{els}, ΔE_{xrep}, ΔE_{orb}, and ΔE_{disp} are -12.15, 13.78, -5.38 and -3.43 kcal/mol, respectively.

The final.gjf/out/chk, promol.gjf/out/chk/fch, fragment1.gjf/out/fch and fragment2.gjf/out/fch in current folder are intermediate files generated by *sobEDA.sh*, commonly you can simply delete them, while you can also check them to try to identify possible reasons if you encountered any error during executing the script or you found the result is strange.

4.2 sobEDA analysis for OC-BH₃ at B3LYP-D3(BJ)/6-311G* level

This section illustrates how to perform a very simple sobEDA analysis for chemical bond interaction, OC-BH₃ is taken as an instance. Structure of this system:
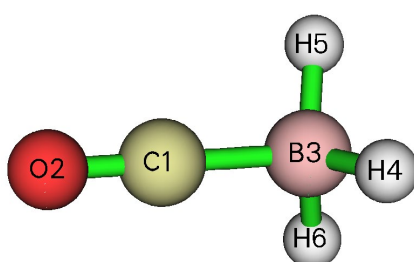
All files of this example have been provided in "OC-BH3" folder, please check them to understand how to set up this analysis. Because in this example we do not use complex basis functions for fragment calculations, therefore "iCP" in *sobEDA.sh* in this case is 0. Because this example involves strong interaction, it is meaningless to conduct sobEDAw analysis, so "sobEDAw" in *sobEDA.sh* is set to 0.

Execute *sobEDA.sh* like last example, you will obtain result very soon:

```
Total interaction energy:    -43.40 kcal/mol

Physical components of interaction energy derived by sobEDA:
Electrostatic (E_els):    -69.50 kcal/mol
Exchange (E_x):    -65.15 kcal/mol
Pauli repulsion (E_rep):    221.03 kcal/mol
Exchange-repulsion (E_xrep = E_x + E_rep):    155.88 kcal/mol
Orbital (E_orb):    -117.36 kcal/mol
DFT correlation (E_DFTc):    -10.89 kcal/mol
Dispersion correction (E_dc):    -1.52 kcal/mol
Coulomb correlation (E_c = E_DFTc + E_dc):    -12.41 kcal/mol
```

As you can see, ΔE_{int} is -43.40 kcal/mol, the sobEDA terms ΔE_{els}, ΔE_x, ΔE_{rep}, ΔE_{orb}, ΔE_{DFTc} and ΔE_{dc} are -69.50, -65.15, 221.03, -117.36, -10.89 and -1.52 kcal/mol, respectively. For simplifying discussion, the ΔE_{xrep} combined from ΔE_x and ΔE_{rep} as well as the ΔE_c combined form ΔE_{DFTc} and ΔE_{dc}, are also shown (155.88 and -12.41 kcal/mol, respectively).

4.3 sobEDA analysis for Cu⁺-H₂O at TPSSh-D3(BJ)/SDD&6-311G* level

This section illustrates sobEDA analysis for a charged system, and we will use mixed basis set and pseudopotential this time. Structure of the example system Cu^+-H_2O is shown below:
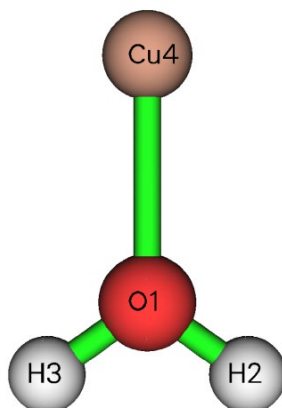
All files of this example have been provided in "Cu+H2O" folder, please check them to understand how to set up this analysis.

The *fragment.txt* of this example is shown below. It can be seen that the fragment 2 (atom 4), namely the Cu(I) cation, is calculated with net charge of 1 and spin multiplicity of 1.

```
2
0 1
1-3
1 1
4
```

The *template.gjf* of this example is evidently more complicated than the previous examples. The content is

```
#p TPSSh/genecp em=gd3bj IOp(3/174=1000000,3/175=2238200,3/177=452900,3/178=4655000)
ExtraLinks=L608 nosymm

opted geometry

1 1
[geometry]

-O -H
6-311G*
****
-Cu
SDD
****


-Cu
SDD

-35 5
```

There are some key points of this template file:

- Because parameters of DFT-D3(BJ) are not built-in for TPSSh in Gaussian 16 C.02 (the version used in the present tutorial), therefore according to Section 2.5, the parameters are supplemented using IOp(3/174=1000000,3/175=2238200,3/177=452900,3/178=4655000).
- *-35* in the last line indicates TPSSh is used, as mentioned in Section 2.5.
- Net charge of 1 and spin multiplicity of 1 defined in this file correspond to the setting used in the calculation of the entire system (while the values for fragment calculations are defined in *fragment.txt*).
- Customized basis sets are used in this example, the same basis set setting is applied to calculations of both entire system and every fragment. Therefore, - must be added before the element names, requesting that Gaussian will not stop if one or more of these elements do not appear in the present calculation.
- Pseudopotential "SDD" is used, due to the same reason as above, - is added prior to Cu.

Run *sobEDA.sh*, you will obtain the following sobEDA result:

```
Total interaction energy:    -51.03 kcal/mol


Physical components of interaction energy derived by sobEDA:
Electrostatic (E_els):    -59.76 kcal/mol
Exchange (E_x):    -20.29 kcal/mol
Pauli repulsion (E_rep):    65.08 kcal/mol
Exchange-repulsion (E_xrep = E_x + E_rep):    44.79 kcal/mol
Orbital (E_orb):    -28.75 kcal/mol
DFT correlation (E_DFTc):    -6.52 kcal/mol
Dispersion correction (E_dc):    -0.78 kcal/mol
Coulomb correlation (E_c = E_DFTc + E_dc):    -7.31 kcal/mol
```
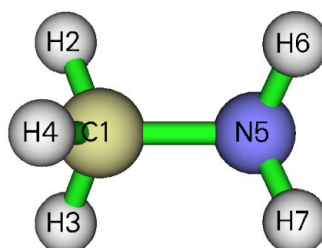
4.4 sobEDA analysis for CH_3-NH_2 at B3LYP-D3(BJ)/def2-TZVP level

This section illustrates sobEDA analysis for open-shell interfragment interaction. Structure of the example system CH_3-NH_2 is shown below:

All files of this example have been provided in "CH3NH2" folder, please check them to understand how to set up this analysis. The *fragment.txt* in this example is given below, it can be seen that both CH_3 and NH_2 fragments are calculated as doublet radical, however, the CH_3 has unpaired electron of α spin, while NH_2 has that of β spin (indicated as negative spin multiplicity).

```
2
0 2
1-4
0 -2
5-7
```

The result of running *sobEDA.sh* is

```
Total interaction energy:    -97.50 kcal/mol

Physical components of interaction energy derived by sobEDA:
Electrostatic (E_els):   -171.02 kcal/mol
Exchange (E_x):   -115.55 kcal/mol
Pauli repulsion (E_rep):    469.61 kcal/mol
Exchange-repulsion (E_xrep = E_x + E_rep):    354.06 kcal/mol
Orbital (E_orb):   -260.78 kcal/mol
DFT correlation (E_DFTc):    -18.38 kcal/mol
Dispersion correction (E_dc):    -1.39 kcal/mol
Coulomb correlation (E_c = E_DFTc + E_dc):    -19.76 kcal/mol
```

By the way, after finish running *sobEDA.sh*, the intermediate files *fragment1.fch* and *fragment2.fch* can be found in current folder, you can use Multiwfn to plot spin density to understand distribution of unpaired electrons of the fragments. For example, boot up Multiwfn, load *fragment2.fch*, and then input

> *5*　　// Calculate grid data
> *5*　　// Spin density
> *2*　　// Medium quality grid
> *-1*　 // Visualize isosurface

Then you will see the following spin density isosurface map, from which we can find unpaired electron distributes above and below the NH_2 plane, which fully meets our expectation.
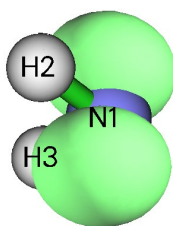
4.5 sobEDAw analysis between multiple fragments: Water tetramer at BHandHLYP-D3(BJ)/6-31+G(d,p) w.CP level

This section illustrates sobEDA analysis for interaction between more than two fragments. Structure of example system water tetramer is shown below:
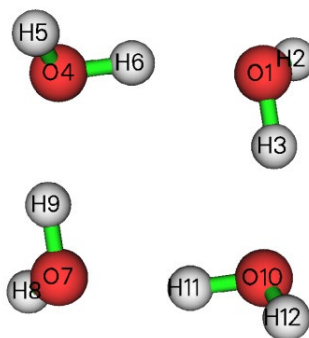
All files of this example have been provided in "water_tetramer" folder, please check them to understand how to set up this calculation. The *fragment.txt* in this example is shown below, it can be seen that four fragments are defined, each one corresponds to a water.

```
4
0 1
1-3
0 1
4-6
0 1
7-9
0 1
10-12
```

The *template.gjf* used in this example is shown below. It can be seen that DFT-D3(BJ) parameters for BHandHLYP are supplemented by IOp options because they are not built-in (at least as of G16 C.02)

```
#p BHandHLYP/6-31+G(d,p) em=gd3bj IOp(3/174=1000000,3/175=1035400,3/177=279300,3/178=4961500)
ExtraLinks=L608 nosymm

opted geometry

0 1
[geometry]

-3 5
```

Note that in the *sobEDA.sh* in this example folder, "iCP" has been set to 1, "sobEDAw" has been set to 1, and the line defining *c*, *a*, *r* parameters for sobEDAw corresponding to the BHandHLYP-D3(BJ)/6-31+G(d,p) w.CP level has been uncommented to make them take effect.

After running *sobEDA.sh*, you will obtain the following result

```
Total interaction energy:    -33.15 kcal/mol

Physical components of interaction energy derived by sobEDA:
Electrostatic (E_els):   -57.56 kcal/mol
Exchange (E_x):   -46.49 kcal/mol
```

```
    Pauli repulsion (E_rep):    116.98 kcal/mol
    Exchange-repulsion (E_xrep = E_x + E_rep):    70.48 kcal/mol
    Orbital (E_orb):    -28.90 kcal/mol
    DFT correlation (E_DFTc):    -14.62 kcal/mol
    Dispersion correction (E_dc):    -2.56 kcal/mol
    Coulomb correlation (E_c = E_DFTc + E_dc):    -17.17 kcal/mol

    Variant of sobEDA for weak interaction (sobEDAw):
    Note:    97.29% DFT correlation is combined with dispersion correction to yield a
SAPT-like dispersion term
    Electrostatic (E_els):    -57.56 kcal/mol
    Exchange-repulsion (including scaled DFT correlation):    70.09 kcal/mol
    Orbital (E_orb):    -28.90 kcal/mol
    Dispersion (E_disp):    -16.78 kcal/mol
```
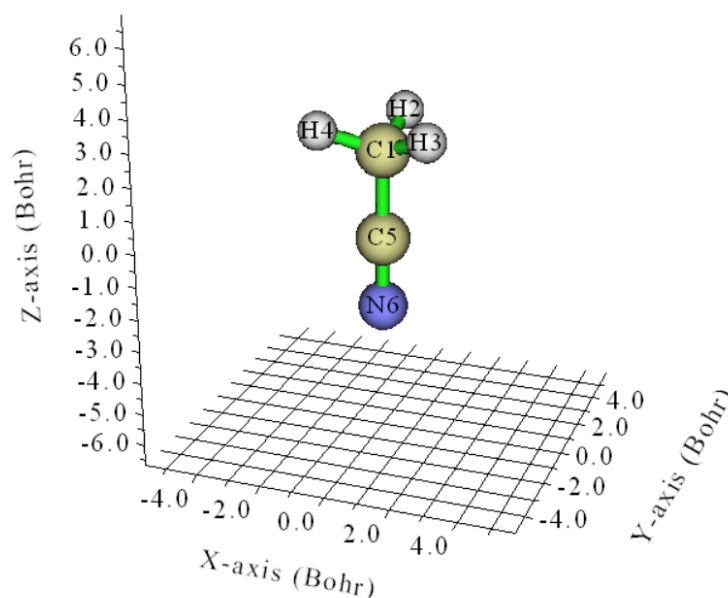
4.6 sobEDA analysis for a series interfragment distances of CH_3-CN

This section illustrates sobEDA analysis for a series interfragment distances of CH_3-CN. Equilibrium structure of this system is shown below:

All files of this example have been provided in "CH3-CN_scan" folder. From the folder you can find *scan.sh*, in which variable *i* is looped from -5 to 40 by 1 each time, corresponding to displacing CH_3 fragment from -0.5 to 4.0 by 0.1 Å each time towards positive direction of Z axis. As can be seen from the script, the displacement of the fragment is realized by automatically invoking Multiwfn, whose option 1 of subfunction 7 of main function 300 is able to make displacement for specific atoms according to a given vector, and then the updated geometry is exported to *system.xyz* in current folder. For the *system.xyz* corresponding to each interfragment distance, *scan.sh* invokes *sobEDA.sh* to perform sobEDA analysis, and the sobEDA terms are extracted from the outputted information to *scan.txt* in current folder. Once running *scan.sh* is fully

finished, the *scan.txt* contains displacement values and various sobEDA terms as different columns. Then you can use the data to plot various physical components of interaction energy with respect to displacements.

Content of the resulting *scan.txt* (the first line labelled meaning of each column)

```
Index E_tot E_els E_x E_rep E_xrep E_orb E_DFTc E_dc E_c
-5 137.62 -288.26 -256.09 1129.33 873.24 -414.49 -31.17 -1.70 -32.87
-4 1.60 -278.48 -205.90 867.43 661.53 -351.29 -28.48 -1.68 -30.16
-3 -74.50 -246.18 -164.36 665.15 500.79 -301.60 -25.86 -1.65 -27.51
-2 -114.27 -207.01 -130.35 508.85 378.50 -260.81 -23.34 -1.61 -24.95
-1 -132.06 -168.66 -102.73 388.11 285.39 -226.27 -20.95 -1.57 -22.51
0 -136.65 -134.51 -80.46 295.00 214.54 -196.47 -18.69 -1.52 -20.21
1 -133.44 -105.64 -62.63 223.39 160.76 -170.50 -16.60 -1.46 -18.06
2 -125.79 -82.02 -48.45 168.54 120.09 -147.78 -14.66 -1.41 -16.07
3 -115.80 -63.14 -37.26 126.72 89.47 -127.86 -12.90 -1.36 -14.25
4 -104.76 -48.31 -28.47 94.99 66.52 -110.35 -11.29 -1.33 -12.62
...ignored
```

It is worth noting that the current scan task does not consider geometry variation of fragments during the change of interfragment distance. To account for this effect, you need to perform relaxed scan, and then perform sobEDA analysis for every resulting geometry.

4.7 sobEDAw analysis for a series interfragment distances of benzene···H₂O

This section illustrates sobEDAw analysis for a series intermolecular distances of benzene···H_2O. The optimized equilibrium structure at B3LYP-D3(BJ)/6-311G** level is shown below.
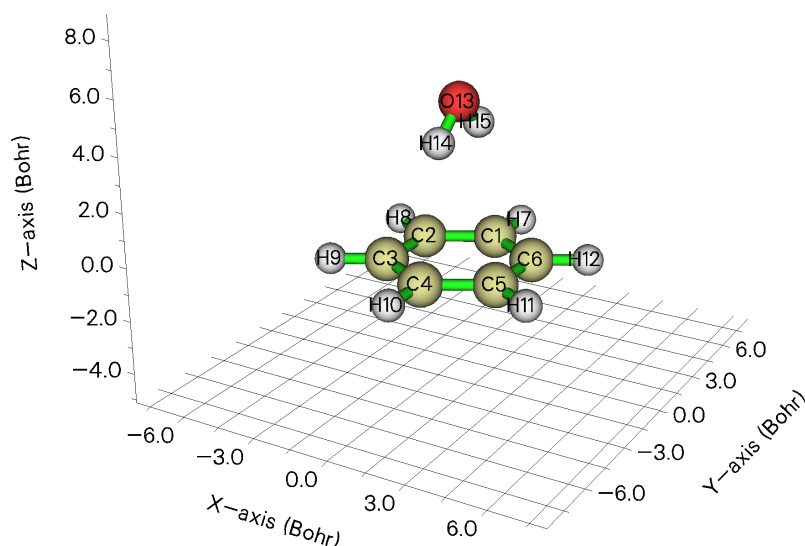
All files of this example have been provided in "benzene-water_scan" folder. From the folder you can find *scan.sh*, in which variable *i* is looped from -5 to 50 by 1 each time, corresponding to displacing water from -0.5 to 5.0 by 0.1 Å each time towards positive direction of Z axis. *equil.xyz*

contains optimized dimer geometry corresponding to above map. As can be seen from *template.gjf* and *sobEDA.sh*, the current sobEDAw analysis will be conducted at B3LYP-D3(BJ)/6-31+G(d,p) w.CB level.

Now run *scan.sh*. Once the calculation is fully finished, the *scan.txt* in current folder will contain displacement values and various sobEDAw terms as different columns. At the same time, you can find *scan.xyz* in current folder, which contains geometry of each calculated structure, you can use VMD program to load it and visualize the structures as trajectory.

Content of the *scan.txt*:

```
Index  E_tot  E_els  E_xrep  E_orb  E_disp
-5 3.83 -11.75 30.09 -5.78 -8.73
-4 1.00 -9.43 22.58 -4.47 -7.69
-3 -0.95 -7.63 16.93 -3.47 -6.78
-2 -2.24 -6.24 12.69 -2.72 -5.98
-1 -3.04 -5.16 9.53 -2.14 -5.27
0 -3.49 -4.31 7.17 -1.69 -4.65
1 -3.69 -3.65 5.41 -1.35 -4.10
2 -3.71 -3.12 4.11 -1.08 -3.62
3 -3.61 -2.70 3.14 -0.87 -3.18
...ignored
```

The distance between center of benzene and oxygen of water in *equil.xyz* is 3.17637 Å, therefore the distance of the structure with index *i* is 3.17637+0.1*i. Plot the various sobEDAw terms with respect to the distance as curve map:
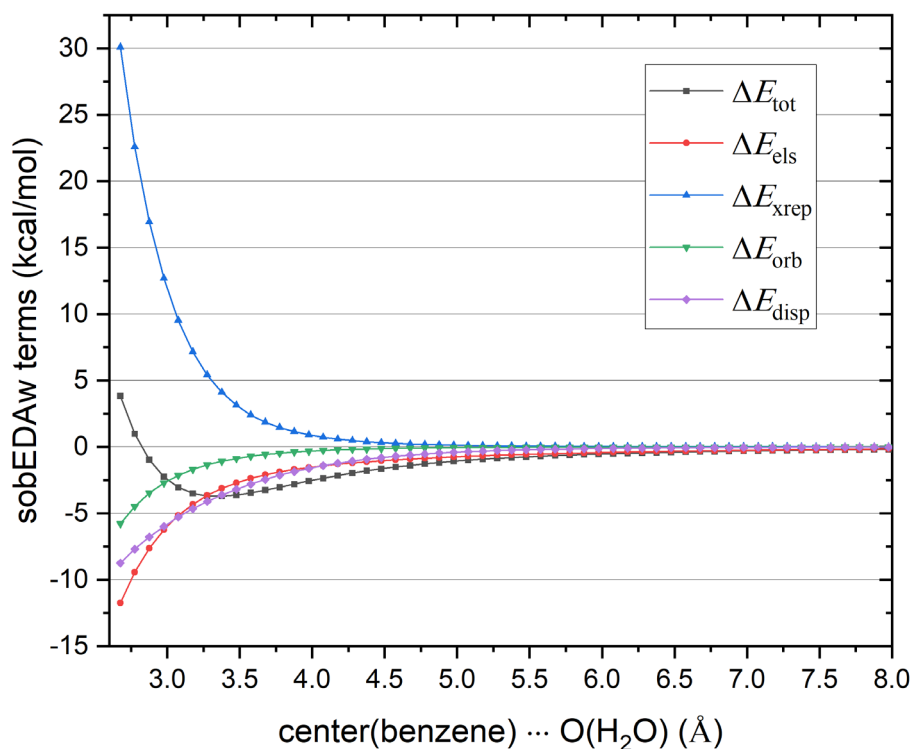
4.8 Obtaining full energy variation terms of interfragment interaction

This example illustrates how to obtain full energy variation terms of interfragment interaction, as exhibited in Fig. 1 of original paper of sobEDA. OC-BH$_3$ is taken as example.

All files of this example have been provided in "OC-BH3_full" folder. As you can see from the *sobEDA.sh* in this folder, "idetail" has been set to 1. After running this script, you will see the following content from the outputted information. It can be seen that variation of various energy components during the three steps of formation of final wavefunction from isolated fragment wavefunctions are shown clearly, they sum up to total interaction energy (-43.40 kcal/mol). Via the detailed information behind sobEDA, you can better understand how sobEDA terms are derived.

```
[...ignored]
Details of energy variations:
                Total      kin       els       exch      corr      disp
isolate->promol:  -147.06     0.00    -69.50    -65.15    -10.89    -1.52 kcal/mol
promol ->frozen:   221.03   427.12   -193.69    -12.46      0.05     0.00 kcal/mol
frozen ->final:   -117.36  -380.34    227.00     37.26     -1.28     0.00 kcal/mol
 Whole process:    -43.40    46.78    -36.19    -40.35    -12.12    -1.52 kcal/mol


*************************
***** Final results *****
*************************


Total interaction energy:    -43.40 kcal/mol
[...ignored]
```

4.9 More examples

Files for additional examples are also provided, please check them yourself
- "C18_O2" folder: sobEDAw for $C_{18}\cdots O_2$ interaction at BHandHLYP-D3(BJ)/6-311+G(2d,p) w.CP level.
- "(CO)5CrCH2" folder: sobEDA for $(CO)_5Cr=CH_2$ interaction at TPSSh/6-311G*&SDD level.
- "C6F6_Cl-" folder: sobEDA for $C_6F_6\cdots Cl^-$ interaction at BHandHLYP-D3(BJ)/6-311+G(2d,p) level.
- "HC-CH" folder: sobEDA for interaction between two quartet CH fragments at B3LYP-D3(BJ)/def2-TZVP level. The files for analyzing interaction between two doublet CH fragments are given in "doublet-fragment" subfolder.

5 Fitting *a*, *c*, *r* parameters

To fit *a*, *c*, *r* parameters of sobEDAw for a specific level, please follow this tutorial: http://sobereva.com/soft/sobEDAw_fit.zip.