ICSSgen

powerd by python

ICSSgen Manual

Input file generator for 2D-ICSS calculation, version 2.1

---------- Developed and Edited by ----------

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[*ICSSgen* Website]

https://www.wangzhe95.net/program-icssgen

1. Overview

1.1 About *ICSSgen*

ICSSgen is an input file generator for 2D-ICSS (2D-NICS) calculation. *ICSSgen* is open-source, free, high-efficient, and user-friendly. *ICSSgen* supports macOS, Linux and Microsoft Windows operating systems. Source code of *ICSSgen* is provided, thus, users can run *ICSSgen* through Python IDE.

ICSSgen can be download at from author's website (https://www.wangzhe95.net/program-icssgen) and author's GitHub homepage (https://github.com/wongzit/ICSSgen).

1.2 How it Works

ICSSgen reads an input file including the target molecular coordinates and adds ghost atom (Bq) to the end of the input file. User can define the plane, altitude, range, and grid quality from *ICSSgen*.

1.3 Testing Platform

ICSSgen has been tested on following platform.

1.3.1 macOS

(1) Mac mini (2020)

CPU: Intel Core i5-8500B 3.00 GHz 6 Cores 6 Threads

Mem: 16 GB 2666 MHz DDR4

GPU: Intel UHD Graphics 630 1536MB

OS: macOS 11.3.1(20E241)

(2) MacBook Air (M1, 2020)

CPU: Apple Silicon M1 8 Cores

Mem: 8 GB

GPU: Apple Silicon M1 8 Cores

OS: macOS 11.3.1(20E241)

1.3.2 Microsoft Windows

(1) Home-built PC I

CPU: Intel Core i7-9700KF 3.60 GHz 8 Cores 8 Threads

Mem: 16 GB 2666 MHz DDR4

GPU: Nvidia RTX 3060 12GB

OS: Windows 10 Education 20H2

(2) Home-built PC II (Physical machine with Windows/Linux dual-boot)

CPU: Intel Core i7-10700 2.90 GHz 8 Cores 16 Threads

Mem: 32 GB 2666 MHz DDR4

GPU: Intel UHD Graphics 630 1536MB

OS: Windows 10 Education 20H2

(3) Mac mini (2020) (Running with Parallels Desktop 16)

CPU: Intel Core i5-8500B 3.00 GHz 6 Cores 6 Threads (2 Cores used)

Mem: 16 GB 2666 MHz DDR4 (4 GB used)

GPU: Intel UHD Graphics 630 1536MB

OS: Windows 10 Education 1909

1.3.3 Linux

(1) Home-built PC I (Running with VMware Workstation Player 16)

CPU: Intel Core i7-9700KF 3.60 GHz 8 Cores 8 Threads (6 Cores used)

Mem: 16 GB 2666 MHz DDR4 (12 GB used)

GPU: Nvidia RTX 3060 12GB

OS: CentOS 8.3

(2) Home-built PC II (Physical machine with Windows/Linux dual-boot)

CPU: Intel Core i7-10700 2.90 GHz 8 Cores 16 Threads

Mem: 32 GB 2666 MHz DDR4

GPU: Intel UHD Graphics 630 1536MB

OS: Red Hat Enterprise Linux 8.3

(3) Mac mini (2020) (Running with Parallels Desktop 16)

CPU: Intel Core i5-8500B 3.00 GHz 6 Cores 6 Threads (3 Cores used)

Mem: 16 GB 2666 MHz DDR4 (4 GB used)

GPU: Intel UHD Graphics 630 1536MB

OS: Ubuntu 20.04, Fedora 34 beta

2. Run *ICSSgen*

2.1 Run with Source Code

If Python IDE is already installed in your computer, you can run *ICSSgen* with the source code. Python 3.7 or newer is recommended. *ICSSgen* may not work normally with Python 2.

For Mac users who want to run *ICSSgen* with source code, please run following command in terminal:

```
python3 /path_to_ICSSgen/ICSSgen_v*.py
```

2.2 Run with Executable File

All executable files are packaged in *execufiles.zip*.

2.2.1 Use Packaged Executable File

The pre-packaged executable file "*ICSSgen_v*_mac*" should be running normally on macOS 10.15 or newer with Intel and Apple M1 chip. You can run *ICSSgen* by double click the icon and *ICSSgen* will be running in terminal window.

2.2.2 Package Source Code into Executable File

If 2.2.1 is not work for some reason, you can try following steps to package *ICSSgen* by yourself:

1) Open terminal, execute `pip3 install pyinstaller` to install necessary packages.
2) Assume the source code file is located at "*/home/user/ICSSgen/ICSSgen_v*_source.py*", execute command below.

```
pyinstaller /home/user/ICSSgen/ICSSgen_v*_source.py --onefile
```

3) After that an executable file would be generated in *dist* folder. (Only executable file is needed, you can delete other files generated by *pyinstaller*.)
4) Now you can run *ICSSgen* by double clicking.

2.3 Run on Linux with Executable File

1) Assume the executable file is located at "*/home/user/ICSSgen/execufiles/ICSSgen_v*_linux*", run below command to add executable permission to it.

```
chmod +x /home/user/ICSSgen/execufiles/ICSSgen_v*_linux
```

2) (Optional) Assume the current shell is bash, add below lines to *~/.bashrc* file.

```
alias icssgen=/home/user/ICSSgen/execufiles/ICSSgen_v*_linux
```

3) After re-entering the terminal, and you can run *ICSSgen* at any dictionary by execute "`icssgen`" command. (If you passed the step (2), you need to execute the full path to *ICSSgen_v*_linux* for running it.)

2.4 Running on Microsoft Windows with Executable File

Find "*ICSSgen_v*_win.exe*" file in program folder, double click it and *ICSSgen* will be running in command line window.

If the Windows Defender stop the *ICSSgen*, please add the *ICSSgen* to the safe file list. More details please

check:

https://faq.nec-lavie.jp/qasearch/1007/app/servlet/relatedqa?QID=018507

3. How to Use

3.1 Before Running

You need prepare a *Gaussian* (Gaussian Inc.,) input file (*.gjf* or *.com*) including route section, and molecular coordinates. Please notice that **only Cartesian coordinates is allowed**. An example input file of benzene is attached in *example* folder:

```
%nprocshared=8
%mem=10GB
#p nmr=giao rb3lyp/6-31g(d)

Benzene_opt

0 1
 C              -1.33923600   -0.39585300    0.00000500
 C              -0.32668500   -1.35773000    0.00006900
 C               1.01242100   -0.96187800   -0.00005500
 C               1.33920200    0.39596500    0.00000800
 C               0.32679800    1.35770000    0.00006200
 C              -1.01250100    0.96179800   -0.00005800
 H              -2.38133000   -0.70401000   -0.00006600
 H              -0.58108600   -2.41424500    0.00007900
 H               1.80037500   -1.71023400   -0.00015400
 H               2.38136700    0.70385800    0.00000700
 H               0.58095200    2.41426700    0.00001800
 H              -1.80027600    1.71035300   -0.00006300
```

3.2 Generate ICSS Input

1) Run *ICSSgen*, the *ICSSgen* will request an (original) input file. You can drag the input file into the command window or input the full path to the input file. User-inputted command are colored in red.

```
Please specify the original input file path:
(e.g.: /ICSSgen/example/benzene.gjf)
/Users/path_to_ICSSgen/example/benzene.gjf
```

2) Specify the plane which ICSS map would be plotted on. The plane is defined in *XY*, *XZ* and *YZ* with no case-sensitivity. So, for user inputting, "xy", "XY" or "xY" are same.

```
Please specify the plane for ICSS map (XY, XZ, YZ):
xy
```

3) Specify the altitude over the molecular plane. The altitude is defined in angstrom (Å).

```
Please input the altitude over the plane (in angstrom):
1
```

4) Specify the ICSS map range. For each direction, minimum and maximum values are needed. After finish, the program will print out the user-determined parameters.

```
Please specify the range of X axis (in angstrom, e.g., -10 10):
-3.5 3.5

Please specify the range of Y axis (in angstrom, e.g., -8 8):
-3.5 3.5

2D-ICSS(XY,1.0) map in [X: -3.5 to 3.5, Y: -3.5 to 3.5].
```

5) Specify the grid quality. The grid quality is defined by the distance between two neighboring ghost atoms. Smaller grid value will give a smoother ICSS map, but more calculation cost is necessary. In my experience, a grid value of 0.25 is enough to produce a perfect ICSS map. The default value in *ICSSgen* is 0.2, you can press enter directly to use 0.2. Negative grid value is allowed but its absolute value would be used. 0 is not allowed, if user inputting is 0, the default value 0.2 would be used.

```
Please specify the grid quality (value smaller than 0.25 is recommended):
(press Enter to use default value 0.2)
(ENTER)
ICSSgen will use grid quality of 0.25.
```

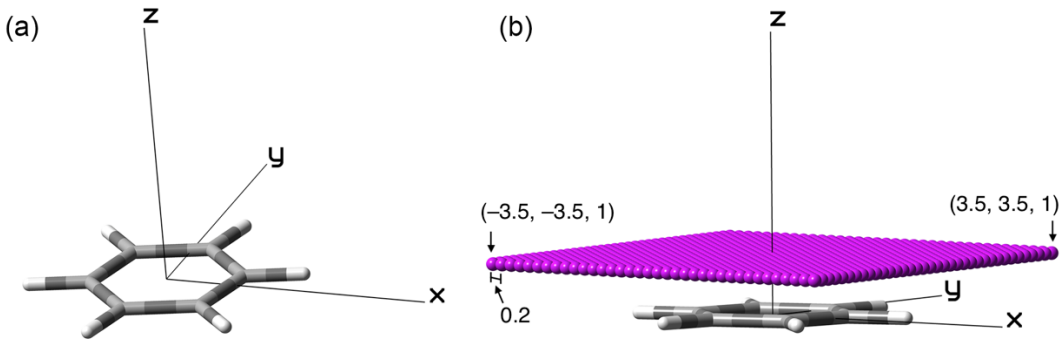

Figure 1. Geometries from (a) original input file and (b) for 2D-ICSS calculation generated with *ICSSgen*.

6) A new input file for ICSS calculation would be generated in the same dictionary as original input file, named with "*xxx_ICSS_plane_altitude.gjf*".

3.3 After Running

Open the ICSS input file with text editor, and check input syntax. Then, submit it to *Gaussian* calculation.