

PySOC

Calculation of Spin-Orbit Coupling

Quick Reference Guide

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How to Use This Document

This document is designed to act as rapid introduction and quick-reference to the PySOC spin-orbit coupling calculation program.

Images are included for comparison and reference.

Supplementary information and helpful tips are displayed separately, as follows:

NOTE: This is a tip.

Commands that should be typed by the user are displayed in the following format:

```
> echo Hello world
```

The arrow character (>) should not be typed; it is used to differentiate commands that should be typed from the resulting output (which will be displayed without the arrow character):

```
> echo Hello world  
Hello world
```

In the above example, the user is being instructed to type: echo Hello world. The computer, in response, gives the output: Hello world.

Ellipses (...) indicate that the real, full output has been truncated:

```
> cat /etc/fstab  
# /etc/fstab: static file system information.  
#  
...
```

About PySOC

PySOC is a program for the calculation of spin-orbit coupling (SOC) values between singlet and triplet excited states. As input, PySOC requires an excited states calculation at any of the following levels of theory:

- Time-dependant DFT (TD-DFT)^{1–7} with Gaussian 09/16^{8,9}
- TD-DFT using the Tamm–Dancoff approximation (TDA)^{1–7,10} with Gaussian 09/16^{8,9}
- Time-dependant Density Functional based Tight Binding (TD-DFTB) with DFTB+¹¹

PySOC consists of two Fortran programs (molsoc and soc_td) and a Python controller (pysoc) with contributions from the following authors:

pysoc: Originally written by Xing Gao *et al.*¹² Rewritten for Python3.6 by the current author.

molsoc: Originally written by Sandro G. Chiodo and Monica Leopoldini,¹³ with modifications by Xing Gao *et al.*¹²

soc_td: Originally written by Xing Gao *et al.*,¹² with modifications by the current author.

Installation

Prerequisites

The four following prerequisites must be installed before PySOC can be used:

- **cclib:** The cclib parsing library,¹⁴ required to parse results from completed Gaussian calculations. The user is directed to the cclib documentation for more information: <https://cclib.github.io/>.
- **Tabulate:** Prints SOC results in a user-friendly table format.
- **Scipy:** Used to provide certain scientific constants for the interconversion of energy units.
- **Periodictable:** Interconverts between atomic number and symbol.

These requirements are most easily satisfied using the pip command:

```
> pip3 install --user cclib tabulate scipy periodictable
```

Download and Link

The latest version of PySOC can be downloaded from github with the git program:

```
> git clone https://github.com/oliver-s-lee/pysoc.git
```

This will create a 'pysoc' folder in the current directory in which PySOC will be downloaded. Within this folder, two further steps are required to 'install' PySOC:

- The 'bin' subdirectory should be added to the user's PATH variable.
- The 'pysoc' top directory should be added to the user's PYTHONPATH variable.

Installation can be made permanent by adding these paths to the user's .bashrc file (located in the user's home directory), for example:

```
# Install PySOC
export PYTHONPATH="$PYTHONPATH:$HOME/pysoc"
PATH="$PATH:$HOME/pysoc/bin"
```

Once modified, the .bashrc file can be reloaded with the source command:

```
source ~/.bashrc
```

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Testing

The installation can be tested with the 'pysoc -v' command, which will print the PySOC version if installation was successful:

```
> pysoc -v  
2.1.4
```

Two example folders are additionally provided, one each for the Gaussian and DFTB+ programs, which can be used to test the calculation of SOC values:

Gaussian

```
> pysoc pysoc/examples/ch2o_gaussian/gaussian.log
```

Singlet	Triplet	RSS (cm-1)	+1 (cm-1)	0 (cm-1)	-1 (cm-1)
S(0)	T(1)	60.7419	42.9510	0.0077	42.9510
S(0)	T(2)	0.0194	0.0137	0.0000	0.0137
S(0)	T(3)	10.6234	0.0133	10.6234	0.0133
S(0)	T(4)	59.8873	42.3467	0.0012	42.3467
S(0)	T(5)	11.7332	0.0013	11.7332	0.0013
S(1)	T(1)	0.0008	0.0006	0.0000	0.0006
S(1)	T(2)	44.3144	31.3350	0.0224	31.3350
S(1)	T(3)	8.6280	6.1009	0.0002	6.1009
S(1)	T(4)	50.7211	0.0151	50.7211	0.0151
S(1)	T(5)	5.5317	3.9115	0.0001	3.9115
S(2)	T(1)	7.3854	5.2223	0.0001	5.2223
S(2)	T(2)	0.2532	0.0008	0.2531	0.0008
S(2)	T(3)	0.0003	0.0002	0.0000	0.0002
S(2)	T(4)	0.2432	0.1720	0.0013	0.1720
S(2)	T(5)	0.0005	0.0004	0.0001	0.0004
S(3)	T(1)	51.2578	0.0335	51.2578	0.0335
S(3)	T(2)	37.2693	26.3534	0.0008	26.3534
S(3)	T(3)	1.4244	1.0072	0.0058	1.0072
S(3)	T(4)	0.0557	0.0394	0.0000	0.0394
S(3)	T(5)	0.9133	0.6458	0.0039	0.6458
S(4)	T(1)	5.8574	4.1418	0.0001	4.1418
S(4)	T(2)	0.2305	0.0018	0.2305	0.0018
S(4)	T(3)	0.0010	0.0007	0.0001	0.0007
S(4)	T(4)	0.9472	0.6698	0.0009	0.6698
S(4)	T(5)	0.0000	0.0000	0.0000	0.0000
S(5)	T(1)	51.1922	36.1984	0.0449	36.1984
S(5)	T(2)	0.0471	0.0333	0.0000	0.0333
S(5)	T(3)	3.1852	0.0023	3.1852	0.0023
S(5)	T(4)	34.6872	24.5276	0.0007	24.5276
S(5)	T(5)	0.7834	0.0021	0.7834	0.0021

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DFTB+

> pysoc pysoc/examples/ch2o_tddftb/ch2o.xyz					
Singlet	Triplet	RSS (cm-1)	+1 (cm-1)	0 (cm-1)	-1 (cm-1)
S(0)	T(1)	77.0964	54.5154	0.0118	54.5154
S(0)	T(2)	0.0300	0.0212	0.0000	0.0212
S(0)	T(3)	76.2779	53.9366	0.0015	53.9366
S(0)	T(4)	26.5506	18.7741	0.0081	18.7741
S(0)	T(5)	21.4371	15.1583	0.0004	15.1583
S(0)	T(6)	10.4277	0.0171	10.4277	0.0171
S(0)	T(7)	0.0016	0.0011	0.0004	0.0011
S(0)	T(8)	1.3659	0.9658	0.0000	0.9658
S(0)	T(9)	0.0224	0.0158	0.0003	0.0158
S(0)	T(10)	11.9821	0.0037	11.9821	0.0037
S(1)	T(1)	0.0011	0.0008	0.0000	0.0008
S(1)	T(2)	53.9735	38.1650	0.0349	38.1650
S(1)	T(3)	56.3777	0.0223	56.3777	0.0223
S(1)	T(4)	0.0011	0.0008	0.0001	0.0008
S(1)	T(5)	23.0942	0.0056	23.0942	0.0056
S(1)	T(6)	14.7378	10.4212	0.0003	10.4212
S(1)	T(7)	36.3932	25.7339	0.0046	25.7339
S(1)	T(8)	0.0101	0.0072	0.0000	0.0072
S(1)	T(9)	8.0243	5.6741	0.0022	5.6741
S(1)	T(10)	1.6583	1.1726	0.0000	1.1726
S(2)	T(1)	56.3777	0.0112	56.3777	0.0112
S(2)	T(2)	42.0284	29.7186	0.0008	29.7186
S(2)	T(3)	0.0384	0.0271	0.0000	0.0271
S(2)	T(4)	25.8912	0.0118	25.8912	0.0118
S(2)	T(5)	0.0122	0.0086	0.0001	0.0086
S(2)	T(6)	2.4438	1.7281	0.0001	1.7281
S(2)	T(7)	1.6462	1.1640	0.0000	1.1640
S(2)	T(8)	0.0317	0.0225	0.0000	0.0225
S(2)	T(9)	11.1961	7.9168	0.0002	7.9168
S(2)	T(10)	13.4967	9.5436	0.0014	9.5436
S(3)	T(1)	0.0013	0.0009	0.0001	0.0009
S(3)	T(2)	39.3959	27.8571	0.0193	27.8571
S(3)	T(3)	25.8912	0.0160	25.8912	0.0160
S(3)	T(4)	0.0010	0.0007	0.0000	0.0007
S(3)	T(5)	17.5933	0.0013	17.5933	0.0013
S(3)	T(6)	1.8475	1.3064	0.0000	1.3064
S(3)	T(7)	6.2101	4.3912	0.0002	4.3912
S(3)	T(8)	0.0164	0.0116	0.0000	0.0116
S(3)	T(9)	17.5326	12.3974	0.0011	12.3974
S(3)	T(10)	13.7304	9.7089	0.0003	9.7089
S(4)	T(1)	59.4613	42.0455	0.0175	42.0455
S(4)	T(2)	0.0418	0.0295	0.0000	0.0295
S(4)	T(3)	44.6992	31.6071	0.0009	31.6071
S(4)	T(4)	42.4153	29.9921	0.0046	29.9921
S(4)	T(5)	24.9459	17.6395	0.0005	17.6395
S(4)	T(6)	0.5542	0.0027	0.5541	0.0027
S(4)	T(7)	0.0036	0.0025	0.0000	0.0025
S(4)	T(8)	16.0856	11.3743	0.0003	11.3743
S(4)	T(9)	0.0350	0.0248	0.0000	0.0248
S(4)	T(10)	3.2489	0.0039	3.2489	0.0039
S(5)	T(1)	23.0942	0.0016	23.0942	0.0016
S(5)	T(2)	24.1241	17.0583	0.0005	17.0583
S(5)	T(3)	0.0096	0.0068	0.0001	0.0068
S(5)	T(4)	17.5933	0.0036	17.5933	0.0036

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S (5)	T (5)	0.0022	0.0016	0.0000	0.0016
S (5)	T (6)	2.6137	1.8482	0.0006	1.8482
S (5)	T (7)	2.2238	1.5725	0.0001	1.5725
S (5)	T (8)	0.0035	0.0025	0.0000	0.0025
S (5)	T (9)	4.1545	2.9377	0.0001	2.9377
S (5)	T (10)	4.5831	3.2407	0.0008	3.2407
S (6)	T (1)	14.5454	10.2851	0.0003	10.2851
S (6)	T (2)	0.1112	0.0020	0.1111	0.0020
S (6)	T (3)	3.4766	2.4583	0.0008	2.4583
S (6)	T (4)	2.6608	1.8815	0.0001	1.8815
S (6)	T (5)	3.3645	2.3790	0.0011	2.3790
S (6)	T (6)	0.0001	0.0000	0.0000	0.0000
S (6)	T (7)	5.0065	0.0163	5.0065	0.0163
S (6)	T (8)	60.1950	42.5642	0.1095	42.5642
S (6)	T (9)	45.7019	0.0742	45.7018	0.0742
S (6)	T (10)	0.0004	0.0003	0.0001	0.0003
S (7)	T (1)	32.5341	23.0051	0.0014	23.0051
S (7)	T (2)	0.0065	0.0046	0.0000	0.0046
S (7)	T (3)	8.1824	5.7858	0.0002	5.7858
S (7)	T (4)	1.7266	1.2209	0.0006	1.2209
S (7)	T (5)	0.8927	0.6312	0.0000	0.6312
S (7)	T (6)	24.5442	0.0176	24.5441	0.0176
S (7)	T (7)	0.0011	0.0008	0.0000	0.0008
S (7)	T (8)	7.9526	5.6234	0.0002	5.6234
S (7)	T (9)	0.0198	0.0140	0.0001	0.0140
S (7)	T (10)	11.4488	0.0003	11.4488	0.0003
S (8)	T (1)	0.0066	0.0047	0.0000	0.0047
S (8)	T (2)	14.6674	10.3714	0.0003	10.3714
S (8)	T (3)	0.0059	0.0041	0.0000	0.0041
S (8)	T (4)	0.0049	0.0035	0.0000	0.0035
S (8)	T (5)	0.0006	0.0004	0.0000	0.0004
S (8)	T (6)	48.2255	34.1006	0.0251	34.1006
S (8)	T (7)	2.6340	1.8625	0.0001	1.8625
S (8)	T (8)	0.0517	0.0366	0.0000	0.0366
S (8)	T (9)	30.0358	21.2385	0.0006	21.2385
S (8)	T (10)	44.5441	31.4974	0.0201	31.4974
S (9)	T (1)	0.0005	0.0003	0.0000	0.0003
S (9)	T (2)	35.5573	25.1428	0.0012	25.1428
S (9)	T (3)	0.0115	0.0082	0.0000	0.0082
S (9)	T (4)	0.0017	0.0012	0.0000	0.0012
S (9)	T (5)	0.0007	0.0005	0.0000	0.0005
S (9)	T (6)	1.0070	0.7120	0.0000	0.7120
S (9)	T (7)	45.5868	32.2347	0.0455	32.2347
S (9)	T (8)	13.6665	0.0397	13.6664	0.0397
S (9)	T (9)	28.9564	20.4753	0.0098	20.4753
S (9)	T (10)	12.1184	8.5690	0.0003	8.5690
S (10)	T (1)	4.3556	3.0798	0.0012	3.0798
S (10)	T (2)	0.0012	0.0008	0.0000	0.0008
S (10)	T (3)	11.9037	8.4172	0.0003	8.4172
S (10)	T (4)	5.0888	3.5983	0.0018	3.5983
S (10)	T (5)	0.9321	0.6591	0.0000	0.6591
S (10)	T (6)	51.7307	0.0198	51.7307	0.0198
S (10)	T (7)	0.0013	0.0009	0.0000	0.0009
S (10)	T (8)	44.0081	31.1184	0.0009	31.1184
S (10)	T (9)	0.0628	0.0444	0.0000	0.0444
S (10)	T (10)	28.6801	0.0189	28.6801	0.0189

Using PySOC

Setup

Before spin-orbit coupling can be calculated, it is first necessary to perform an excited states calculation with either the Gaussian or DFTB+ quantum mechanical (QM) calculation programs. The next section will briefly cover the necessary options to perform SOC calculations with each, but the reader is expected to be familiar with the basic operation of the QM program of choice.

NOTE: Shells higher than the f shell are not currently supported by PySOC. The user should ensure that the basis set used in the QM program does not contain g (or higher) shells.

Gaussian

Time-dependant DFT excited states calculations both with and without the Tamm–Dancoff approximation are supported for Gaussian versions 09 and 16. Older versions of Gaussian and alternative calculation methods (CIS etc.) may additionally be supported, but have not been tested.

PySOC requires that the following options be specified in the input file:

Option	Type	Description
%rwf=file.rwf	Link 0 option	Indicates that the read-write intermediate file should be created with the name 'file.rwf'. PySOC expects the rwf file to have the same name as the log file (except for the extension), but this can be specified manually to pysoc if a different name is used.
6D	Route keyword	Specifies that pure (rather than Cartesian) d functions should be used.
10F	Route keyword	Specifies that pure (rather than Cartesian) f functions should be used.
GFInput	Route keyword	Specifies that the basis set should be printed in the calculation output.

In addition, either the 'TD' or 'TDA' keywords should be given to calculate excited states. An example input file is given below:

```
%mem=1GB
%chk=gaussian.chk
%rwf=gaussian.rwf
# TD(50-50,nstates=5) wB97XD/TZVP 6D 10F nosymm GFInput

test

0 1
C      -0.131829      -0.000001      -0.000286
O       1.065288       0.000001       0.000090
H      -0.718439       0.939705       0.000097
H      -0.718441      -0.939705       0.000136
```

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DFTB+

Please note that this section is under revision.

NOTE: PySOC requires Gaussian type orbitals (GTOs) to perform the SOC calculation, yet DFTB+ uses Slater-type orbitals (STOs). Thus the parameter set used for the DFTB+ calculation must be fitted to GTOs for use with PySOC. PySOC contains a fitted set for the mio-1-1 parameter set which will be used by default, alternative fitted sets can be specified with the '--fitted_basis' option:

```
> pysoc ch2o.xyz --fitted_basis /path/to/directory
```

An example dftb_in.hsd file is given below:

```
Geometry = GenFormat {
  <<< "ch2o.gen"
}

Driver = {}

Hamiltonian = DFTB {
  SCC = Yes
  SCCTolerance = 1e-10 # Very tight for test purposes only
  MaxAngularMomentum = {
    H = "s"
    C = "p"
    O = "p"
  }
  SlaterKosterFiles = Type2FileNames {
    Prefix =
"/fsnfs/users/xinggao/work/gsh/thiothymine/gtsh/test_python/tddftb/sk/
mio-1-1/"
    Separator = "-"
    Suffix = ".skf"
  }
  LinearResponse {
    NrOfExcitations = 10
    StateOfInterest = 0
    Symmetry = both
    HubbardDerivatives {
      H = 0.347100 0.491900
      C = 0.341975 0.387425
      O = 0.467490 0.523300
    }
    WriteTransitions = Yes
    WriteTransitionDipole = Yes
    WriteXplusY = Yes
  }
}

Options {
  WriteEigenvectors = Yes
  WriteHS = No
}
```

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```
ParserOptions {  
  ParserVersion = 4  
}
```

After performing the DFTB+ calculation, set WriteHS = Yes and run the calculation a second time.

Spin-Orbit Coupling Calculation

Once the QM calculation of choice has completed successfully, SOC can be calculated using the 'pysoc' program. This program has one mandatory argument which is the principle output file from the completed QM calculation. For Gaussian, this is the .log file, while for DFTB+ this is the .xyz geometry file. PySOC will automatically find the additional input files it requires from the location of the .log or .xyz file.

NOTE: When computing SOC from a Gaussian calculation, the location of the .rwf file can be given explicitly using the '--rwf_file' argument:

```
> pysoc ch2o.log --rwf_file gaussian.rwf
```

For example, to calculate SOC for a file in the current directory with the name ch2o.log:

```
> pysoc ch2o.log
```

Or to calculate SOC from a completed DFTB+ calculation:

```
> pysoc ch2o.xyz
```

Each calculation has a typical duration of a few minutes, and the output will be presented in a user-friendly table format:

```
> pysoc ch2o.log
Singlet      Triplet      RSS (cm-1)      +1 (cm-1)      0 (cm-1)      -1 (cm-1)
-----
S0           T1           60.7419         42.9510         0.0077         42.9510
S0           T2           0.0194          0.0137          0.0000          0.0137
S0           T3          10.6234          0.0133          10.6234          0.0133
S0           T4          59.8873         42.3467          0.0012         42.3467
S0           T5          11.7332          0.0013          11.7332          0.0013
S1           T1           0.0008          0.0006          0.0000          0.0006
S1           T2          44.3144         31.3350          0.0224         31.3350
S1           T3           8.6280          6.1009          0.0002          6.1009
S1           T4          50.7211          0.0151          50.7211          0.0151
S1           T5           5.5317          3.9115          0.0001          3.9115
S2           T1           7.3854          5.2223          0.0001          5.2223
S2           T2           0.2532          0.0008          0.2531          0.0008
S2           T3           0.0003          0.0002          0.0000          0.0002
S2           T4           0.2432          0.1720          0.0013          0.1720
...
```

Here, each line indicates SOC between one singlet and one triplet state, which are given by the 'Singlet' and 'Triplet' columns respectively. The last three columns each contain the calculated spin-orbit coupling with quantum numbers +1, 0 and -1 respectively for those two states, which are summarised by the RSS column containing the root sum square of these three values. All SOC values are given in wavenumbers (cm⁻¹).

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Alternatively, a comma-separated values (CSV) format can be requested with the '-c' option, which can be more easily imported into a spreadsheet for analysis:

```
> pysoc ch2o.log -c
Singlet,Triplet,RSS (cm-1),+1 (cm-1),0 (cm-1),-1 (cm-1)
S0,T1,60.7419154885397,42.95102,0.00769,42.95102
S0,T2,0.019431296920174937,0.01374,1e-05,0.01374
S0,T3,10.623396701112124,0.01332,10.62338,0.01332
S0,T4,59.887319900989056,42.34673,0.00124,42.34673
S0,T5,11.733160146260683,0.00131,11.73316,0.00131
...
```

To write to a file instead of to the screen, use standard Linux file redirection with the '>' or '>>' characters (to overwrite or append to an existing file respectively):

```
> pysoc ch2o.log -c > SOC.csv
```

Intermediate Files

PySOC generates a number of intermediate files during operation. By default, these are deleted at the end of the calculation and only the final SOC values are displayed. To override this behaviour and keep these intermediate files, use the '-o' (output) option with a path to a directory where the intermediate files should be stored. One may use '-o .' to write the intermediate files to the current directory. The '-o' option has no effect on the final SOC values:

```
> pysoc ch2o.log -o ./
Singlet      Triplet      RSS (cm-1)      +1 (cm-1)      0 (cm-1)      -1 (cm-1)
-----
S0           T1           60.7419         42.9510         0.0077         42.9510
S0           T2           0.0194         0.0137         0.0000         0.0137
S0           T3           10.6234         0.0133         10.6234         0.0133
S0           T4           59.8873         42.3467         0.0012         42.3467
S0           T5           11.7332         0.0013         11.7332         0.0013
...
```

Referencing PySOC

Scientific publications which make use of PySOC in their work should cite the original PySOC publication by Xing Gao *et al.* as well as the cclib publication by O'Boyle *et al.*:

Evaluation of Spin-Orbit Couplings with Linear-Response Time-Dependent Density Functional Methods, Xing Gao, Shuming Bai, Daniele Fazzi, Thomas Niehaus, Mario Barbatti, and Walter Thiel, *J. Chem. Theory Comput.*, 2017, **13** (2), 515–524. DOI: 10.1021/acs.jctc.6b00915

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