Siam Quantum

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Homepage

The project homepage contains the complete info. The project is located at GitHub as well.
https://sites.google.com/site/siamquantum/
https://github.com/Siam-Quantum/SQ-4.0-Development

Source

Source code is available in the project homepage and at GitHub.
https://sites.google.com/site/siamquantum/
https://github.com/Siam-Quantum/SQ-4.0-Development

Reference

Chachiyo, T. et al.: Siam Quantum: a compact open-source quantum simulation software for molecules, Thailand (2016);
see https://sites.google.com/site/siamquantum.

Description & Use

Siam Quantum offers wide computational methodology possibilities from ab initio through DFT, perturbation theory up to molecular dynamics. Both single point and geometry optimization procedures are available.

Quick start

Siam Quantum accepts as the input file directly the .xyz coordinate file produced by e.g. Atomdroid. The basis in the GAMESS-US style is saved as a text file. The keywords controlling the calculation are listed below, and are not a part of the input .xyz file, but they are filled in the execution command.

Use in command line / shell:

```
sq [input file].xyz [basis file].txt [options] > [output file]
```
(in Windows command line)

or

```
./sq [input file].xyz [basis file].txt [options] > [output file]
```
(in Android shell).

The result will appear in the same location.

Available switches:

```
[x] Ab Initio Method:
-HF             Hartree-Fock (default)
                Density Functional Theory
-LDA=S:VWN5       ex: Slater          corr: VWN5
-LDA=S:CHACHIYO   ex: Slater          corr: Chachiyo
-DFT=HALF         ex: 0.5*(HF+Slater) corr: VWN5
-DFT=PBE          ex: PBE             corr: PBE
-DFT=BLYP         ex: Becke88         corr: LYP
-DFT=CHACHIYO     ex: Chachiyo        corr: Chachiyo
-DFT=B3LYP        The famous Becke's three parameters hybrid
-LIBXC=STR        Use LibXC with specific ex. and corr.
                  See its website for the avialable functionals
                  Example, -LIBXC=GGA_X_CHACHIYO+GGA_C_CHACHIYO
                           -LIBXC=HYB_GGA_XC_B3LYP
-Q=INT          Set total molecular charge (default=0)
-M=INT          Set molecular spin multiplicity (M=2S+1)
-R              Use restricted   orbitals (default if singlet)
-U              Use unrestricted orbitals (default if  M > 1 )


[x] Compute DFT exchange from Hartree-Fock densities:
-xSlater        Slater LDA exchange
-xPerdewYue     J.P.Perdew and W.Yue 1986 exchange
-xPBE           Perdew‐Burke‐Ernzerhof exchange
-xBecke88       A.D.Becke 1988 exchange
-xMVS           meta-GGA Made Very Simple exchange
-xChachiyo      T.Chachiyo and H.Chachiyo exchange


[x] Post SCF:
-FORCE          Compute forces acting on nuclei
-OPT            Request geometry optimization
-MP2            Request MP2 energy calculations
-MECP=INT,INT   Request MECP between two spin multiplicities
-EXCITE         Request excited state calculations
-QMD            Request quantum molecular dynamics simulation
```

```
[x] SCF Cycle:
-GUESS=DIAG     Use identity density matrix as initial guess (default)
-GUESS=CORE     Use density from core hamiltonian as initial guess
-GUESS=CHECK    Use density from checkpoint as initial guess
-SCFDIIS        Use 4-point DIIS method for convergence (default)
-SCFDIIS3       Use 3-point DIIS method for convergence
-SCFDIIS2       Use 2-point DIIS method for convergence
-SCFDAMP        Use simple weighting method for convergence
-SCFDRAG=REAL   Set SCF drag coefficient between 0 to 1 (default=0.25)
-SCFCONV=REAL   Set SCF convergence threshold (default=1.0E-6)
-SCFMAX=INT     Set maximum number of scf cycle (default=80)
-SCFACC=3STEP   Use increasing integral accuracy in 3 steps (default)
-SCFACC=1STEP   Use fixed integral accuracy
-MAXMEM=INT     Set maximum memory per CPU in Mbyte (default=250)


[x] Grid:
-GRIDSIZE=S     Good enough for a few milli-hartree accuracy
-GRIDSIZE=M     Below milli-hartree (default for energy run)
-GRIDSIZE=L     A few micro hartree (default for optimization)
-GRIDSIZE=XL    Good for testing (96/590 radial/anuglar point)
-GRID=BALLS     Use Becke partition + uniform radius (default)
-GRID=BECKE     Use Becke partition + bragg radius


[x] Checkpoint File:
-LCHECK         Do not perform SCF but load info from checkpoint
-SCHECK         Save checkpoint file at the end (default=no)
-SCHECK=ALL     Save checkpoint file every scf cycle (default=no)
-FCHECK=STR     Set file name for checkpoint (default=checkpoint.txt)
-LDMATRIX       Load density matrix at the beginning (default=no)
-SDMATRIX       Save density matrix at the end (default=no)
-FDMATRIX=STR   Set file name for density matrix (default=dmatrix.txt)


[x] Output:
-DENSITY        Print electron density   volume information
-POTENTIAL      Print electric potential volume information
-GRADOVER43     Gradient over rho^4/3    volume information
-GRADRS         Gradient electron radius volume information
-MOUP=INT       Print spin up mo. volume info (index starts at 1)
-MODN=INT       Print spin dn mo. volume info (index starts at 1)
-VOLCUT=REAL    Set accuracy for computing volume info (default=1.0E-4)
-VOLGRID=INT    Set the number of grid points per angstrom (default=10)
-XSF            Volume info. will be in XSF  format to 'volume.xsf'
-CUBE           Volume info. will be in CUBE format to 'volume.cube'
-GAUSSIAN       Emulate Gaussian output to 'gaussian.log' (for GabEdit)


[x] Parallel Run:
-NCPU=INT       Set the number of CPUs (default=1)
-PREFIX=STR     Set prefix string for the job (default=SQ)
```

```
[x] Geometry Optimization:
-OPTMAX=INT     Maximum number of iterations (default=30)


[x] Minimum Energy Crossing Point (MECP):
-MECPMAX=INT    Maximum number of iterations (default=30)
-FCHECKA=STR    State A checkpoint file name (default=checkpointA.txt)
-FCHECKB=STR    State B checkpoint file name (default=checkpointB.txt)
-FDMATRIXA=STR  State A density matrix file name (default=dmatrixA.txt)
-FDMATRIXB=STR  State B density matrix file name (default=dmatrixB.txt)
-GAUSSINA=STR   State A Gaussian input file name (excluding .com)
-GAUSSINB=STR   State B Gaussian input file name (excluding .com)
-GAUSSEXE=STR   Gaussian program execution string


[x] External Field:
-EF=EX,EY,EZ    Uniform electric field in AU (default=0.0,0.0,0.0)
                Electric field 1 AU = 51.4220652 Volt/Angstrom


[x] Quantum Molecular Dynamics (QMD):
-INITVEL=STR    Initial velocity from the file in xyz format  (nm/ps)
-INITTEMP=REAL  Initial velocity at random using the temp.   (kelvin)
-KEEPTEMP=REAL  Rescale velocity to maintain the temp. (default=none)
-TRAJ=STR       Set output trajectory file         (default=traj.xyz)
-DT=REAL        Set time step in pico-sec             (default=0.001)
-QMDMAX=INT     Set maximum number of steps           (default=25)
-EFREQ=REAL     Set electric field frequency in THz   (default=0.0)

[x] Some of available functionals from LIBXC:
XC_LDA_C_2D_AMGB
XC_LDA_C_BR78
XC_LDA_C_CHACHIYO
XC_LDA_C_GL
XC_LDA_C_HL
XC_LDA_C_LP_A
XC_LDA_C_LP_B
XC_LDA_C_MCWEENY
XC_LDA_C_ML1
XC_LDA_C_ML2
XC_LDA_C_OB_PW
XC_LDA_C_OB_PZ
XC_LDA_C_OW
XC_LDA_C_OW_LYP
XC_LDA_C_PK09
XC_LDA_C_PW
XC_LDA_C_PW_MOD
XC_LDA_C_PW_RPA
XC_LDA_C_PZ
XC_LDA_C_PZ_MOD
XC_LDA_C_RC04
XC_LDA_C_vBH
XC_LDA_C_VWN
XC_LDA_C_VWN_1
XC_LDA_C_VWN_2
XC_LDA_C_VWN_3
XC_LDA_C_VWN_4
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XC_LDA_C_VWN_RPA
XC_LDA_C_XALPHA
XC_LDA_K_LP
XC_LDA_K_TF
XC_LDA_K_ZLP
XC_LDA_X
XC_LDA_X_1D
XC_LDA_X_2D
XC_LDA_X_ERF
XC_LDA_X_RAE
XC_LDA_X_REL
XC_LDA_XC_GDSMFB
XC_LDA_XC_KSDT
XC_LDA_XC_TETER93
XC_GGA_C_AM05
XC_GGA_C_APBE
XC_GGA_C_BCGP
XC_GGA_C_BMK
XC_GGA_C_FT97
XC_GGA_C_GAM
XC_GGA_C_GAPLOC
XC_GGA_C_HCTH_A
XC_GGA_C_LM
XC_GGA_C_LYP
XC_GGA_C_N12
XC_GGA_C_N12_SX
XC_GGA_C_OPTC
XC_GGA_C_OP_B88
XC_GGA_C_OP_PW91
XC_GGA_C_OP_PBE
XC_GGA_C_P86
XC_GGA_C_PBE
XC_GGA_C_PBEFE
XC_GGA_C_PBEINT
XC_GGA_C_PBELOC
XC_GGA_C_PBE_JRGX
XC_GGA_C_PBE_MOL
XC_GGA_C_PBE_SOL
XC_GGA_C_PW91
XC_GGA_C_Q2D
XC_GGA_C_REGTPSS
XC_GGA_C_RGE2
XC_GGA_C_SCAN_E0
XC_GGA_C_SG4
XC_GGA_C_SOGGA11
XC_GGA_C_SOGGA11_X
XC_GGA_C_SPBE
XC_GGA_C_TAU_HCTH
XC_GGA_C_TCA
XC_GGA_C_TM_PBE
XC_GGA_C_TM_LYP
XC_GGA_C_W94
XC_GGA_C_WI0
XC_GGA_C_WI
XC_GGA_C_WL
XC_GGA_C_XPBE
XC_GGA_C_ZPBEINT

XC_GGA_C_ZPBESOL
XC_GGA_C_ZVPBEINT
XC_GGA_C_ZVPBESOL
XC_GGA_K_ABSP1
XC_GGA_K_ABSP2
XC_GGA_K_ABSP3
XC_GGA_K_ABSP4
XC_GGA_K_BALTIN
XC_GGA_K_DK
XC_GGA_K_ERNZERHOF
XC_GGA_K_GE2
XC_GGA_K_GOLDEN
XC_GGA_K_GP85
XC_GGA_K_GR
XC_GGA_K_LIEB
XC_GGA_K_LUDENA
XC_GGA_K_MEYER
XC_GGA_K_OL2
XC_GGA_K_TFVW
XC_GGA_K_VJKS
XC_GGA_K_VSK
XC_GGA_K_VW
XC_GGA_K_YT65
XC_GGA_X_FT97_A
XC_GGA_X_FT97_B
XC_GGA_X_GAM
XC_GGA_X_HERMAN
XC_GGA_X_HJS_B88
XC_GGA_X_HJS_B88_V2
XC_GGA_X_HJS_B97X
XC_GGA_X_HJS_PBE
XC_GGA_X_HJS_PBE_SOL
XC_GGA_X_HTBS
XC_GGA_X_KT1
XC_GGA_X_N12
XC_GGA_X_OL2
XC_GGA_X_SOGGA11
XC_GGA_X_SSB
XC_GGA_X_SSB_D
XC_GGA_X_VMT84_GE
XC_GGA_X_VMT84_PBE
XC_GGA_X_WPBEH
XC_GGA_XC_B97_D
XC_GGA_XC_B97_GGA1
XC_GGA_XC_BEEFVDW
XC_GGA_XC_EDF1
XC_GGA_XC_HCTH_120
XC_GGA_XC_HCTH_147
XC_GGA_XC_HCTH_407
XC_GGA_XC_HCTH_407P
XC_GGA_XC_HCTH_93
XC_GGA_XC_HCTH_P14
XC_GGA_XC_HCTH_P76
XC_GGA_XC_HLE16
XC_GGA_XC_KT1
XC_GGA_XC_KT2
XC_GGA_XC_MOHLYP

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XC_GGA_XC_MOHLYP2
XC_GGA_XC_MPWLYP1W
XC_GGA_XC_OBLYP_D
XC_GGA_XC_OPBE_D
XC_GGA_XC_OPWLYP_D
XC_GGA_XC_PBE1W
XC_GGA_XC_PBELYP1W
XC_GGA_XC_TH1
XC_GGA_XC_TH_FL
XC_GGA_XC_XLYP
XC_MGGA_C_B88
XC_MGGA_C_DLDF
XC_MGGA_C_KCIS
XC_MGGA_C_M05
XC_MGGA_C_M05_2X
XC_MGGA_C_M06
XC_MGGA_C_M06_2X
XC_MGGA_C_M06_HF
XC_MGGA_C_M06_L
XC_MGGA_C_PKZB
XC_MGGA_C_REVTPSS
XC_MGGA_C_TPSS
XC_MGGA_C_TPSSLOC
XC_MGGA_X_M11
XC_MGGA_X_M11_L
XC_MGGA_X_MBEEF
XC_MGGA_X_MBEEFVDW
XC_MGGA_X_MK00B
XC_MGGA_X_TM
XC_MGGA_X_VT84
XC_MGGA_XC_B97M_V
XC_MGGA_XC_OTPSS_D
XC_MGGA_XC_TPSSLYP1W
```

Program status

The current package contains Siam Quantum binaries of version 1.2.14 compiled for the particular Android hardware platforms and adapted for running in terminal environment.

License

Siam Quantum

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The basis files were taken from the Basis Set Exchange Portal (GAMESS-US style).
https://bse.pnl.gov/bse/portal

MinGW

The Windows version contains unix2dos binary which is a part of MinGW runtime.
http://www.mingw.org/

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BLAS

Siam Quantum binaries offered by us were statically linked to BLAS library (freely-available software package, available in the homepage).
http://www.netlib.org/blas/

LAPACK

Siam Quantum binaries offered by us were statically linked to LAPACK library (released under modified BSD license, check the homepage for details).
http://www.netlib.org/lapack/

LibXC

Siam Quantum binaries offered by us were statically linked to LibXC library (released under the MPL license (v. 2.0), check the homepage for details).
https://gitlab.com/libxc/libxc

Note: The 32-bit versions of SiamQuantum were compiled without support for mgga_x_2d_prhg07 functional due to cross-compiler issues.

X11-Basic

GUI of the Windows version was built using X11-Basic (by Markus Hoffmann) framework (GPL v.3). For correct functionality, SDL library (available under GNU LGPL license) is included in package.
http://x11-basic.sourceforge.net/
https://www.libsdl.org/

Advanced Installer

The MSI installer for Windows was created using the Advanced Installer (Freeware edition).
https://www.advancedinstaller.com/
https://www.advancedinstaller.com/top-freeware-features.html

Contact

Compilation of the source code for Android/Windows as well as the Android/Windows app development was done by Alan Liška (alan.liska@jh-inst.cas.cz) and Veronika Růžičková (sucha.ver@gmail.com), J. Heyrovský Institute of Physical Chemistry of the CAS, v.v.i., Dolejškova 3/2155, 182 23 Praha 8, Czech Republic.
Website: http://www.jh-inst.cas.cz/~liska/MobileChemistry.htm