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Semiempirical Hartree-Fock in NWChem (semiemp module)

Below is a sample input for a single point calculation for INDO Hamiltonian:

```
start benzene_scf

charge 0
geometry noautosym noautoz
C       -0.804616000     0.000000000    -2.637508000
C       -1.968653000    -0.357135000    -1.934532000
C        0.359421000     0.357135000    -1.934532000
H       -2.876005000    -0.635517000    -2.482493000
H        1.266773000     0.635517000    -2.482493000
C       -1.968653000    -0.357135000    -0.528579000
C        0.359421000     0.357135000    -0.528579000
H       -2.876005000    -0.635517000     0.019382000
H        1.266773000     0.635517000     0.019382000
C       -0.804616000     0.000000000     0.174397000
H       -0.804616000     0.000000000     1.270320000
H       -0.804616000     0.000000000    -3.733431000
end

semiemp
mult 1
apx INDO/1
scftype rhf
maxiter 50
end


task semiemp energy
```

No basis set is needed.

MULT- MULTIPLICITY

Multiplicity of the system can be defined here.

APX-Approximate Hamiltonian

Currently available methods are CNDO/1, CNDO/2, INDO/1 and INDO/2. (1 and 2 indicates two different parametrization for one centre core integrals).

SCFTYPE-Wave function type

Currently only RHF and UHF is available.

MAXITER-Iteration limit.

This keyword indicate maximum allowed iterations. Default is 50.

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SCFTOL-Convergence criteria for density.

Default value is 10^{-7}.

INTTYP- Integral type

0 (default) for ground state calculations

1 for spectroscopic calculations (INDO/S etc)

INTPOL-Control for interpolation step in SCF

Default is FAST.

If SCF iteration shows instability, INTPOL should be set to SLOW. It might help with the convergence.

RT-INDO/S

Input for RT-INDO/S

start benzene_y

charge 0
geometry noautosym noautoz
C -0.804616000 0.000000000 -2.637508000
C -1.968653000 -0.357135000 -1.934532000
C 0.359421000 0.357135000 -1.934532000
H -2.876005000 -0.635517000 -2.482493000
H 1.266773000 0.635517000 -2.482493000
C -1.968653000 -0.357135000 -0.528579000
C 0.359421000 0.357135000 -0.528579000
H -2.876005000 -0.635517000 0.019382000
H 1.266773000 0.635517000 0.019382000
C -0.804616000 0.000000000 0.174397000
H -0.804616000 0.000000000 1.270320000
H -0.804616000 0.000000000 -3.733431000
end

semiemp
mult 1.0
apx INDO/1
scftype rhf
maxiter 100
inttyp 1
end

rt_semiemp
nrestarts 100

```
tmax 1000
dt 0.1
tag "kick_y"
field_type delta
field_max 0.0001
polarization y
print dipole
end

task semiemp rt_semiemp
```

RT-INDO/S is currently available only for RHF wave functions.

NRESTARTS

This sets the number of run-time check points where the time-dependent complex density matrix is saved to file, allowing the simulation to be restarted from that point.

PROPAGATOR

If nothing is mentioned modified Chebyshev propagator will be used. Only other option available for now is conventional Chebyshev propgator. The keyword “Propagator Chebyshev” will activate the conventional Chebyshev propagator. For understanding the difference between two propagators please check our original paper (J. Chem. Phys. 2019, 150, 104103).

TMAX

This option specifies the maximum time (in au) to run the simulation before stopping, which must be a positive real number.

DT

This specifies the electronic time step for time integration.

TAG -- Output label

This option sets a label for the output for convenient parsing (e.g., with "grep").

Tag “kick_y”

It appears in the output as:

```
Kick_ytotal 0.1 2.20000  -7.589146713114E+001 -7.589146713114E+001 -7.589146713114E+001  #Dipole moment [system]
```

FIELD_TYPE

This option sets type of external electric field. Two options currently available are “delta” and “Gaussian”.

Gaussian field (only works with “propagator Chebyshev” keyword) has some other options-

FREQUENCY 0.12 au #frequency of laser in au (e.g., 0.12 au = 3.27 eV)

CENTER 200.0 #center of Gaussian envelop (in au time)

WIDTH 50.0 #width of Gaussian pulse (in au time)

FIELD_MAX

This option sets the maximum value of the electric field

SPIN

SPIN TOTAL has to be used for UHF wave function.

Polarization

This option sets the polarization direction. It can be x, y or z.

PRINT

This option sets the different time-dependent properties to be computed and printed at each time step.

Dipole: Dipole moment