EMSL

Gaussian Basis AIMD

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Gaussian Basis AIMD: QMD Module

- **Finite Cluster Molecular Dynamics**
- Compatible with all Gaussian basis function based electronic structure methods in NWChem
  - DFT, LR-TDDFT, MP2
  - Will switch to numerical gradients if analytical gradients are absent
- Velocity Verlet
- Constant Energy & Constant Temperature Ensembles
  - Berendsen, Langevin, and Stochastic Velocity Rescaling

https://nwchemgit.github.io/Gaussian-Basis-AIMD.html

Details: *Journal of Physical Chemistry B*, *120*(8), 1429 (2015)

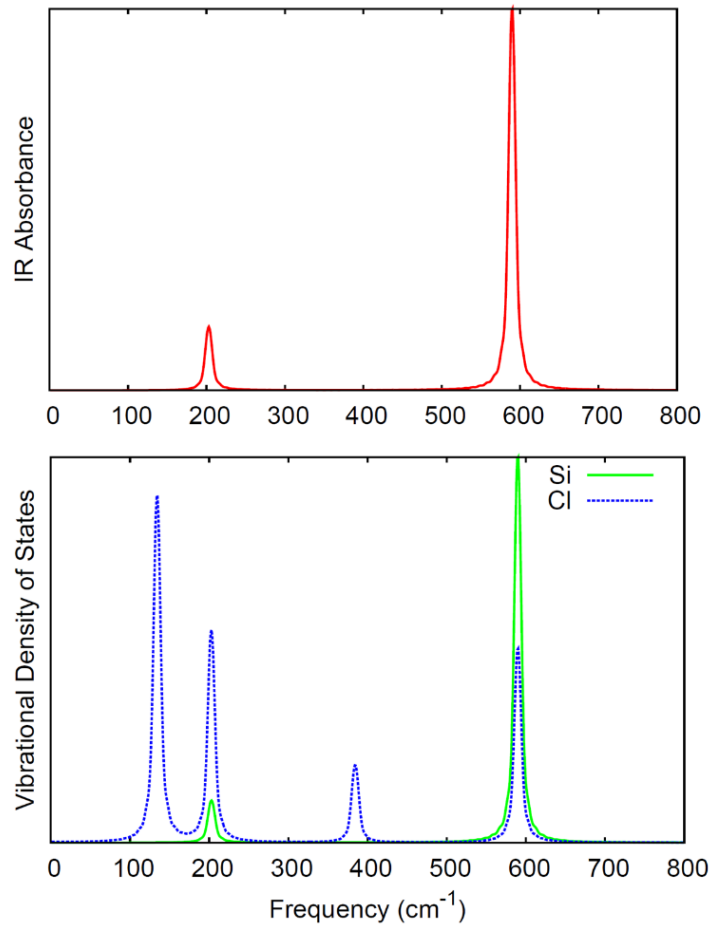
QMD: Sample Input

```
geometry noautosym noautoz
 O    0.00000000    -0.01681748     0.11334792
 H    0.00000000     0.81325914    -0.34310308
 H    0.00000000    -0.67863597    -0.56441201
end

dft; xc hfexch; end
basis; * library 6-31g* ;end

qmd
 nstep_nucl   200
 dt_nucl      10.d0
 targ_temp    200.d0
 com_step     10
 rand_seed    12345
 thermostat   svr
 print_xyz    5
end

task dft qmd
```

```
#
# water - S0 HF/6-31G* geometry
# ground state HF/6-31G* MD
# time step = 10 a.u.
# number of steps = 200
# SVR thermostat, default tau
# 200 K
# translations and rotations every 10 steps
# print trajectory every 5 steps
# random seed set to 12345
#
```

QMD Detailed Example: $SiCl_4$

```
geometry noautosym noautoz
 Si                -0.00007905     0.00044148     0.00000001
 Cl                 0.71289590     1.00767685     1.74385011
 Cl                -2.13658008    -0.00149375    -0.00000001
 Cl                 0.71086735    -2.01430142    -0.00000001
 Cl                 0.71289588     1.00767684    -1.74385011
end
basis
* library 6-31G
end
dft
xc hfexch 1.0
end
qmd
 nstep_nucl   20000
 dt_nucl      10.0
 targ_temp    20.0
 com_step     10
 rand_seed    12345
 thermostat   none
end
task dft qmd
```



See Documentation & Analysis:
https://nwchemgit.github.io/Gaussian-Basis-AIMD.html

Combining QMD with Properties

```
start qmd_props
...

qmd
 nstep_nucl  200
 dt_nucl     10.d0
 targ_temp   200.d0
 com_step    10
 rand_seed   12345
 thermostat  berendsen
# calculate properties as defined in
# the properties block every 5 steps
 property 5
end

property
 dipole
 aoresponse  1 .0911267060
 velocity
 damping 0.007
 shielding 1 1
end

task dft qmd
```

NOTE: The choice of property can slow down the QMD depending on how oftern you want to calculate it

Combining QMD with TDDFT

```
...
qmd
 nstep_nucl   200
 dt_nucl      10.d0
 targ_temp    200.d0
 com_step     10
 rand_seed    12345
 thermostat   berendsen
# calculate TDDFT every 3 steps
 tddft 3
end

tddft
 nroots 2
 notriplet
end

task dft qmd
```

NOTE: The choice of property/response can slow down the QMD depending on how often you want to calculate it

Questions?

Thank you