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PWmat RT-TDDFT optical absorption spectrum calculation-- absorpy

1. **basic settings**
   1. **definitions of rt-TDDFT optical absorption spectrum：**

Electric field:

,

Dipole moment:

Linear polarizability:

absorption corss-section:

dipole-strength function:

Note: i. all above variables in atomic units.

ii. dipole-strength function is used for plotting the spectrum.

* 1. **-ppath, --pwmat\_path**

if the PWmat PATH has been exported to the environment, ignore this setting. Check through:

which PWmat

* 1. **–upath,--utils\_path**

if the PWmat utils PATH has been exported to the environment, ignore this setting. Check through:

which absorption\_spec\_R.x

* 1. **–g,--gpus**

number of gpus used to run PWmat. Default=1.

* 1. **–psp,--psp\_files**

psudopotential files

* 1. **–a,-atom\_file**

structure config file

* 1. **–mt,--max\_time**

the max simulating time,unit fs. Default=5fs.

* 1. **-pr ,--polar**

the polarization direction. Default=x

* 1. **-pd,--periodic**

whether or not periodic structure. Default=false

1. **example Si**

atom.config:

|  |
| --- |
| ***8***  ***Lattice vector***  ***0.5429999828E+01 0.0000000000E+00 0.0000000000E+00***  ***0.0000000000E+00 0.5429999828E+01 0.0000000000E+00***  ***0.0000000000E+00 0.0000000000E+00 0.5429999828E+01***  ***Position, move\_x, move\_y, move\_z***  ***14 0.000000000 0.000000000 0.000000000 0 0 0***  ***14 0.000000000 0.500000000 0.500000000 0 0 0***  ***14 0.500000000 0.500000000 0.000000000 0 0 0***  ***14 0.500000000 0.000000000 0.500000000 0 0 0***  ***14 0.750000000 0.250000000 0.750000000 0 0 0***  ***14 0.250000000 0.250000000 0.250000000 0 0 0***  ***14 0.250000000 0.750000000 0.750000000 0 0 0***  ***14 0.750000000 0.750000000 0.250000000 0 0 0*** |

pseudopotential files:

|  |
| --- |
| Si.SG15.NCPP.PBE.UPF |

run:

|  |
| --- |
| absorpy -a atom.config -psp Si.SG15.NCPP.PBE.UPF -pd true |

outputs:

|  |  |  |
| --- | --- | --- |
| results/ | absorption(S) |  |
| rundir\_x/  rundir\_y  rundir\_z | dipole\_fft.data(D)  E\_fft.data(f)  MDDIPOLE.RSPACE(D)  MDDIPOLE.KSPACE(D)  dipole\_tau.data(D)  OUT.TDDFT\_TIME(f) | Note:  if periodic structure:  use MDDIPOLE.KSPACE  if non-periodic structure:  use MDDIPOLE.RSPACE |

plot:

|  |  |
| --- | --- |
| absorption | dipole-x |
|  |  |

1. **example CH4**

atom.config: (molecule at the center of lattice)

|  |
| --- |
| ***5***  ***Lattice vector***  ***0.6000000000E+01 0.0000000000E+00 0.0000000000E+00***  ***0.0000000000E+00 0.6000000000E+01 0.0000000000E+00***  ***0.0000000000E+00 0.0000000000E+00 0.6000000000E+01***  ***Position, move\_x, move\_y, move\_z***  ***6 0.500000000 0.500000000 0.500000000 0 0 0***  ***1 0.439206913 0.334139912 0.544457272 0 0 0***  ***1 0.439206929 0.544457281 0.334139895 0 0 0***  ***1 0.439327692 0.621514088 0.621514041 0 0 0***  ***1 0.682180157 0.500017053 0.500017021 0 0 0*** |

pseudopotential files:

|  |
| --- |
| C.SG15.NCPP.PBE.UPF H.SG15.NCPP.PBE.UPF |

run:

|  |
| --- |
| absorpy -a atom.config -psp C.SG15.NCPP.PBE.UPF,H.SG15.NCPP.PBE.UPF -pr x,y,z -nb 40 |

outputs:

|  |  |  |
| --- | --- | --- |
| results/ | absorption(S) |  |
| rundir\_x/  rundir\_y  rundir\_z | dipole\_fft.data(D)  E\_fft.data(f)  MDDIPOLE.RSPACE(D)  MDDIPOLE.KSPACE(D)  dipole\_tau.data(D)  OUT.TDDFT\_TIME(f) | Note:  if periodic structure:  use MDDIPOLE.KSPACE  if non-periodic structure:  use MDDIPOLE.RSPACE |

plot:

|  |  |
| --- | --- |
| absorption | dipole-x |
|  |  |

1. **detailed settings**
   1. **–m, --mode**

default is run. If --mode=post, just read the PWmat TDDFT outputs and calculate the spectrum. One can use the mode=post to adjust the spectrum output figure.

Note: the basic parameters(used to run PWmat TDDFT) of ‘–m run’ and ‘–m post’ should be the same, including -dt,-a,-psp,-g,-ef,-pd etc.

* 1. **–nb, --num\_band**

if want to get the spectrum of a specified range of frequency, one should change the NUM\_BAND which is used to run PWmat.

Note: there is no way to exactly set the spectrum range of frenquency in this version of absorpy.

* 1. **-dt,--dt**

if is the max frequency of spectrum, then , so . One should use smaller dt to get more accurate and stable results.

* 1. **–ef, --efield –s,--sigma –c, --center –f,--frequency –k,--kphase**

|  |  |
| --- | --- |
| -ef EFIELD, --efield EFIELD | the strength of efield,unit  (default: 0.1) |
| -s SIGMA, --sigma SIGMA | sigma of gaussian pulse,unit fs  (default: dt) |
| -c CENTER, --center CENTER | center of gaussian pulse,unit fs  (default: 10\*sigma) |
| -f FREQUENCY, --frequency FREQUENCY | frequency of sin, sin(f\*t+k)  (default: 0.0) |
| -k KPHASE, --kphase KPHASE | k of sin, sin(f\*t+k)  (default: pi/2) |

The external electric field is expressed as:

|  |
| --- |
|  |
|  |
|  |
|  |
|  |
|  |

* 1. **–bf,--broaden\_factor**

used for damping the dipole curves and broadening the peaks.

* 1. **–dtr,--dt\_restart –tr,--t\_restart**

|  |  |
| --- | --- |
| -dtr DT\_RESTART, --dt\_restart DT\_RESTART | dtr\*dt, first round MD step time  (default: 0.5) |
| -tr T\_RESTART, --t\_restart T\_RESTART | tr\*max\_time, first round MD time length  (default: 0.1) |

the running of rt-tddft is splited into two stage, in order to get more time points of the pulse:

round one :

time\_length=tr\*max\_time

time\_step=dtr\*dt

round two:

time\_length=(1-tr)\*max\_time

time\_step=dt

* 1. **-fzp ,--fft\_zero\_padding**

used for smoothing the curves, the FFT operations will use fzp\*stepMD points. (stepMD=(1-tr)\*max\_time/dt+tr\*max\_time/(dtr\*dt))

* 1. **--pwmat PWMAT**

any input in PWmat etot.input can be set with –pwmat, eg. --pwmat=’N123=40 40 40’

1. **detailed data**

check rundir\_x(or maybe rundir\_y, rundir\_z) for dipole, efield and their fft data.

1. **parameter range**

|  |  |
| --- | --- |
| GaAs | absorpy -pd true -pr x |
|  | |
| range | |
| **-ef,--efiled** : absorpy -a atom.config -psp Ga,As -ef \* -pd true | |
|  |  |
| **-s,--sigma** : absorpy -a atom.config -psp Ga,As -c 0.25 -s \* -pd true | |
|  |  |
| **-mt,--max\_time** : absorpy -a atom.config -psp Ga,As -mt \* -pd true | |
|  |  |
| **-nb,--num\_band** : absorpy -a atom.config -psp Ga,As -nb \* -pd true | |
|  |  |
| **-fzp,--fft\_zero\_pad** : absorpy -a atom.config -psp Ga,As -fzp \* -pd true | |
|  |  |
| **-bf,--broaden\_factor** : absorpy -a atom.config -psp Ga,As -bf \* -pd true | |
|  |  |
| **k-points** : absorpy -a atom.config -psp Ga,As --pwmat='mp\_n123=\*, in.symm=f' -pd true | |
|  |  |
| CH4 | absorpy -pd false -pr x,y,z |
|  | |
| **box size** : absorpy -a atom.config -psp C,H -pr x,y,z -nb 80 | |
|  |  |

1. **absorpy –h**

|  |  |
| --- | --- |
| -h, --help | show this help message and exit |
| -m {post,run},--mode {post,run} | mode post: just post processing;  mode run: run PWmat + post processing  (default: run) |
| -g GPUS, --gpus GPUS | number of gpus used to run PWmat  (default: 1) |
| -prec{double,single}, --precision {double,single} | precision settings used to run PWmat  (default: single) |
| -conv {easy,difficult}, --convergence {easy,difficult} | convergence settings used to run PWmat  (default: difficult) |
| -coul COULOMB, --coulomb COULOMB | coulomb settings used to run PWmat  (default: 0) |
| -nb NUM\_BAND, --num\_band NUM\_BAND | NUM\_BAND settings used to run PWmat  (default: 0) |
| -ppath PWMAT\_PATH, --pwmat\_path PWMAT\_PATH | path of PWmat  (default: ) |
| -upath UTILS\_PATH, --utils\_path UTILS\_PATH | path of PWmat utils  (default: ) |
| -psp PSP\_FILES, --psp\_files PSP\_FILES | psudopotential files  (format 'file1,file2,...')  (default: None) |
| -a ATOM\_FILE, --atom\_file ATOM\_FILE | structure config file  (default: None) |
| -dt DT, --dt DT | tddft time step length,unit fs  (default: 0.01) |
| -mt MAX\_TIME, --max\_time MAX\_TIME | the max simulating time,unit fs  (default: 5) |
| -pr POLAR, --polar POLAR | the polarization direction  (format 'x,y,z')  (default: x) |
| -ef EFIELD, --efield EFIELD | the strength of efield,unit  (default: 0.1) |
| -s SIGMA, --sigma SIGMA | sigma of gaussian pulse,unit fs  (default: dt) |
| -c CENTER, --center CENTER | center of gaussian pulse,unit fs  (default: 10\*sigma) |
| -f FREQUENCY, --frequency FREQUENCY | frequency of sin, sin(f\*t+k)  (default: 0.0) |
| -k KPHASE, --kphase KPHASE | k of sin, sin(f\*t+k)  (default: pi/2) |
| -bf BROADEN\_FACTOR, --broaden\_factor BROADEN\_FACTOR | factor for broadening peaks  (default: 10)  { bf\*Dipole(t)\*exp(-t/max\_time) } |
| -pd {true,false}, --periodic {true,false} | whether or not periodic structure  (default: false) |
| -dtr DT\_RESTART, --dt\_restart DT\_RESTART | dtr\*dt, first round MD step time  (default: 0.5) |
| -tr T\_RESTART, --t\_restart T\_RESTART | tr\*max\_time, first round MD time length  (default: 0.1) |
| -fzp FFT\_ZERO\_PADDING, --fft\_zero\_padding FFT\_ZERO\_PADDING | fzp\*stepMD, fft zero padding points  (default: 10) |
| --pwmat PWMAT | PWmat etot.input settings  (default: ) |