the octopus

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4.10.5 `TDLanczosTol` (real, 5e-4)

The main developing team of this program is composed of:

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1 Inroducion

1.1 Description of

`oct`

determines the time-dependent density, just as in the Hohenberg-Kohn formalism the static ground state density is given by the minimum of the total energy ($\delta E[\rho]/\delta\rho(r) = 0$)

5. gsl: Finally that someone had the nice idea of making a public sci

if you are using the Absoft Fortran 90 compiler on a linux machine. Also, if you have some of the required libraries in some unusual directories, these directories may be placed in the variable LDFLAGS (e.g., export LDFLAGS=$LDFLAGS:/opt/lib/).

The configuration script will try to find out which compiler you are using. Unfortunately, and due to the nature of the primitive language that octopus is programmed in, the automatic test fails very often. Often it is better to set the variable FCFLAGS

- `--with-fft-lib=<lib>`: **Instruct the**

2.3 Di□erent octopus executables

By performing the standard install, you will get an executable called `octopus`**, and a set of utility programs called** `oct-`**something**

Whatever went wrong...: Up to now, we cannot really make a list of commonly found problems. So if something else went wrong, please subscribe to `octopus-users`

If `octopus` **tries to read a variable that is not defined in the input file, it automatically assigns to it a default value. All variables read are output to the file "**`out.oct`**". If you are not sure of what the program is reading, just take a look at it. Everything following**

4.1.6 UnitsOutput

the

—

4.4.6 DerivativesSpace (integer, real_space)

Defines in which space gradients and the Laplacian are calcul

4.5.3 ExtraStates (integer, 0)

The number of states is in principle calculated considering the minimum numbers of states necessary to hold the electrons present in the system. The nu

4.6.3 LocalPotentialSpace (integer, fourier_space)

If `fourier_space`**, generate the local part of the pseudo-potential in Fourier space; Otherwise do it directly in real space. The autiliary bot defined vi a the** `DoubleFFTParameter` **is used fothis purpose.**

4.6.4

4.8.10 EigenSolver (integer, cg):

At each SCF cycle step, a diagonalisation of the Hamiltonian is performed. Th468(7.71715(h)0.3.337(l55

where T

the larger the dimension of the Arnoldi subspac.23051(n)0e. If the maximum dimension allowed by TDExpOrder is not enough to me.23051(n)0et the c.23051(n)0rite.23051(n)0rion, the above-mntio

Some methods, however, do require the knowledge of the Hamiltonian at some point of the interval $[t, t + \delta t]$. This problem is solved by making use of extrapolation: given a number

- aetrs: **Approximated Enforced Time-Reversal Symmetry (AETRS).**

4.10.20 AbsorbingBoundaries (integer, no)

To improve the quality of the spectra by avoiding the formation of standing density waves, one can make the boundaries of the simulation box absorbing.

4.12.12 OutputPlaneZ

5.8 oct-make-st

make_st **reads** tmp/restart.static **and replaces some of the Kohn-Sham states by Gaus-**

7 Examples

7.0.1 Hello world

As a firsexample,3-312.92(w)28.3974(e)-308.779(w)0.346884(i)-0.2[illegible]

pseudopotential file (“Na.vps,3-284.046(o)0.

“Na.asii” m0[illegible]187(y)-339.297(b)-27.717

install was ised after ma

sould find it. Otherwis,3-45

```
C  0.000 -1.396  0.000
C -1.209 -0.698  0.000
C -1.209  0.698  0.000
H  0.000  2.479  0.000
H  2.147  1.240  0.000
H  2.147 -1.240  0.000
H  0.000 -2.479  0.000
H -2.147 -1.240  0.000
H -2.147  1.240  0.000
```

Options Inde

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