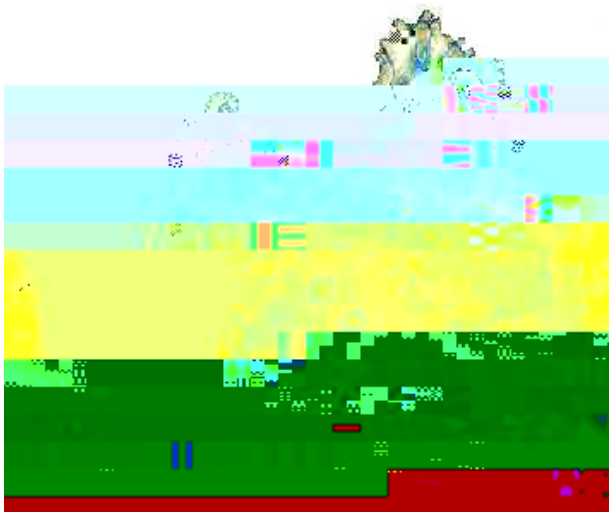
the octopus **manual**

Electronic Structure
Molecular Dynamics
Excited-State Dynamics
Recipes-Generator
March 2002



Male Hapalocheen lunuet (tp)
an female Hapalocheen lunuet (bottm)..246175(e)]TJ38.169-13.149Td[(P)-0.0693767

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1 Copying

3.2 Time dependent density functional theory

Several reviews of time-dependent density function theory (TDDFT) and its applications have appeared recently, like the works by Gross et al.[2], Casida[3], Dobson et al,[4] , and Burke et al[5].

The Hohenberg-Kohn-Sham theory as described is a ground state theory, and it is hence not meant for the calculation of electronic excitations. However, one can extend the ideas of static DFT. When one asks for the evolution of the system under the influence of a time-

determines the time-dependent density, just as in the Hohenb

4 Installation

browse at `http://nautilus.fis.uc.pt/cgi-bin/cvsweb.cgi/marques/octopus/`**. The**

Section 6.1.7 [Verbose], page 14 and see Section 6.1.8 [Debu

5 The parser

All input opion shud be in a file called “ `inp` **”, in the directory** `octopus` **is run from. Alterntively, if ths fies not fund, standard input is re**

6.1.6 UnitsOutput (string, 'a.u.')

Same as Units**, but only refers to the values in the output files. That is, if** UnitsOutput = "eVA"**, all physical values in the output files will be written in eV and Å.**

6.1.7 Verbose (integer, 30)

Verbosity level of the program. The higher, the more verbose octopus **is.**

- **Oxygen labelled 'O'. Next number is the atomic mass (in atomic mass units), and third field, the atomic number (8, in this case). Afterwar**

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- f886(o)0.299886(p)0.29urier_space

6.8.15 TypeOfMixing (integer, broyden)

Selects the mixing procedure to be used during the SCF cycle. Possible values are:

- linear: **Linear mixing.**
- gr_pulay

Being the equation linear, one may formally define a linear "evolution" operator, which trasforms the initial vector into the solution at time T:

$$\psi_i(T) = Uer$$

6.10.6 TDEvolutionMethod

- no: **Do not move the ions.**
- verlet: **Newtonian dynamics using Verlet.**
- vel_verlet: **Newtonian dynamics using velocity Verlet.**

6.10.20 AbsorbingBoundaries (integer, no)

To improve the quality of the spectra by avoiding the formati

`OutputPlaneX` **etc. has always the (side) length of the longest axis; this is independent from the chosen geometry. Data points which are inexistent in the actual geometry have**

6.12.11 OutputPlaneY

6.13.5

7.10 wf.net

8 Undocumeted Variable

If you want to ue the variables you will have to go to the cod e to find out what they do. If you d it, pee take the time o write hort descript ion and end patc31331423(h)-358.543f the maul to u ;) BTW, at may not work, or

9 Examples

9.0.1 Hello world

the

Options Index

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