the o•topus developer's

Chapter 2: xc

 f_der : This is the f_der_type structure: the structure that knows how to do the derivatives. It is de ned i nout for technical reasons, but it should not

xc_functl

3.1 xc_functl_type

integer :: family

integer :: id

integer :: spin_channels integer(POINTER_SIZE) :: conf integer(POINTER_SIZE) :: info

The integer family may take one of the four following families:

XC_FAMI LY_LDA = >or LDA functionals.

XC_FAMI LY_GGA = >or **GGA** functionals.

¥C3 FAMIMAG CGAG Afunctionals.

Y_OEP = > or OEP functionals (i.e. orbital dependent functionals).

et in either the xc_functl_init_exchange and xc_functl_init_ iding on the functional requested, read from the input le, and which integer identi er.

the identi er for the functional (wing) TF may tak e the following

ıncionals:

• XC_FAMILY_LDA family, any of the exchange functionals listed in Sec-

_DA functionals], page 11. In fact, only one: XC_LDA_X (wing)TF

ILY_GGA family, any of the exchange functionals listed in Sec-

ctionals], page 12.

hhy MB6/exchange functionals listed in Sec-nout Car Curati Anson Sinn Lunionari Zec-. In fact, only one: XC_MGGA_X_TPSS

ลธ์&9.3527 0 Td (=)Tj 9.3490 (wing)T300 (wing)TF)Tj 6.1090817.2473 0 Td (,)Tj 6.94907 0 Td (corresp)Tj 34.36

3.2 subroutine xc_functl_init_exchange

type(xc_functl_type), intent(out) :: functl

integer, intent(in) :: spin_channels

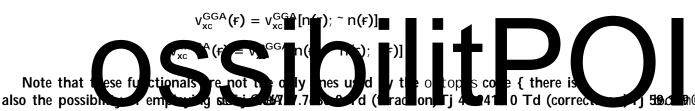
This subroutine initializes one xc_functl_type structure

₄ lib_xc

This module is in charge of providing the simple functionals, i.e. the LDA, GGA and mGGA functionals. It is in fact nothing else than an interface to the libxc. a C library.

The LDA, GGA and mGGA functionals de ned here are local (yes, the GGA and MGGA are also local), in the sense that the value of the potential at a given point depends only on the values of the density { and the gradient of the density and the kinetic energy density, for the GGA and mGGA cases { at a given point:

$$V_{xc}^{LDA}(\mathbf{f}) = V_{xc}^{LDA}[\mathbf{n}(\mathbf{f})];$$



4.2 subroutine xc_l da

It initializes the p handler to hold one of the MGGA functionals, which theepnspinh

4.11 GGA functionals

Exchange:

```
XC\_GGA\_X\_PBE = 101 =>  Perdew, Burke & Ernzerhof exchange XC\_GGA\_XC\_LB = 103 =>  van Leeuwen & Baerends
```

Correlation:

XC_GGA_C_PBE = 102 => Perdew, Burke & Ernzerhof correlation

4.12 MGGA functionals

Exchange:

```
XC_MGGA_X_TPSS = 201 => Perdew, Tao, Staroverov & Scuseria exchange
```

Correlation:

 $XC_MGGA_C_TPSS =$