LIBXC: a library of exchange and correlation functionals for density functional theory

Miguel A. L. Marques∗
Université de Lyon, F-69000 Lyon, France and LPMCN, CNRS, UMR 5586,
Université Lyon 1, F-69622 Villeurbanne, France

Micael J. T. Oliveira
Center for Computational Physics, University of Coimbra,
Rua Larga, 3004-516 Coimbra, Portugal

Tobias Burnus
Peter Grünberg Institut and Institute for Advanced Simulation,
Forschungszentrum Jülich, and Jülich Aachen Research Alliance, 52425 Jülich, Germany

The central quantity of density functional theory is the so-called exchange-correlation functional. This quantity encompasses all non-trivial many-body effects of the ground-state and has to be approximated in any practical application of the theory. For the past 50 years, hundreds of such approximations have appeared, with many successfully persisting in the electronic structure community and literature. Here, we present a library that contains routines to evaluate many of these functionals (around 180) and their derivatives.

I. INTRODUCTION

Density functional theory (DFT) is perhaps one of the most successful theories in Physics and in Chemistry of the last half-century [1-4]. It is currently used to predict the structure and the properties of atoms, molecules, and solids; it is a key ingredient of the new field of Materials Design, where one tries to create new materials with specific properties; it is making its way in Biology as an important tool in the investigation of proteins, DNA, etc. These are only a few examples of a discipline that even now, almost 50 years after its birth, is growing at an exponential rate.

Almost all applications of DFT are performed within the so-called Kohn-Sham scheme [5], that uses a non-interacting electronic system to calculate the density of the interacting system [6]. The Kohn-Sham scheme leads to the following equations. (Hartree atomic units are used throughout the paper, i.e. $\hbar = m_e = 1$.)

$$\left[-\nabla^2 + v_{\text{ext}}(r) + v_{\text{Hartree}}[n](r) + v_{\text{xc}}[n](r)\right] \psi_i(r) = \varepsilon_i \psi_i(r),$$

where the first term represents the kinetic energy of the electrons; the second is the external potential usually generated by a set of Coulombic point charges (sometimes described by pseudopotentials); the third term is the Hartree potential that describes the classical electrostatic repulsion between the electrons,

$$v_{\text{Hartree}}[n](r) = \int d^3 r' \frac{n(r')}{|r-r'|},$$

and the exchange-correlation (xc) potential $v_{\text{xc}}[n]$ is defined by

$$v_{\text{xc}}[n](r) = \frac{\delta E_{\text{xc}}[n]}{\delta n(r)}.$$  

$E_{\text{xc}}[n]$ is the xc energy functional. Note that by $[n]$ we denote that the quantity is a functional of the electronic density,

$$n(r) = \sum_i^{\text{occ.}} |\psi_i(r)|^2,$$

where the sum runs over the occupied states.

*Corresponding author. Electronic address: marques@tddft.org
The central quantity of this scheme is the xc energy $E_{\text{xc}}[n]$ that describes all non-trivial many-body effects. Clearly, the exact form of this quantity is unknown and it must be approximated in any practical application of DFT. We emphasize that the precision of any DFT calculation depends solely on the form of this quantity, as this is the only real approximation in DFT (neglecting numerical approximations that are normally controllable).

The first approximation to the exchange energy, the local density approximation (LDA), was already proposed by Kohn and Sham in the same paper where they described their Kohn-Sham scheme [5]. It states that the value of xc energy density at any point in space is simply given by the xc energy density of a homogeneous electron gas (HEG) with electronic density $n(r)$. Mathematically, this is written as

$$E_{\text{LDA}}^{\text{xc}} = \int d^3r n(r) e_{\text{HEG}}^{\text{xc}}(n(r)),$$

where $e_{\text{HEG}}^{\text{xc}}(n)$ is the xc energy per electron of the HEG. Note that this quantity is a function of $n$. While the exchange contribution $e_{\text{HEG}}^{\text{xc}}(n)$ can be easily calculated analytically, the correlation contribution is usually taken from Quantum Monte-Carlo simulations [7, 8]. As defined, the LDA is unique, but, as we will see in the A, even such precise definition can give rise to many different parameterizations.

During the past 50 years, hundreds of different forms appeared [9] and they are usually arranged in families, which have names such as generalized-gradient approximations (GGAs), meta-GGAs, hybrid functionals, etc. In 2001, John Perdew came up with a beautiful idea on how to illustrate these families and their relationship [10]. He ordered these families as rungs in a ladder that leads to the heaven of “chemical accuracy”, and that he christened the Jacob’s ladder of density functional approximations for the xc energy (see Fig. 1). Every rung adds a dependency on another quantity, thereby increasing the precision of the functional but also increasing the numerical complexity and the computational time.

At the bottom of the ladder we find the LDA, a functional that depends locally on the density only. The second rung is occupied by the GGA

$$E_{\text{xc}}^{\text{GGA}} = \int d^3r n(r) e_{\text{xc}}^{\text{GGA}}(n(r), \nabla n(r)).$$

As one can see, one now adds the gradient of the density, a semi-local quantity that depends on an infinitesimal region around $r$, as a parameter to the energy density. Note that there is a considerable amount of craftsmanship and physical/chemical intuition going into the creation of the function $e_{\text{xc}}^{\text{GGA}}(n, \nabla n)$, but also a fair quantity of arbitrariness. It is therefore not surprising that many different forms were proposed over the years. The same is true for the functionals on the next rung, the meta-GGAs

$$E_{\text{xc}}^{\text{mGGA}} = \int d^3r n(r) e_{\text{xc}}^{\text{mGGA}}(n(r), \nabla n(r), \nabla^2 n(r), \tau(r)).$$

FIG. 1: Jacob’s ladder of density functional approximations for the xc energy.
This time one adds the Laplacian of the density $\nabla^2 n(r)$ and also (twice) the kinetic energy density
\[
\tau(r) = \sum_i^{\text{occ}} |\nabla \psi_i(r)|^2.
\]
Note that the meta-GGAs are effectively orbital functionals due to the dependence in $\tau(r)$.

The forth rung is occupied by functionals that include the exact-exchange (EXX) contribution to the energy
\[
E^{\text{EXX}}_x = -\frac{1}{2} \int d^3r \int d^3r' \frac{\psi_i(r)\psi_j^*(r')\psi_j^*(r)\psi_i(r)}{|r-r'|}.
\]
These functionals can include the whole $E^{\text{EXX}}_x$ or only a fraction of it, and $E^{\text{EXX}}_x$ can be evaluated with the bare Coulomb interaction or with a screened version of it. Furthermore, one can add a (semi-)local xc term or one that depends on the orbitals. In any case, the fourth rung only includes functionals that depend on the occupied orbitals only. Notorious examples of functionals on this rung are the hybrid functionals
\[
E^{\text{Hyb}}_{xc} = a_x E^{\text{EXX}}_x + E^{\text{GGA}}_{xc}[n(r), \nabla n(r), \nabla^2 n(r), \tau(r)].
\]
Note that the local part of this functional can be a meta-GGA, a GGA, or even an LDA.

Finally, on the last rung of Jacob’s ladder one finds functionals that depend on the empty (virtual) Kohn-Sham orbitals. Perhaps the best known example of these functionals is the random-phase approximation (RPA).

In a practical DFT calculation one needs typically to evaluate both $E_{xc}$ and $\nabla_{xc}$. Furthermore, to obtain response properties higher derivatives of $E_{xc}$ are required. For example, in first order one can get the electric polarizability, the magnetic susceptibility, phonon frequencies, etc., and these usually require the knowledge of the xc kernel
\[
f_{xc}(r, r') = \frac{\delta E_{xc}}{\delta n(r)\delta n(r')}.
\]
In second order one can obtain, e.g., hyperpolarizabilities, Raman tensors, etc., but these calculations usually require
\[
k_{xc}(r, r', r'') = \frac{\delta E_{xc}}{\delta n(r)\delta n(r')\delta n(r'')}.
\]
The calculation of these derivatives is fairly straightforward by using basic functional analysis and the chain rule for functional derivatives. We give here as an example the case of the xc potential for a GGA
\[
v_{xc}^{\text{GGA}}(r) = \epsilon_{xc}^{\text{GGA}}(n(r), \nabla n(r)) + \int d^3r n(r) \frac{\partial \epsilon_{xc}^{\text{GGA}}}{\partial n} \bigg|_{n=n(r)} \nabla n = \nabla n(r)
\]
\[
+ \int d^3r n(r) \frac{\partial \epsilon_{xc}^{\text{GGA}}}{\partial \nabla n} \bigg|_{n=n(r)} \nabla n = \nabla n(r)
\]
\[
\nabla n = \nabla n(r)
\]
\[
= \epsilon_{xc}^{\text{GGA}}(n(r), \nabla n(r)).
\]
Integrating by parts the third term, one finally arrives at
\[
v_{xc}^{\text{GGA}}(r) = \epsilon_{xc}^{\text{GGA}}(n(r), \nabla n(r)) + n(r) \frac{\partial \epsilon_{xc}^{\text{GGA}}}{\partial n} \bigg|_{n=n(r)} \nabla n = \nabla n(r)
\]
\[
- \nabla \left[n(r) \frac{\partial \epsilon_{xc}^{\text{GGA}}}{\partial \nabla n} \bigg|_{n=n(r)} \nabla n = \nabla n(r)\right] = \epsilon_{xc}^{\text{GGA}}(n(r), \nabla n(r)).
\]
Clearly, higher functional derivatives of $E_{xc}$ involve higher partial derivatives of $\epsilon_{xc}$.

By now it is clear what a code needs to implement for the functionals of the first three rungs: given $n(r)$, and possibly $\nabla n(r)$, $\nabla^2 n(r)$, and $\tau(r)$, one needs the xc energy density $\epsilon_{xc}(r)$ and all relevant partial derivatives of this quantity. This is indeed the information that is provided by Libxc. For hybrid functionals the library also returns, besides the semi-local part, also the mixing coefficient $a_x$. Unfortunately, EXX and other functionals of the forth and fifth rank are too dependent on the actual numerical representation of the wave-functions and can not be easily included in a generic library.

Finally, we would like to mention that some applications of DFT do not use the Kohn-Sham scheme, but try to approximate the kinetic energy functional directly in terms of the density. This approach follows the path that was laid down in the 1927 by Thomas and Fermi \[11, 12\], and is sometimes referred to as “orbital-free DFT” \[13\]. In this case, we also need a functional form (either an LDA or a GGA) for the kinetic energy, and many of these are present in Libxc. A good review of functionals for the kinetic energy density can be found in Ref. [14].

Note that even if the discussion above was restricted to spin-compensated systems for the sake of simplicity, all functionals of Libxc can also be used with spin-polarization.
II. SOME HISTORY

LIBXC started as a spin-off project during the initial development of the (time-dependent) DFT code OCTOPUS \cite{13-18}. At that point it became clear that the task of evaluation of the xc functional was completely independent of the main structure of OCTOPUS, and could therefore be transformed into a library. The first steps into the development of LIBXC were taken in September 2006, and the first usable version of the library included a few of the most popular LDA and GGA functionals.

At the same time, the European Theoretical Spectroscopy Facility was carrying a coordinate effort to improve code interoperability and re-usability of its software suite, so efforts were almost immediately made to interface those codes with LIBXC. This catalyzed the development of the library and accelerated its dissemination in the community.

During the following years, the library was expanded following two main lines:

(i) To include as many functionals as possible (by now we include around 180 — see \cite{A}). This was done for several reasons. First, we implemented nearly all of the “old” functionals that played an important role in the development of DFT. From this perspective, we can look at LIBXC as a “living museum” of the history of this important discipline. It also allows users to reproduce old results with little effort. Secondly, many of the functionals that are proposed nowadays are implemented in LIBXC within weeks from the moment they are published. In this way new developments are very rapidly available in several different codes, allowing for these new functionals to be quickly tested and benchmarked. Note that we have an agnostic policy, i.e. we try to include the maximum possible number of functionals, without making any judgment of value concerning their beauty, elegance, or usefulness. This judgment is left for the final user to perform.

(ii) To include derivatives of the xc energy up to high orders. As we stated before, to perform a standard Kohn-Sham calculation one only requires the xc energy functional and its first derivatives. However, higher derivatives are essential in order to obtain response properties. Of course, these higher derivatives can be calculated numerically from lower-order derivatives, but this procedure tends to introduce unnecessary errors and instabilities in the calculations. We therefore implemented derivatives up to the third order for the LDAs and up to second order for the other functionals. We note that these derivatives are hard-coded, and not automatically generated from the output of symbolic manipulation software \cite{19, 20}. Even if the latter approach is excellent in order to test implementations, the automatically generated code is often extremely verbose, inefficient, and unreadable. Note that LIBXC includes automatic procedures to check the implementation of the analytic derivatives.

At the beginning, LIBXC was used exclusively in the code OCTOPUS. However, since then several other codes from both the Solid-State Physics and Quantum Chemistry communities started to use this library. The list of codes that use LIBXC at the time of writing is as follows (in alphabetical order):

- **ABINIT** \cite{21, 22} ([http://www.abinit.org/](http://www.abinit.org/)) — This is a general purpose plane-wave code. Besides the basic functionality, ABINIT also includes options to optimize the geometry, to perform molecular dynamics simulations, or to calculate dynamical matrices, Born effective charges, dielectric tensors, and many more properties.

- **APE** \cite{24} ([http://www.tddft.org/programs/APE](http://www.tddft.org/programs/APE)) — The atomic pseudopotential engine (APE) is a tool for generating atomic pseudopotentials within DFT. It is distributed under the GPL and it produces pseudopotential files suitable for use with several codes.

- **ATOMPAW** \cite{21} ([http://www.wfu.edu/~natalie/papers/pwpaw/man.html](http://www.wfu.edu/~natalie/papers/pwpaw/man.html)) — The computer program ATOMPAW generates projector and basis functions which are needed for performing electronic structure calculations based on the projector augmented wave (PAW) method. The program is applicable to materials throughout the periodic table.

- **ATOMISTIX ToolKit** \cite{26, 27} ([http://quantumwise.com](http://quantumwise.com)) — This is a software package that uses nonequilibrium Green’s functions simulations to study transport properties like I-V characteristics of nanoelectronic devices. It uses a powerful combination of DFT, semi-empirical tight-binding, and classical potentials.

- **BigDFT** \cite{28, 29} ([http://inac.cea.fr/L_Sim/BigDFT/](http://inac.cea.fr/L_Sim/BigDFT/)) — BigDFT is a DFT massively parallel electronic structure code using a wavelet basis set. Wavelets form a real space basis set distributed on an adaptive mesh. Thanks to its Poisson solver based on General Green’s function formalism, periodic systems, surfaces and isolated systems can be simulated with the proper boundary conditions.

- **DP** \cite{30} ([http://www.dp-code.org/](http://www.dp-code.org/)) — Dielectric properties (DP) is a Linear Response TDDFT code, in frequency-reciprocal and frequency-real space, that uses a plane-wave basis set.

- **ELK** ([http://elk.sourceforge.net/](http://elk.sourceforge.net/)) — An all-electron full-potential linearized augmented-plane wave (FP-LAPW) code with many advanced features. This code is designed to be as simple as possible so that new
developments in the field of density functional theory (DFT) can be added quickly and reliably. The code is freely available under the GNU General Public License.

- **ERKALE** [http://erkale.googlecode.com] — ERKALE is a quantum chemistry program developed by J. Lehtola used to solve the electronic structure of atoms, molecules and molecular clusters. The main use of ERKALE is the computation of X-ray properties, such as ground-state electron momentum densities and Compton profiles, and core (X-ray absorption and X-ray Raman scattering) and valence electron excitation spectra of atoms and molecules.

- **EXCITING** [31, 32] [http://exciting-code.org/] — EXCITING is a full-potential all-electron DFT package based on the linearized augmented plane-wave (LAPW) method. It can be applied to all kinds of materials, irrespective of the atomic species involved, and also allows for the investigation of the atomic-core region.

- **GPAW** [33, 34] [https://wiki.fysik.dtu.dk/gpaw] — GPAW is a DFT Python code based on the projector-augmented wave (PAW) method and the atomic simulation environment (ASE). It uses real-space uniform grids and multigrid methods or atom-centered basis-functions.

- **HIPPO** [35–37] — This is an electronic structure code, developed by N. Lathiotoakis, that implements Reduced Density Matrix Functionals for atomic and molecular systems using Gaussian-type orbitals.

- **OCTOPUS** [15–18] [http://www.tddft.org/programs/octopus/] — OCTOPUS is a scientific program aimed at the *ab initio* virtual experimentation on a hopefully ever-increasing range of system types. Electrons are described quantum-mechanically within density-functional theory (DFT), and in its time-dependent form (TDDFT) when doing simulations in time. Nuclei are described classically as point particles. Electron-nucleus interaction is described within the pseudopotential approximation.

- **YAMBO** [38] [http://www.yambo-code.org/] — YAMBO is a Fortran/C code for many-body calculations in solid state and molecular physics. The code was originally developed in the Condensed Matter Theoretical Group of the Physics Department at the University of Rome “Tor Vergata” by A. Marini. Previous to its release under the GPL license, YAMBO was known as SELF.

This diversity of codes is extremely important, because in this way a certain functional can be tested and used with a variety of methods in different physical situations. For example, a meta-GGA developed within a certain code to get good band-gaps of solids can be immediately used in a different code (often after a simple recompilation) to obtain the ionization potential of molecules.

LIBXC is freely available from [http://www.tddft.org/programs/Libxc](http://www.tddft.org/programs/Libxc), and it is distributed under the GNU Lesser General Public License v3.0. This license not only allows everyone to read, modify, and distribute the code, but also allows LIBXC to be linked from close-source codes. The reader is also referred to the web site to obtain more information, updated documentation, examples, new versions, etc.

As most open source projects, we strongly encourage contributions from researchers willing to contribute with the implementation of new functionals, higher derivatives, bug corrections, or even bug reports.

## III. AN EXAMPLE

### A. Calling **LIBXC**

Probably the best way to explain the usage of LIBXC is through an example. The following small program calculates the xc energy for a given functional for several values of the density; the available C bindings can be found in header file *xc.h*. More information and examples can be found in the manual and in the header files.

```c
#include <stdio.h>
#include <xc.h>

int main()
{
    xc_func_type func;
    double rho[5] = {0.1, 0.2, 0.3, 0.4, 0.5};
    double sigma[5] = {0.2, 0.3, 0.4, 0.5, 0.6};
    double ek[5];
```
int i, func_id = 1;

/* initialize the functional */
if(xc_func_init(&func, func_id, XC_UNPOLARIZED) != 0) {
    fprintf(stderr, "Functional 'd' not found\n", func_id);
    return 1;
}

/* evaluate the functional */
switch(func.info->family)
{
    case XC_FAMILY_LDA:
        xc_lda_exc(&func, 5, rho, ek);
        break;
    case XC_FAMILY_GGA:
    case XC_FAMILY_HYB_GGA:
        xc_gga_exc(&func, 5, rho, sigma, ek);
        break;
}
for(i=0; i<5; i++) {
    printf("%lf %lf\n", rho[i], ek[i]);
}

/* free the functional */
xc_func_end(&func);
}

The functionals are divided in families (LDA, GGA, etc.). Given a functional identifier, func_id, the functional is initialized by xc_func_init, and evaluated by xc_XXX_exc, which returns the energy per unit volume (ek). Finally, the function xc_func_end cleans up. We note that we follow the convention used in Quantum Chemistry and, instead of passing the full gradient of the density, we use the variable

$$\sigma(r) = \nabla n(r) \cdot \nabla n(r).$$

Converting between partial derivatives with respect to \(\sigma\) and \(\nabla n\) is trivially done with the use of the chain rule. All the quantities passed to and returned by the library are in atomic units.

Fortran 90 bindings are also included in Libxc. These can be found in the file libxc_master.F90. In general, calling Libxc from Fortran is as simple as from C. Here is the previous example in Fortran:

```fortran
program lxctest
    use xc_f90_types_m
    use xc_f90_lib_m

    implicit none

    TYPE(xc_f90_pointer_t) :: xc_func
    TYPE(xc_f90_pointer_t) :: xc_info
    real(8) :: rho(5) = (/0.1, 0.2, 0.3, 0.4, 0.5/)
    real(8) :: sigma(5) = (/0.2, 0.3, 0.4, 0.5, 0.6/)
    real(8) :: ek(5)
    integer :: i, func_id

    func_id = 1

    ! initialize the functional
    call xc_f90_func_init(xc_func, xc_info, func_id, XC_UNPOLARIZED)

    ! evaluate the functional
```
```c
select case (xc_f90_info_family(xc_info))
case(XC_FAMILY_LDA)
  call xc_f90_lda_exc(xc_func, 5, rho(1), ek(1))
case(XC_FAMILY_GGA, XC_FAMILY_HYB_GGA)
  call xc_f90_gga_exc(xc_func, 5, rho(1), sigma(1), ek(1))
end select

do i = 1, 5
  write(*, "(F8.6,1X,F9.6)") rho(i), ek(i)
end do

! free the functional
call xc_f90_func_end(xc_func)

end program lxctest
```

### B. The info structure

Besides the mathematical formulas necessary to evaluate the functional and its derivatives, **Libxc** includes a considerable amount of metadata that is quite useful for both the calling program and for the end user. This information is contained for each functional in the structure `xc_func_info_type`. The relevant part of this structure for the end user is defined as

```c
/* flags that can be used in info.flags */
#define XC_FLAGS_HAVE_EXC (1 << 0) /* 1 */
#define XC_FLAGS_HAVE_VXC (1 << 1) /* 2 */
#define XC_FLAGS_HAVE_FXC (1 << 2) /* 4 */
#define XC_FLAGS_HAVE_KXC (1 << 3) /* 8 */
#define XC_FLAGS_HAVE_LXC (1 << 4) /* 16 */
#define XC_FLAGS_1D (1 << 5) /* 32 */
#define XC_FLAGS_2D (1 << 6) /* 64 */
#define XC_FLAGS_3D (1 << 7) /* 128 */
#define XC_FLAGS_STABLE (1 << 9) /* 512 */
#define XC_FLAGS_DEVELOPMENT (1 << 10) /* 1024 */

typedef struct{
  int number;    /* identifier number */
  int kind;      /* XC_EXCHANGE and/or XC_CORRELATION */
  char *name;    /* name of the functional, e.g. "PBE" */
  int family;    /* type of the functional, e.g. XC_FAMILY_GGA */
  char *refs;    /* references */
  int flags;     /* see above for a list of possible flags */
  ...
} xc_func_info_type;
```

For example, for the Slater exchange functional, this structure is defined as

```c
const XC(func_info_type) XC(func_info_lda_x) = {
  XC_LDA_X,
  XC_EXCHANGE,
  "Slater exchange",
  XC_FAMILY_LDA,
  "PAM Dirac, Proceedings of the Cambridge Philosophical Society 26, 376 (1930)"
  "F Bloch, Zeitschrift fuer Physik 57, 545 (1929)",
  /* other flags */
};
```
Note that the references are separated by a newline. The user of the library can access the information in the following way:

```c
#include <stdio.h>
#include <xc.h>

int main()
{
    xc_func_type func;
    xc_func_init(&func, XC_GGA_X_B88, XC_UNPOLARIZED);
    printf("The functional '%s' is defined in the reference(s):\n%s\n", func.info->name, func.info->refs);
    xc_func_end(&func);
}
```

IV. CONCLUSIONS AND THE FUTURE

`Libxc` is by now seven years old, and the code is quite stable and in use by hundreds of scientists around the world. We are committed to continue the development of the library in the future, mainly by following the two lines mentioned before: include all functionals, and their derivatives of the highest possible order. By now essentially all LDA and GGA functionals ever proposed in the literature are already included in the library. Unfortunately, important gaps still remain especially in the meta-GGAs and hybrid functionals. We will fill in those gaps in the near future. It is not clear if `Libxc` will ever include all functionals ever developed (especially, as several new functionals come out every year), but we will of course try...

V. ACKNOWLEDGEMENTS

`Libxc` profited considerably from other projects dedicated to xc functionals (such as the density-functional repository in Daresbury of H. J. J. van Dam), from generally available code (such as the library of xc functionals of the Minnesota group [http://comp.chem.umn.edu/info/dft.htm](http://comp.chem.umn.edu/info/dft.htm), xc routines of Abinit [21] [22], Espresso [33], etc.), and several individuals that contributed either with code, bug fixes, or even bug reports. To all of these we would like to express our gratitude.

MJTO thankfully acknowledges financial support from the Portuguese FCT (contract #SFRH/BPD/44608/2008).

Appendix A: Available functionals

For convenience, functionals in `Libxc` are divided in exchange, correlation, and exchange-correlation functionals. This division is sometimes arbitrary, but it is often useful for the end user (who may fancy strange mixtures of functionals) and for the code developers.

Below we give a complete list of the functionals the library currently knows about. We note that many of these were tested against reference implementations, when available, or against published results. The functionals have a label that is used to identify the functional inside `Libxc`. Furthermore, the third column indicates the time in seconds required for 50,000,000 evaluations of the (spin-unpolarized) xc potential in a single core of an Intel Core 2 processor running at 2.83 GHz. As one can see, the typical execution time within `Libxc` is much smaller than the total time required in the whole calculation.

### TABLE I: Functionals available in `Libxc`

#### LDA Functionals
### LDA Exchange

- **LDA Exchange**: LDA exchange
- **XC,LDA,X,2D**: Slater exchange in 2D
- **XC,LDA,X,1D**: Slater exchange in 1D

### LDA Correlation

- **XC,LDA,C,WIGNER**: Wigner parametrization
- **XC,LDA,C,RPA**: Random Phase Approximation
- **XC,LDA,C,HL**: Hedin & Lundqvist
- **XC,LDA,C,GL**: Gunnarsson & Lundqvist
- **XC,LDA,C,XALPHA**: Slater’s Xα (X-alpha)
- **XC,LDA,C,VWN**: Vosko, Wilk, & Nussair
- **XC,LDA,C,VWN,RPA**: Vosko, Wilk, & Nussair (RPA)
- **XC,LDA,C,PRM**: Pittalis, Räsänen, and Marques (LDA for 2D systems)
- **XC,LDA,C,C2D**: Attaccalite, Moroni, Gori-Giorgi, and Bachelet (LDA for 2D systems)
- **XC,LDA,C,C2D,PRM**: Pittalis, Räsänen, and Marques (LDA for 2D systems)
- **XC,LDA,C,vBH**: von Barth & Hedin
- **XC,LDA,C,1D,CSC**: Casula, Sorella & Senatore (LDA correlation for 1D systems)
- **XC,LDA,C,ML1**: Modified LDA (version 1) of Proynov and Salahub
- **XC,LDA,C,ML2**: Modified LDA (version 2) of Proynov and Salahub
- **XC,LDA,C,GOMBAS**: Gombas

### LDA Exchange-Correlation

- **XC,LDA,XC,TETER93**: Teter 1993

### LDA Kinetic Energy

- **XC,LDA,K,TF**: Thomas-Fermi kinetic energy
- **XC,LDA,K,LP**: Lee and Parr Gaussian ansatz for the kinetic energy

### GGA Functionals

#### GGA Exchange

- **XC,GGA,X,PBE**: Perdew, Burke & Ernzerhof exchange
- **XC,GGA,X,PBE,R**: Perdew, Burke & Ernzerhof exchange (revised)
- **XC,GGA,X,MPBE**: Adamo & Barone modification to PBE
- **XC,GGA,X,XPBE**: Extended PBE by Xu & Goddard III
- **XC,GGA,X,B86**: Becke 86 Xalpha,beta,gamma
- **XC,GGA,X,B88,MGC**: Becke 86 Xalpha,beta,gamma (with mod. grad. correction)
- **XC,GGA,X,B88**: Becke 88
- **XC,GGA,X,G96**: Gill 96
- **XC,GGA,X,PW86**: Perdew & Wang 86
- **XC,GGA,X,PW91**: Perdew & Wang 91
- **XC,GGA,X,OPTX**: Handy & Cohen OPTX 01
- **XC,GGA,X,DK87,R1**: dePristo & Kress 87 (version R1)
- **XC,GGA,X,DK87,R2**: dePristo & Kress 87 (version R2)
- **XC,GGA,X,G93**: Lacks & Gordon 93
- **XC,GGA,X,FT97,A**: Filatov & Thiel 97 (version A)
- **XC,GGA,X,FT97,B**: Filatov & Thiel 97 (version B)
- **XC,GGA,X,PE,BESOL**: Perdew, Burke & Ernzerhof exchange (for solids)

#### GGA Correlation

- **XC,GGA,C,PBE**: Perdew, Burke & Ernzerhof exchange
- **XC,GGA,C,RPBE**: Hammer, Hansen & Norsk (PBE-like)
- **XC,GGA,C,WC**: Wu & Cohen
| Method                        | Description                                                                 | Energy | Source     |
|-------------------------------|-----------------------------------------------------------------------------|--------|------------|
| XC_GGA_X_Am05                 | Armiento & Mattsson 05 exchange                                              | 61.38  | [78, 79]   |
| XC_GGA_X_PBEA                 | Madsen 07                                                                   | 30.98  | [80]       |
| XC_GGA_X_mpW91                | mPW91 of Adamo & Barone                                                     | 47.19  | [81]       |
| XC_GGA_X_2D_B86_MGC           | Becke 86 with modified gradient correction for 2D                           | 13.49  | [82]       |
| XC_GGA_X_BAYESIAN             | Bayesian best fit for the enhancement factor                                | 18.91  | [83]       |
| XC_GGA_X_PBE_JSR              | Reparametrized PBE by Pedroza, Silva & Capelle                              | 18.71  | [84]       |
| XC_GGA_X_OPTB88_VDW           | opt-Becke 88 for vdW                                                         | 25.24  | [85]       |
| XC_GGA_X_PBEK1_VDW            | Reparametrized PBE for vdW                                                  | 18.72  | [85]       |
| XC_GGA_X_OPTPBE_VDW           | Reparametrized PBE for vdW                                                  | 40.62  | [85]       |
| XC_GGA_X_JRG2                 | Regularized PBE                                                             | 14.65  | [86]       |
| XC_GGA_X_RPW86                | Refitted Perdew & Wang 86                                                   | 30.61  | [87]       |
| XC_GGA_X_KT1                  | Keal and Tozer, version 1                                                    | 23.96  | [88]       |
| XC_GGA_X_HERMAN               | Herman Xalphabeta GGA                                                        | 17.44  | [89, 90]   |
| XC_GGA_X_LBM                  | van Leeuwen & Baerends modified                                            | 30.98  | [91]       |
| XC_GGA_X_OL2                  | Exchange form based on Ou-Yang and Levy v.2                                 | 15.09  | [92]       |
| XC_GGA_X_MB88                 | Modified Becke 88 for proton transfer                                       | 24.86  | [94]       |
| XC_GGA_X_APBE                 | mu fixed from the semiclassical neutral atom                                | 18.71  | [95]       |
| XC_GGA_X_HTBBS                | Haas, Tran, Blaha, and Schwarz                                            | 26.17  | [96]       |
| XC_GGA_X_Airy                 | Constantin et al based on the Airy gas                                     | 47.48  | [97]       |
| XC_GGA_X_Lag                  | Local Airy Gas                                                              | 49.75  | [98]       |
| XC_GGA_X_SOGGA11              | Second-order generalized gradient approximation 2011                       | 20.40  | [99]       |
| XC_GGA_X_C09X                 | C09x to be used with the VdW of Rutgers-Chalmers                           | 19.86  | [100]      |

**GGA Correlation**

| Method                        | Description                                                                 | Energy | Source     |
|-------------------------------|-----------------------------------------------------------------------------|--------|------------|
| XC_GGA_C_PBE                  | Perdew, Burke & Ernzerhof correlation                                        | 39.69  | [59, 60]   |
| XC_GGA_C_XPBE                 | Extended PBE by Xu & Goddard III                                            | 43.85  | [63]       |
| XC_GGA_C_LYP                  | Lee, Yang & Parr                                                           | 25.88  | [101, 102] |
| XC_GGA_C_P86                  | Perdew 86                                                                   | 51.36  | [103]      |
| XC_GGA_C_PBE_SOL              | Perdew, Burke & Ernzerhof correlation SOL                                    | 55.32  | [75]       |
| XC_GGA_C_PW91                 | Perdew & Wang 91                                                            | 51.17  | [70, 104]  |
| XC_GGA_C_Am05                 | Armiento & Mattsson 05 correlation                                          | 25.88  | [78]       |
| XC_GGA_C_LM                   | Langreth & Mehl                                                            | 42.87  | [105]      |
| XC_GGA_C_PBE_JRGX             | Reparametrized PBE by Pedroza, Silva & Capelle                              | 55.74  | [84]       |
| XC_GGA_C_RGE2                 | Regularized PBE                                                             | 40.55  | [86]       |
| XC_GGA_C_WL                   | Wilson & Levy                                                               | 20.95  | [106]      |
| XC_GGA_C_WI                   | Wilson & Ivanov                                                             | 16.48  | [107]      |
| XC_GGA_C_WI0                  | Wilson & Ivanov initial version                                             | 19.42  | [107]      |
| XC_GGA_C_APBE                 | mu fixed from the semiclassical neutral atom                               | 40.86  | [95]       |
| XC_GGA_C_SOGGA11              | Second-order generalized gradient approximation 2011                       | 40.67  | [99]       |
| XC_GGA_C_SOGGA11_X            | to be used with                                                             | 37.05  | [108]      |

**GGA Exchange-Correlation**

| Method                        | Description                                                                 | Energy | Source     |
|-------------------------------|-----------------------------------------------------------------------------|--------|------------|
| XC_GGA_XC_LB                  | van Leeuwen & Baerends                                                      | 29.27  | [109]      |
| XC_GGA_XC_HCTH_93             | HCTH functional fitted to 93 molecules                                       | 155.10 | [110]      |
| XC_GGA_XC_HCTH_120            | HCTH functional fitted to 120 molecules                                     | 151.57 | [111]      |
| XC_GGA_XC_HCTH_147            | HCTH functional fitted to 147 molecules                                     | 143.57 | [111]      |
| XC_GGA_XC_HCTH_147            | HCTH functional fitted to 147 molecules                                     | 155.60 | [112]      |
| XC_GGA_XC_EDF1                | Empirical functional from Adamson, Gill, and Pople                          | 69.03  | [113]      |
| XC_GGA_XC_XLYP                | XLYP functional                                                             | 106.30 | [114]      |
| XC_GGA_XC_PBE1W               | PBE1W (functional fitted for water)                                         | 94.72  | [115]      |
| XC_GGA_XC_MPWLXYP1W            | mPWLYP1w (functional fitted for water)                                      | 106.74 | [115]      |
| Functional Form | Description | Value |
|-----------------|-------------|-------|
| PBELYP1W        | (functional fitted for water) | 79.12 |
| KT2             | Keal and Tozer, version 2 | 31.73 |
| TH1             | Tozer and Handy v. 1 | 383.44 |
| TH2             | Tozer and Handy v. 2 | 352.52 |
| TH3             | Tozer and Handy v. 3 | 332.24 |
| TH4             | Tozer and Handy v. 4 | 337.86 |
| KT2             | Keal and Tozer, version 2 | 31.73 |

**GGA Kinetic Energy**

| Functional Form | Description | Value |
|-----------------|-------------|-------|
| GGA Kinetic Energy | von Weiszaecker correction to Thomas-Fermi | 18.49 |
| GE2             | Second-order gradient expansion of the kinetic energy density | 16.08 |
| GOLDEN          | TF-lambda-vW form by Golden \((l = 13/45)\) | 16.39 |
| YT65            | TF-lambda-vW form by Yonei and Tomishima \((l = 1/5)\) | 13.29 |
| BALTIN          | TF-lambda-vW form by Baltin \((l = 5/9)\) | 13.24 |
| LIEB            | TF-lambda-vW form by Lieb \((l = 14.68)\) | 16.08 |
| ABSR1           | gamma-TFvW form by Acharya et al \([g = 1 - 1.412/N^{1/3}]\) | 15.74 |
| ABSR2           | gamma-TFvW form by Acharya et al \([g = 1 - 1.332/N^{1/3}]\) | 18.01 |
| GR              | gamma-TFvW form by Gázquez and Robles | 13.89 |
| LUDENA          | gamma-TFvW form by Ludeña | 18.73 |
| GP85            | gamma-TFvW form by Ghosh and Parr | 18.19 |
| LP              | Becke 88 | 22.69 |
| FRB88           | Fuentealba & Reyes \((B88\) version) | 19.97 |
| FRPW86          | Fuentealba & Reyes \((PW86\) version) | 32.24 |
| PEARSON         | Pearson 1992 | 13.30 |
| OL1             | Ou-Yang and Levy v.1 | 20.43 |
| OL2             | Ou-Yang and Levy v.2 | 20.26 |
| DK              | DePristo and Kress | 18.64 |
| PERDEW          | Perdew | 16.21 |
| VSK             | Vitos, Skriver, and Kollar | 17.05 |
| JKS             | Vitos, Johansson, Kollar, and Skriver | 18.61 |
| ERNZERHOF       | Ernzerhof | 18.72 |
| LC94            | Lembarki & Chermette | 46.63 |
| PBE             | \(\mu\) fixed from the semiclassical neutral atom | 19.48 |
| THAKKAR         | Thakkar 1992 | 24.92 |
| TW1             | Tran and Wesolowski set 1 \((Table II)\) | 18.70 |
| TW2             | Tran and Wesolowski set 2 \((Table II)\) | 18.30 |
| TW3             | Tran and Wesolowski set 3 \((Table II)\) | 19.01 |
| TW4             | Tran and Wesolowski set 4 \((Table II)\) | 19.97 |

**MetaGGA Exchange**

| Functional Form | Description | Value |
|-----------------|-------------|-------|
| LT A            | Local tau approximation | 24.07 |
| TPS S           | Perdew, Tao, Staroverov & Scuseria exchange | 28.88 |
| TAU HCTH        | Tau HCTH | 23.45 |
| GVT4            | GVT4 \((\text{exchange part of VSXC})\) | 26.85 |
| M06-L           | M06-L | 29.74 |
| BR89            | Becke-Roussel 89 | 49.39 |
| BJ06            | Becke & Johnson 06 | 35.28 |
| TB09            | Tran & Blaha 09 | 31.96 |
| Functional Type | Name | Notes |
|-----------------|------|-------|
| B3PW91 | The original hybrid proposed by Becke | 99.90 |
| B3LYP | (in)famous hybrid similar to B3PW91 | 93.55 |
| B97 | Perdew 86 hybrid similar to B3PW91 | 105.17 |
| B1WC | Hybrid using the optx functional | 78.60 |
| B97-1 | Hybrid based on SOGGA11 form | 158.49 |
| B97-2 | | 154.97 |
| B97-K | Boese-Martin for Kinetics | 151.12 |
| B3LYP | Becke 97-3 | 155.92 |
| B1PW91 | Becke 97-2 | 155.12 |
| mPW1PW | Becke 97-1 | 158.38 |
| mPW3PW | Becke 97-K | 150.13 |
| mPW1K | Becke 97-4 | 112.08 |

References:

1. P. Hohenberg, W. Kohn, Phys. Rev. 136 (1964) B864.
2. R. G. Parr, W. Yang, Density-Functional Theory of Atoms and Molecules, Oxford Univ. Press, New York, 1989.
3. R. Dreizler, E. Gross, Density Functional Theory, Springer, Berlin, 1990.
4. M. Marques, C. Fiolhais, M. Marques (Eds.), A Primer in Density Functional Theory, Springer, Berlin, 2003.
5. W. Kohn, L. J. Sham, Phys. Rev. 140 (1965) A1133.
6. R. van Leeuwen, volume 43 of Advances in Quantum Chemistry, Academic Press, 2003, pp. 25 – 94.
7. D. M. Ceperley, B. J. Alder, Phys. Rev. Lett. 45 (1980) 566.
8. G. Ortiz, P. Ballone, Phys. Rev. B 50 (1994) 1391.
9. G. E. Scuseria, V. N. Staroverov, in: C. E. Dykstra, G. Frenking, K. S. Kim, G. E. Scuseria (Eds.), Theory and Applications of Computational Chemistry: The First Forty Years, Elsevier, Amsterdam, 2005, p. 669.
10. J. P. Perdew, K. Schmidt, AIP Conf. Proc. 577 (2001) 1.
O. Gunnarsson, B. I. Lundqvist, Phys. Rev. B 13 (1976) 4274.
M. Gell-Mann, K. A. Brueckner, Phys. Rev. 106 (1957) 364.
E. Wigner, Trans. Faraday Soc. 34 (1938) 678.
J. P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 77 (1996) 3865.
J. P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 78 (1997) 1396.
L. Hedin, B. I. Lundqvist, J. Phys. C: Solid State Phys. 4 (1971) 2064.
P. Gombás, Pseudopotentielle, Springer, New York, 1967.
S. Goedecker, M. Teter, J. Hutter, Phys. Rev. B 54 (1996) 1703.
S. H. Vosko, L. Wilk, M. Nusair, Can. J. Phys. 58 (1980) 1200.
L. Genovese, B. Videau, M. Ospici, T. Deutsch, S. Goedecker, J.-F. Méhaut, Comptes Rendus Mécanique 339 (2011) 149.
P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, G. L. Chiarotti, M. Cococcioni, A. Marini, C. Ambrosch-Draxl, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. De Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, M. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, R. M. Wentzcovitch, J. Phys.: Cond. Matt. 21 (2009) 395502.
X. Gonzé, J.-M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G.-M. Rignanese, L. Sindic, M. Verstraete, G. Zerah, F. Jollet, M. Torment, A. Roy, M. Mikami, P. Goesez, J.-Y. Raty, V. Olevano, F. Bruneval, L. Reining, R. Godby, G. Onida, D. Hamann, D. Allan, Zeit. Kristallogr. 220 (2005) 558.
X. Gonzé, J.-M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G.-M. Rignanese, L. Sindic, M. Verstraete, G. Zerah, F. Jollet, M. Torment, A. Roy, M. Mikami, P. Goezez, J.-Y. Raty, D. Allan, Comp. Mat. Sci. 25 (2002) 478.
J. P. Perdew, Y. Wang, Phys. Rev. B 45 (1992) 13244.
G. Ortiz, P. Ballone, Phys. Rev. B 56 (1997) 9970.
X. Gonze, G.-M. Rignanese, M. Verstraete, J.-M. Beuken, Y. Pouillon, R. Caracas, F. Jollet, M. Torrent, G. Zerah, M. Mikami, P. Goezez, M. Veithen, J.-Y. Raty, V. Olevano, F. Bruneval, L. Reining, R. Godby, G. Onida, D. Hamann, D. Allan, Zeit. Kristallogr. 220 (2005) 558.
X. Gonze, J.-M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G.-M. Rignanese, L. Sindic, M. Verstraete, G. Zerah, F. Jollet, M. Torrent, A. Roy, M. Mikami, P. Goezez, J.-Y. Raty, D. Allan, Comp. Mat. Sci. 25 (2002) 478.
J. P. Perdew, Y. Wang, Phys. Rev. B 45 (1992) 13244.
| Reference | Author(s) | Journal | Volume | Year | Page |
|-----------|-----------|---------|--------|------|------|
| [61]      | Y. Zhang, W. Yang | Phys. Rev. Lett. | 80 (1998) | 890. |
| [62]      | C. Adamo, V. Barone | J. Chem. Phys. | 116 (2002) | 5933. |
| [63]      | X. Xu, W. A. Goddard | J. Chem. Phys. | 121 (2004) | 4068. |
| [64]      | A. D. Becke | J. Chem. Phys. | 84 (1986) | 4524. |
| [65]      | A. D. Becke | J. Chem. Phys. | 107 (1997) | 8554. |
| [66]      | A. D. Becke | J. Chem. Phys. | 85 (1986) | 7184. |
| [67]      | A. D. Becke | Phys. Rev. A | 38 (1988) | 3098. |
| [68]      | P. M. W. Gill | Mol. Phys. | 89 (1996) | 433. |
| [69]      | J. P. Perdew, W. Yue | Phys. Rev. B | 33 (1986) | 8800. |
| [70]      | J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, C. Fiolhais | Phys. Rev. B | 46 (1992) | 6671. |
| [71]      | N. C. Handy, A. J. Cohen | Mol. Phys. | 99 (2001) | 403. |
| [72]      | A. E. DePristo, J. D. Kress | J. Chem. Phys. | 86 (1987) | 1425. |
| [73]      | D. J. Lacke, R. G. Gordon | Phys. Rev. A | 47 (1993) | 4681. |
| [74]      | M. Filatov, W. Thiel | Mol. Phys. | 91 (1997) | 847. |
| [75]      | J. P. Perdew, A. Ruzsinszky, G. I. Csonka, O. A. Vydrov, G. E. Scuseria, L. A. Constantin, X. Zhou, K. Burke | Phys. Rev. Lett. | 100 (2008) | 136406. |
| [76]      | G. K. H. Madsen | Phys. Rev. B | 75 (2007) | 195108. |
| [77]      | C. Adamo, V. Barone | J. Chem. Phys. | 108 (1998) | 664. |
| [78]      | S. Pittalis, E. Räsänen, J. G. Vilhena, M. A. L. Marques | Phys. Rev. A | 79 (2009) | 012503. |
| [79]      | J. J. Mortensen, K. Kaasbjerg, S. L. Frederiksen, J. K. Nørskov, J. P. Sethna, K. W. Jacobsen | Phys. Rev. Lett. | 95 (2005) | 216401. |
| [80]      | L. S. Pedroza, A. J. R. da Silva, K. Capelle | Phys. Rev. B | 79 (2009) | 201106. |
| [81]      | J. Klimes, D. R. Bowler, A. Michaelides | J. Phys.: Cond. Matt. | 22 (2010) | 022201. |
| [82]      | A. Ruzsinszky, G. I. Csonka, G. E. Scuseria | J. Chem. Theo. Comp. | 5 (2009) | 763. |
| [83]      | E. D. Murray, K. Lee, D. C. Langreth | J. Chem. Theory Comput. | 5 (2009) | 2754. |
| [84]      | T. W. Keal, D. J. Tozer | J. Chem. Phys. | 119 (2003) | 3015. |
| [85]      | F. Herman, J. P. Van Dyke, L. B. Ortenburger | Phys. Rev. Lett. | 22 (1969) | 807. |
| [86]      | F. Herman, I. B. Ortenburger, J. P. Van Dyke | Int. J. Quant. Chem. | 4 (1969) | 827. |
| [87]      | P. R. T. Schipper, O. V. Gritsenko, S. J. A. van Gisbergen, E. J. Baerends, J. Chem. Phys. | 112 (2000) | 1344. |
| [88]      | P. Fuentebalba, O. Reyes | Chem. Phys. Lett. | 232 (1995) | 31. |
| [89]      | H. Ou-Yang, M. Levy | Int. J. Quantum Chem. | 40 (1991) | 379. |
| [90]      | V. Tognotti, C. Adamo | J. Phys. Chem. A | 113 (2009) | 14415. PMID: 19518066. |
| [91]      | L. A. Constantin, E. Fabiano, S. Laricchia, F. Della Sala | Phys. Rev. Lett. | 106 (2011) | 184006. |
| [92]      | P. Haas, F. Tran, P. Blaha, K. Schwarz | Phys. Rev. B | 83 (2011) | 205117. |
| [93]      | L. A. Constantin, A. Ruzsinszky, J. P. Perdew | Phys. Rev. B | 80 (2009) | 035125. |
| [94]      | L. Vitos, B. Johansson, J. Kollár, H. L. Skriver | Phys. Rev. B | 62 (2000) | 10046. |
| [95]      | R. Beverati, Y. Zhao, D. G. Truhlar | J. Phys. Chem. Lett. | 2 (2011) | 1991. |
| [96]      | R. Peverati, D. G. Truhlar | J. Phys. Chem. Lett. | 135 (2011) | 191102. |
| [97]      | L. Vitos, B. Johansson, J. Kollár, H. L. Skriver | J. Phys. Chem. Lett. | 2 (2011) | 1991. |
| [98]      | D. Langreth, M. J. Mehl | Phys. Rev. Lett. | 47 (1981) | 446. |
| [99]      | L. C. Wilson, M. Levy | Phys. Rev. B | 41 (1990) | 12930. |
| [100]     | L. C. Wilson, S. Ivanov | Int. J. Quant. Chem. | 69 (1998) | 523. |
| [101]     | R. Beverati, D. G. Truhlar | J. Chem. Phys. | 135 (2011) | 191102. |
| [102]     | R. van Leeuwen, E. J. Baerends | Phys. Rev. A | 49 (1994) | 2421. |
| [103]     | F. A. Hamprecht, A. J. Cohen, D. J. Tozer, N. C. Handy | J. Chem. Phys. | 109 (1998) | 6204. |
| [104]     | A. D. Boese, N. I. Doltusins, N. C. Handy, M. Sprik | J. Chem. Phys. | 112 (2000) | 1670. |
| [105]     | A. D. Boese, N. C. Handy | J. Chem. Phys. | 114 (2001) | 5497. |
| [106]     | R. D. Adamson, P. M. Gill, J. A. Pople | Chem. Phys. Lett. | 284 (1998) | 6. |
| [107]     | X. Xu, W. A. Goddard | Proc. Nat. Ac. Sci. USA | 101 (2004) | 2673. |
| [108]     | E. E. Dahlke, D. G. Truhlar | J. Chem. Phys. | 109 (2005) | 15677. |
| [109]     | D. J. Tozer, N. C. Handy, W. H. Green | Chem. Phys. Lett. | 273 (1997) | 183. |
| [110]     | D. J. Tozer, N. C. Handy | J. Chem. Phys. | 108 (1998) | 2545. |
| [111]     | D. J. Tozer, N. C. Handy | J. Phys. Chem. A | 102 (1998) | 3162. |
| [112]     | N. C. Handy, D. J. Tozer | Mol. Phys. | 94 (1998) | 707. |
C. F. v. Weizsäcker, Z. Phys. A: Hadrons Nucl. 96 (1935) 431.

A. S. Kompaneets, E. S. Pavlovskii, Zh. Eksp. Teor. Fiz. 31 (1956) 427. [Sov. Phys. JETP 4, 328 (1957)].

D. A. Kirzmit, Zh. Eksp. Teor. Fiz. 32 (1957) 115. [Sov. Phys. JETP 5, 64 (1957)].

S. Golden, Phys. Rev. 105 (1957) 604.

K. Yonei, Y. Tomishima, J. Phys. Soc. Jpn. 20 (1965) 1051.

R. Baltin, Z. Naturforsch. 27 (1972) 1176.

E. H. Lieb, Rev. Mod. Phys. 53 (1981) 603.

P. K. Acharya, L. J. Bartolotti, S. B. Sears, R. G. Parr, Proc. Nat. Acad. Sci. 77 (1980) 6978.

J. L. Gázquez, J. Robles, J. Chem. Phys. 76 (1982) 1467.

E. V. Lukeția, in: F. B. Malik (Ed.), Cond. Matt. Theor., volume 1, Plenum, New York, 1986, p. 183.

S. K. Ghosh, R. G. Parr, J. Chem. Phys. 82 (1985) 3307.

H. Lee, C. Lee, R. G. Parr, Phys. Rev. A 44 (1991) 768.

D. J. Lacks, R. G. Gordon, J. Chem. Phys. 100 (1994) 4446.

E. W. Pearson, R. G. Gordon, J. Chem. Phys. 82 (1985) 881.

A. E. DePristo, J. D. Kress, Phys. Rev. A 35 (1987) 438.

J. P., Perdew, Phys. Lett. A 165 (1992) 79.

L. Vitos, H. L. Skriver, J. Kollár, Phys. Rev. B 57 (1998) 12611.

M., Ernzerhof, J. Mol. Struct.: THEOCHEM 501–502 (2000) 59.

A. Lembarki, H. Chermette, Phys. Rev. A 50 (1994) 5328.

A. J. Thakkar, Phys. Rev. A 46 (1992) 6920.

F. Tran, T. A. Wesolowski, Int. J. Quantum Chem. 89 (2002) 441.

M. Ernzerhof, G. E. Scuseria, J. Chem. Phys. 111 (1999) 911.

J. Tao, J. P., Perdew, V. N. Staroverov, G. E. Scuseria, Phys. Rev. Lett. 91 (2003) 146401.

J. P. Perdew, J. Tao, V. N. Staroverov, G. E. Scuseria, J. Chem. Phys. 120 (2004) 6898.

A. D. Boese, N. C. Handy, J. Chem. Phys. 116 (2002) 9559.

T. V. Voorhis, G. E. Scuseria, J. Chem. Phys. 109 (1998) 400.

Y. Zhao, D. G. Truhlar, J. Chem. Phys. 125 (2006) 194101.

Y. Zhao, D. Truhlar, Theor. Chem. Acc. 119 (2008) 523.

A. D. Becke, M. R. Roussel, Phys. Rev. A 39 (1989) 3761.

A. D. Becke, E. R. Johnson, J. Chem. Phys. 124 (2006) 221101.

F. Tran, P. Blaha, Phys. Rev. Lett. 102 (2009) 226401.

E. Räsänen, S. Pittalis, C. R. Proetto, J. Chem. Phys. 132 (2010) 044112.

S. Pittalis, E. Räsänen, N. Helbig, E. K. U. Gross, Phys. Rev. B 76 (2007) 235314.

A. D. Becke, J. Chem. Phys. 98 (1993) 5648.

P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, J. Phys. Chem. 98 (1994) 11623.

A. J. Cohen, N. C. Handy, Mol. Phys. 99 (2001) 607.

M. Ernzerhof, G. E. Scuseria, J. Chem. Phys. 110 (1999) 5029.

D. I. Bilc, R. Orlando, R. Shaltaf, G.-M. Rignanese, J. Íñiguez, P. Ghosez, Phys. Rev. B 77 (2008) 165107.

P. J. Wilson, T. J. Bradley, D. J. Tozer, J. Chem. Phys. 115 (2001) 9233.

A. D. Boese, J. M. L. Martin, J. Chem. Phys. 121 (2004) 3405.

T. W. Keal, D. J. Tozer, J. Chem. Phys. 123 (2005) 121103.

C. Adamo, V. Baronc, Chem. Phys. Lett. 274 (1997) 242.

Y. Zhao, D. G. Truhlar, J. Phys. Chem. A 108 (2004) 6908.

H. L. Schneider, A. D. Becke, J. Chem. Phys. 108 (1998) 9624.

B. J. Lynch, P. L. Fast, M. Harris, D. G. Truhlar, J. Phys. Chem. A 104 (2000) 4811.