A Safari Through Density Functional Theory

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Abstract Density functional theory is widely used to treat quantum many body problems in many areas of physics and related fields. A brief survey of this method covering foundations, functionals and applications is presented here.

1 The Astonishing Rise of Density Functional Theory

The first text books on density functional theory contain at most 750 references ([1, 2]). In 2011 a search via Google yields the astonishing number of about 5 200 000 entries if one searches for 'density functional theory'. A selection of the topics, that are included in the Google listing, is

- Ground (and some excited) state properties of nuclei, atoms, molecules, clusters and solids
- Surface physics (adsorption, absorption)
- Properties of plasmas
- Superconducting systems
- Multicomponent systems
- Laser excitation
- DFT in molecular dynamics approaches
- Collision problems, e.g., ion-atom collisions
- Nano tubes, quantum dots

One may add that the Nobel Prize in Chemistry of the year 1998 has been awarded to W. Kohn and J. A. Pople for the development of density functional theory.

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W. Greiner (ed.), *Exciting Interdisciplinary Physics*,
FIAS Interdisciplinary Science Series, DOI: 10.1007/978-3-319-00047-3_37,

All this raises the question: 'Why is density functional theory so popular?' The short answer is: It allows the reformulation of a quantum many body problem in terms of a set of equivalent one particle problems, which can be handled more easily.

In view of the complexity of the many body problem one might well ask: Is this really possible? The answer to this question is: An *exact* mapping is in principle possible, but—and this is the reason for the popularity of the method—in reality in terms of approximations that yield excellent results.

2 Basic Version: Ground State Properties

The starting point of the discussion is a standard many body Hamiltonian with kinetic energy, motion of the particles in an external potential and an interaction between all pairs of particles[1]

$$\hat{H} = \hat{T} + \hat{V} + \hat{W}.$$

The foundation of density functional theory is provided by the proof of the Hohenberg-Kohn Theorem [3], which states that the groundstate expectation value of any observable is a unique functional of the groundstate density

$$A_0[n_0] = \langle\, \psi_0[n_0]\, |\hat{A}|\, \psi_0[n_0]\, \rangle.$$

Furthermore: the functionals for the kinetic $T[n_0]$ and the interaction energies $W[n_0]$ are universal. This means: the kinetic energy functional has the same form for any (nonrelativistic fermion) system and the interaction energy functional is the same for any Coulomb system, however complicated the functionals are. The groundstate energy of a specific system (e.g. atom, molecule, solid) is therefore characterised by the one particle potential

$$V[n_0] = \langle\, \psi_0[n_0]\, |\hat{V}|\, \psi_0[n_0]\, \rangle = \int \mathrm{d}^3 r\ v(\mathbf{r}) n_0(\mathbf{r}),$$

in the sense that there exists a unique, bijective mapping $V[n] \Longleftrightarrow n$.

On the basis of the theorem one may, given an energy functional, attempt to determine the groundstate energy variationally. The variational problem

$$\frac{\delta}{\delta n(\mathbf{r})} \left\{ E_0[n] - \mu \int \mathrm{d}^3 r\ n(\mathbf{r}) \right\} = 0,$$

with the subsidiary condition of a fixed particle number N, allows the determination of the ground state density $n_0(\mathbf{r})$ and the ground state energy E_0. This direct path to the ground state energy was attempted by the precursors of modern density functional

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[1] Questions of additional degrees of freedom as, e.g., spin will be suppressed here.

theory, the Thomas-Fermi model (and its extensions, see e.g. [1]). So far only results of modest accuracy have been obtained. The reason is: the kinetic energy functional $T[n]$ is not known well enough.

A way around the difficulties with the kinetic energy was suggested by Kohn and Sham [4]. The Kohn-Sham method can be summarized in the following fashion[2]:

- Step 1: Represent the ground state density (again suppressing questions of spin or other degrees of freedom)

  $$n(\mathbf{r}) \equiv n_0(\mathbf{r}) = N \int \mathrm{d}^3 r_2 \ldots \int \mathrm{d}^3 r_N \ \Psi_0^\dagger(\mathbf{r},\ \mathbf{r}_2,\ \ldots)\Psi_0(\mathbf{r},\ \mathbf{r}_2,\ \ldots)$$

  in terms of a set of orbital functions

  $$n(\mathbf{r}) = \sum_{i=1}^{N} \varphi_i^*(\mathbf{r})\varphi_i(\mathbf{r}).$$

- Step 2: Rearrange the expression for the groundstate energy

  $$E_0[n] = T[n] + W[n] + \int \mathrm{d}^3 r \ v(\mathbf{r})n(\mathbf{r})$$

  after addition and subtraction of the *noninteracting* kinetic energy

  $$T_s[n] = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \int \mathrm{d}^3 r \ \varphi_i^*(\mathbf{r})\nabla\varphi_i(\mathbf{r})$$

  and the Hartree energy

  $$W_H(n) = \frac{1}{2} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \, n(\mathbf{r}_1)w(\mathbf{r}_1, \mathbf{r}_2)n(\mathbf{r}_2)$$

  in the form

  $$E_0[n] = T_s[n] + W_H[n] + V[n] + E_{xc}[n]$$

  with the *exchange-correlation energy*

  $$E_{xc}[n] = T[n] - T_s[n] + W[n] - W_H[n].$$

  This central energy term is given by the difference between the full kinetic energy and its noninteracting counterpart as well as the difference between the full interaction energy and the Hartree energy. In other words, it contains all serious many

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[2] The actual argumentation is more subtle. The subtlety is discussed under the heading of v-representability, which concerns the question of the existence of functional derivatives of kinetic energy functionals [5].

body aspects of the problem. On the other hand, through the rearrangement, the large and easy to obtain parts of the ground state energy have been separated neatly from the smaller, but for all finer points important, exchange-correlation contribution.

- Step 3: By variation with respect to the orbitals (and the subsidiary condition of orthonormality—which turns out to be sufficient) one arrives at the Kohn-Sham orbital equations

  $$\left\{-\frac{\hbar^2}{2m}\nabla + v(\mathbf{r}) + v_H([n];\mathbf{r}) + v_{xc}([n];\mathbf{r})\right\}\varphi_i(\mathbf{r}) = \varepsilon_i\varphi_i(\mathbf{r}).$$

  This single particle equation contains three potential terms. Next to the given external potential and the Hartree potential one has to deal with the *exchange-correlation potential* $v_{xc}([n];\mathbf{r})$, which is defined by the functional derivative of the exchange-correlation energy

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

The Kohn-Sham equations constitute the map of the many body problem on effective single particle problems. They invite the following comments:

- The full, effective Kohn-Sham potential

  $$v_{KS}([n];\mathbf{r}) = v(\mathbf{r}) + v_H([n];\mathbf{r}) + v_{xc}([n];\mathbf{r})$$

  is determined by the density. The Kohn-Sham problem is, as the Hartree-Fock problem, a selfconsistency problem: an initial guess of the density (given the density dependence of the potentials) has to be iterated until selfconsistency.
- The Hartree approximation is recovered for $v_{xc} = 0$, the Hartree-Fock approximation—cum grano salis—for $v_{xc} = v_x$. The Kohn-Sham scheme deals, however, with correlation effects beyond these approximations.
- One welcome feature of the Kohn-Sham potential v_{KS} is the fact, that it is multiplicative. It is much simpler to handle such a potential for geometrically complicated systems as compared to the Hartree-Fock potential, which includes a 'nonlocal' exchange term.
- Although it might be very tempting to endow some physical significance to the Kohn-Sham orbitals, the genesis of the approach does not support this point of view. As a matter of principle, the orbitals are just mathematical constructs aimed at generating the ground state density. In the same vein: the determinant constructed from the lowest energy Kohn-Sham orbitals does not represent the groundstate of the problem at hand.

3 Survey of xc-Functionals

The xc-energy functionals or potentials are at the heart of the ensuing discussion. Most functionals found in the literature address nonrelativistic, many particle Coulomb systems. This field of activity will serve for the introduction of the four types of functionals which have been used to date. Some sample results are found in Sect. 5.

The functionals, that are most often used and easiest to apply, are based on the local density approximation.

3.1 LDA: Local Density Approximation

The LDA assumes that xc-energy densities ($e_{xc} = E_{xc}$/volume) obtained for homogeneous systems (the electron gas, nuclear matter) can be transfered locally to situations which are not so homogeneous

$$e_{xc}^{hom}(n) \longrightarrow e_{xc}^{LDA}(n(\mathbf{r})) \quad \text{so that} \quad E_{xc}^{LDA}[n] = \int \mathrm{d}^3r \; e_{xc}^{LDA}(n(\mathbf{r})).$$

The global functional dependence of the energy density on the constant density is supposed to be (approximately) correct locally. One may then use results from many body perturbation theory or Monte Carlo simulations of the homogeneous systems for the formulation of the functionals. This approach leads to functionals, which lead to very acceptable results, so that one is bound to ask for the reason. The reason for the success of the LDA is a cancelation of errors between the exchange and the correlation contributions. This, in turn, is due to the fact that the corresponding exchange and correlation holes (correlation functions between *pairs* of particles) of the LDA satisfy exact sum rules

$$\rho_x(\mathbf{r}_1, \mathbf{r}_2) \leq 0 \qquad \int \mathrm{d}^3r' \rho_x(\mathbf{r}, \mathbf{r} + \mathbf{r}') = -1 \qquad \int \mathrm{d}^3r' \rho_c(\mathbf{r}, \mathbf{r} + \mathbf{r}') = 0$$

on the average.

There are, nonetheless, deficiencies of the LDA. The major one is a problem with selfinteraction effects, due to a lack of cancelation of the selfinteraction between the direct and the exchange energies. This leads to an incorrect asymptotic limit of the xc-potential, for instance for neutral Coulomb systems

$$\lim_{r\to\infty} v_{xc}^{LDA} \longrightarrow -\varepsilon^{-\gamma r} \quad \text{instead of} \quad \lim_{r\to\infty} v_{xc}^{exact} \longrightarrow -\frac{1}{r}.$$

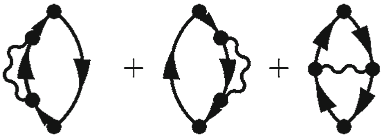
If one particle is removed far from the system, one should observe a Coulomb potential as an effect of the hole left behind. This feature is also the reason for a poor representation of negative ions.

3.2 GE: Gradient Expanded Functionals

If the homogeneous system does not provide an acceptable input, it is natural to look at corrections due to inhomogeneities. An expansion of the xc-energy to low order in derivatives of the density can be written as

$$\begin{aligned} E_{xc}[n] &= E_{xc}^{(0)}[n] + E_{xc}^{(2)}[n] + E_{xc}^{(4)}[n] + \ldots \\ &= \int \mathrm{d}^3 r \left\{ e_{xc}^{LDA}(n(\mathbf{r})) + B_{xc}^{(2)}(n(\mathbf{r}))(\nabla n(\mathbf{r}))^2 + \ldots \right\} . \end{aligned}$$

The technique used to evaluate the details is many body perturbation theory. For instance, the coefficient of the second order contribution in the exchange-only limit $B_x^{(2)}$ is determined by evaluation of the three diagrams of the irreducible polarisation insertion



Even the evaluation of these contributions did not turn out to be straightforward due to the singular structure of the Coulomb interaction at small momenta. The same must be said for low order correlation contribution. After much work, the gradient expansion was found to converge slowly and lead to unsatisfactory results. One of the reasons for this disappointing feature is the fact that the sum rules for the exchange and correlation hole (see above) are not satisfied if evaluated with input obtained by gradient expansion [6].

3.3 GGA: Generalised Gradient Functionals

The study of the gradient expansion of the xc-energy demonstrates that low order correction beyond the LDA contribution can be expressed in terms of two quantities, the density and a second order density gradient, usually called s

$$s(\mathbf{r}) = \left(\frac{\nabla n(\mathbf{r}) \cdot \nabla n(\mathbf{r})}{n(\mathbf{r})^{8/3}} \right)^{1/2} .$$

A standard ansatz takes the form

$$\Delta E_{xc}^{GGA}[n] = \int \mathrm{d}^3r \; e_{xc}^{LDA}(n(\mathbf{r})) f_{xc}(n(\mathbf{r}), s(\mathbf{r})).$$

For Coulomb problems there exists a large number of well and not so well founded suggestions for the function f_{xc}. Parameters are, for instance, fitted by optimal reproduction of atomic data. The resulting functions can then, relying on the universality of the functionals in question, be used for other Coulomb systems, from molecules to solids. Again it is found that the sum rules for the pair correlation holes play an important part. They can be enforced by a 'real space cut-off', which is achieved technically by limiting the integrations to a suitable section of space [7].

3.4 OF: Orbital Functionals

Orbital or implicit functionals are introduced with the argument that the ground state density is also a functional of the Kohn-Sham orbitals. It might, for this reason, be worthwhile to use the orbitals as the basic variables. It is then possible to define the Kohn-Sham exchange (with Kohn-Sham rather than Hartree-Fock orbitals)

$$E_x^{KS} = -\frac{1}{2}\sum_{i,j}\int \mathrm{d}^3r_1 \int \mathrm{d}^3r_2 \varphi_i^*(\mathbf{r}_1)\varphi_j^*(\mathbf{r}_2) W(\mathbf{r}_1,\mathbf{r}_2)\varphi_i(\mathbf{r}_2)\varphi_i(\mathbf{r}_1),$$

so that the exchange-only limit is selfinteraction-free. The calculation of the xc-potential is now more involved, as the application of the chain rule for the functional derivatives

$$\frac{\delta}{\delta n(\mathbf{r})} = \int \mathrm{d}^3r' \sum_j \frac{\delta}{\delta\varphi_j(\mathbf{r}')}\frac{\delta\varphi_j(\mathbf{r}')}{\delta n(\mathbf{r})} + \text{herm. conj.}$$

leads to integral equations for the xc-potential. The appearance of the integral equations is the reason for the alternative name of the orbital approach: Optimised Potential Method. For instance in the x-only limit one obtains the equation

$$\int \mathrm{d}^3r_1 v_x^{OF}(\mathbf{r}_1) K(\mathbf{r}_1,\mathbf{r}_2) = Q(\mathbf{r}_2) \; ,$$

where the kernel K and the inhomogeneous term Q depend explicitly on occupied as well as unoccupied Kohn-Sham orbitals. The solution of the integral equations for the effective potentials has to be repeated within each selfconsistency cycle. As this is quite time-consuming, efficient shortcuts [8] on the basis of closure have been invented and tested. The correlation contribution is usually evaluated in terms of a perturbative approach a posteriori.

4 Extensions

Extensions of the basic theory have been formulated and explored in many directions. As examples one might name

- Time-dependent density functional theory [9] for the exploration of excitation and collision processes: The basis is in this case the Runge-Gross Theorem [10], which can be viewed as a nontrivial extension of the Hohenberg-Kohn Theorem. The action functional

  $$A[n(t)] = \langle \psi[n(t)] | \hat{A}(t) | \psi[n(t)] \rangle$$

  replaces the energy functional. The extension is, among others reasons, nontrivial, as retarded and advanced time structures have to be separated properly.
- Relativistic density functional theory [11, 12], e.g. for the investigation of systems involving heavy elements: the formulation (basic existence theorem, structure of the functionals, orbital equations) has to be based on a proper quantum field theoretical background (as quantum electrodynamics) in order to deal with questions of renormalisation, vacuum polarisation etc. A relativistic four-current replaces the density. In addition viable schemes have to be explored with the aim of handling the solution of the underlying single particle Dirac-Kohn-Sham equations with particle as well as hole states.
- Current/Spin-polarised density functional theory by inclusion of spin degrees of freedom.
- Thermal density functional theory based on use of the free energy and the grand potential.
- The list could be extended (see e.g. [5]).

5 Some Applications and Results

In this chapter a small selection of results, partly in the form of tables and partly by illustrations are presented, with minimal comments. As usual, the devil hides in the detail. Details are not be outlined here. Therefore interested readers are encouraged to consult the references for explicit methods used and for further examples.

5.1 Nuclei

The question of the energy situation in heavy or superheavy nuclei has been investigated with an approach termed Quantum-Hadro-Dynamics [13], that is a non-renormalisable, field-theoretical meson-exchange model. The nucleons interact via the exchange of massive scalar and vector mesons. The coupling constants are

Table 1 Binding energy/nucleon (MeV) and charge radius (fm) of element 114, [14]

	Binding energy (MeV)			Charge radius (fm)		
	HF	LDA	Exp	HF	LDA	Exp
${}_{16}$O	5.11	7.63	7.98	2.74	2.74	2.73
${}_{40}$Ca	6.46	8.26	8.55	3.46	3.52	3.46
${}_{48}$Ca	6.72	8.53	8.67	3.45	3.53	3.45
${}_{90}$Zr	7.11	8.73	8.71	4.23	4.33	4.23
${}_{208}$Pb	6.49	7.87	7.87	5.47	5.60	5.47
114		7.10			6.32	

Table 2 Mean absolute deviation of atomisation energies (kcal/mol) for the 32 'standard' molecules, [15]

HF	MP2	MP2+	LSD	GGA/LSD	GGA
85.9	22.4	28.8	35.7	4.4	5.6

determined so that they reproduce the properties of lighter nuclei. The model is then used to predict properties of heavier nuclei and superheavies. The results for the binding energy per nucleon (in [MeV]) and the charge radius (in [fm]) of a density functional calculation with the QHD model at the LDA level [14] are shown in Table 1.

5.2 Molecules

An investigation of various properties of 32 'standard molecules' by Johnson et al. [15] convinced the community of Chemists of the usefulness and predictive power of density functional theory. Table 2 shows results for the mean absolute deviation of atomisation energies (in units of kcal/mol), comparing three standard many body methods (Hartree-Fock and many body perturbation theory to second order, direct and augmented by selected fourth order contributions) with three different density functional approaches (local-spin-density, generalised gradient approximation for exchange plus local-spin-density for correlation and a generalised gradient functional for both exchange and correlation).

The same picture emerges on the level of individual molecules, for instance at the atomisation energies (in units of eV) of carbohydrates [16] as a function of the number of bonds (N) shown in Table 3.

Direct insight into the distribution of the electrons in the ground state of a molecule can be gleened by looking at the gradients of the density, as illustrated for instance in the two parts of Fig. 1. The figure shows the variation of the two gradient functions s and d

Table 3 Atomisation energies (eV) of selected carbohydrates, [16]

	N	Exp	HF	LDA	GGA
H_2	1	4.75	3.63	4.89	4.55
C_2	1	6.36	0.73	7.51	6.55
C_2H_2	3	17.69	13.00	20.02	18.09
CH_4	4	18.04	14.39	20.09	18.33
C_2H_4	5	24.65	18.71	27.51	24.92
C_2H_6	7	31.22	24.16	34.48	31.24
C_6H_6	12	59.67	45.19	68.42	61.34

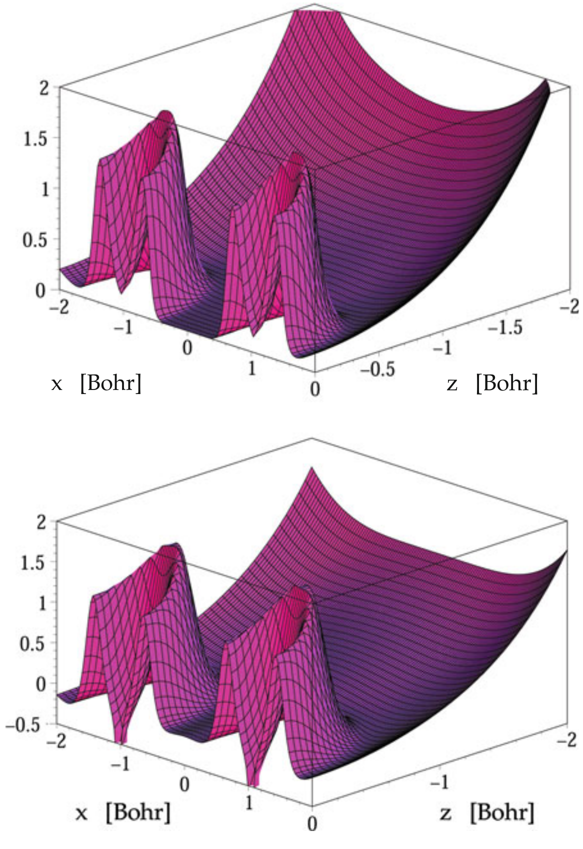
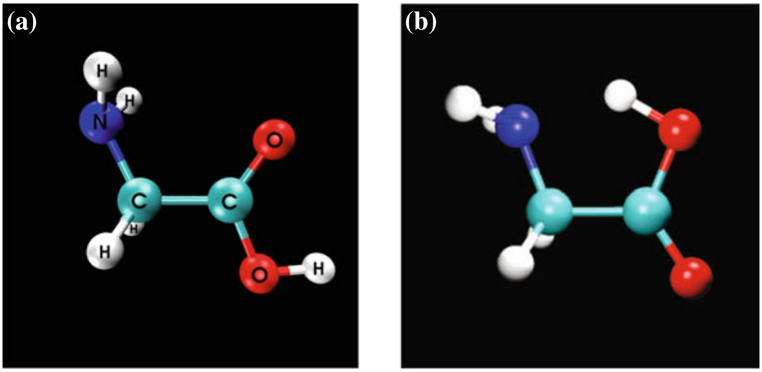


Fig. 1 Characteristic gradients s and d of the density in the N_2-molecule, [5]

$$s = \left(\frac{\nabla n \cdot \nabla n}{n^{8/3}}\right)^{1/2} \quad \text{and} \quad d = \frac{\Delta n}{n^{5/3}}$$

for the nitrogen molecule N_2 (over the x-y plane). The density has been obtained by a Kohn-Sham calculation with exact exchange [5]. The two nuclei are located at $x = \pm 1.035$ Bohr, $y = z = 0$.



Glycine Ip Glycine IIp

Fig. 2 The conformers glycine Ip and glycine IIp

An example for the treatment of more complex molecules is the calculation of the structure of small amino acids like glycine. The chemical formula

$$\mathbf{NH_2\,CH_2\,COOH}$$

does not tell the full story, as there exist a number of conformers as for instance glycine Ip and glycine IIp shown[3] in Fig. 2.

These molecules were treated like solids with a supercell technique (with 23 Å) using a plane wave expansion of the orbitals and a pseudopotential approach of the Troullier-Martins type. Results for the various bond lengths and bond angles in glycine Ip are collected in Table 4. LDA results [17] are compared with experimentally determined values [18]. A corresponding calculation for glycine IIp, presented in Table 5, emphasises the variation of results with the size of the basis (cut-off of the plane wave basis at 60 versus 100 Rydbergs). This illustrates on one side the accuracy that can be obtained with reasonably modest means (within the LDA) and (in comparison with the Table 4) the difference in the structure of the two conformers. The results of [17] can be summarised in the form: the structure of all the conformers of all small amino acids is well reproduced by density functional theory. The effect of contributions of gradient corrections is not very dramatic.

The total groundstate energies of the two conformers in LDA are found to be (in Hartree)

$$E_0(Ip) = -55.8006\mathrm{H} \quad E_0(IIp) = -55.9047\mathrm{H}.$$

The energy difference $E_0(IIp) - E_0(Ip) = -0.05\mathrm{H} = -0.14$ eV $= -3.12$ kcal/mol does however not agree with the experimental value $E_0(IIp) - E_0(Ip) = +0.06$ eV $= +1.4$ kcal/mol. The conformer Ip has the lower energy.

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[3] p stands for the fact that the heavy constituents are planar.

Table 4 Structure of glycine Ip, [17]

Ip Bond	Bond lengths (Ångstrøm) Expt	LDA	Angle	Bond angles (degrees) Expt	LDA
N–H	(1.001)	1.020	H–N–H	(110.3)	106.5
N–C	1.467	1.431	H–N–C	(113.3)	111.0
C–H	(1.081)	1.101	N–C–C	112.1	115.0
C–C	1.526	1.506	H–C–H	(107.0)	104.4
C–O	1.355	1.332	C–C–O	111.6	114.9
C = O	1.205	1.200	C–C = O	125.1	125.7
O–H	(0.966)	0.976	C–O–H	(112.3)	104.7

Table 5 Structure of glycine IIp, [17]

IIp Bond	Bond lengths (Ångstrøm) LDA60	LDA100	Angle	Bond angles (degrees) LDA60	LDA100
N–H	1.026	1.019	H–N–H	107.9	108.7
N–C	1.453	1.449	H–N–C	113.1	113.7
C–H	1.103	1.099	N–C–C	109.9	110.4
C–C	1.518	1.518	H–C–H	106.2	106.1
C–O	1.338	1.324	C–C–O	112.2	112.0
C = O	1.228	1.203	C–C = O	122.5	123.1
O–H	1.046	1.023	C–O–H	100.0	101.8

5.3 Solids

Different options for density functional potentials in solids reproduce in general the gross features but differ sufficiently in detail, so that they give rise to different band structures. This point is illustrated in Fig. 3, which shows the exchange potential obtained by a plane wave pseudo potential calculations for Si [5]. The plot illustrates the difference between two GGA potentials, one LDA potential and the more involved (and more accurate) OPM potential. The potentials are plotted along the [111] direction of a diamond structure.

The band structure resulting from the OPM potential is displayed in Fig. 4, together with rather close results obtained with the simpler, very efficient KLI approximation.

5.4 Final Remark

Obviously it is only possible to scratch the surface of a vast field in such a short communication. For further reading and study we naturally recommend the

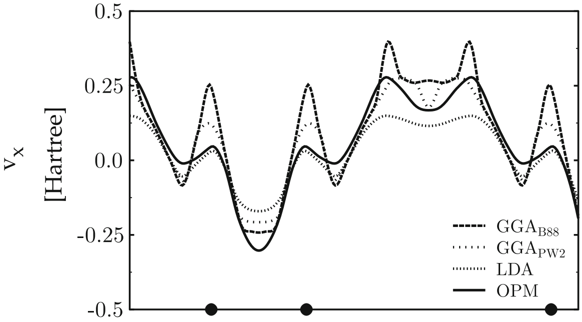

Fig. 3 Exchange potential of Si, plotted along the [111] direction for a diamond structure, [5]

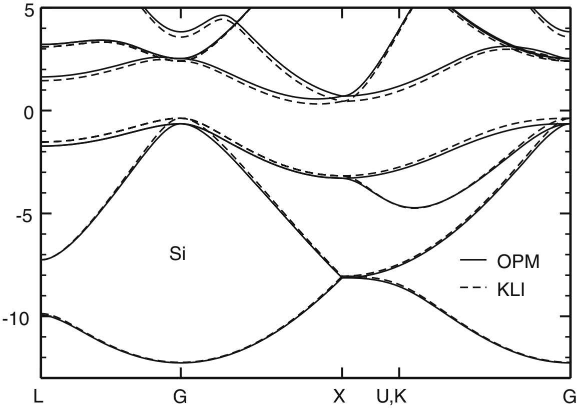

Fig. 4 Band structure of Si obtained for the OPM and for the KLI approximation, [5]

book [5], which presents a fuller overview, addresses many finer points and provides the explanation of the figures, which are included here. The book also contains references to additional texts and reviews.

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