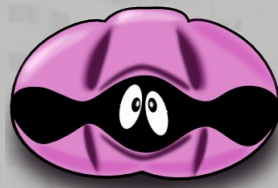


Density-Functional Theory: Basic concepts and approximations

Andrea Marini

October 21, Barranquilla, Colombia



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della Materia



Ultrafast Science Laboratory of the
Material Science Institute National Research Council
(Monterotondo Stazione, Italy)

<http://www.yambo-code.eu/andrea>

Outline

Mean-Field made exact: the Hohenberg-Kohn Theorem



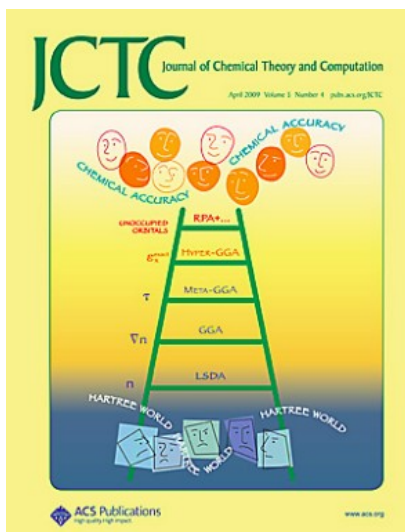
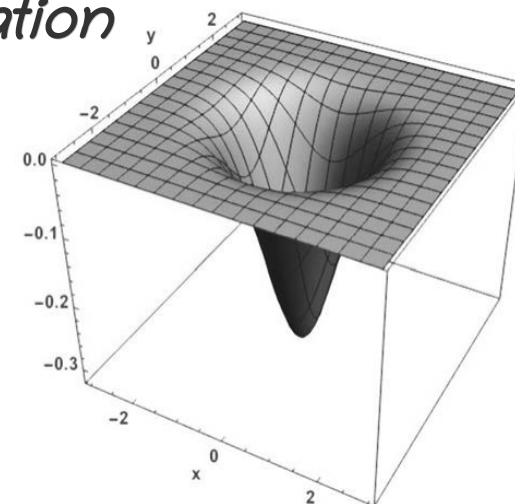
Lu Jeu Sham
28 April 1938



Walter Kohn
1923-2016

DFT in practice via the Kohn-Sham equations

The Exchange-Correlation Energy Functional

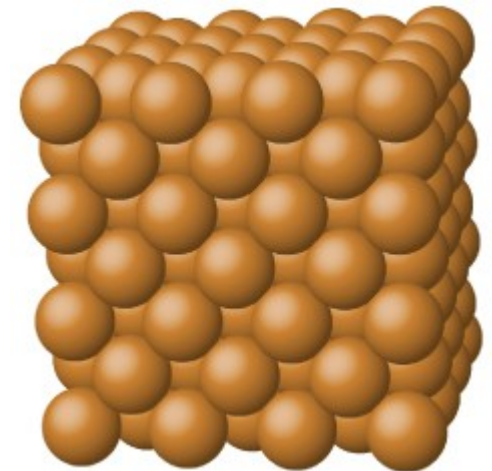
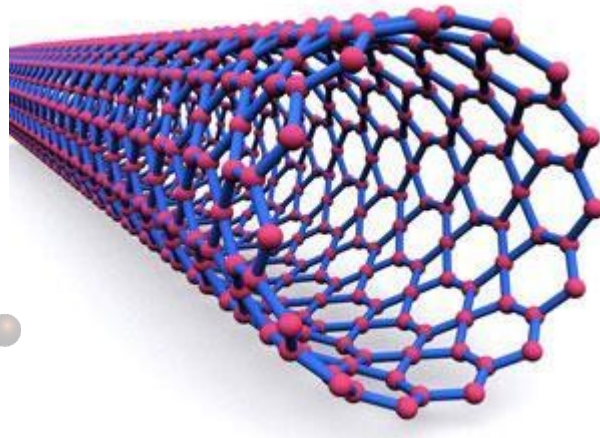
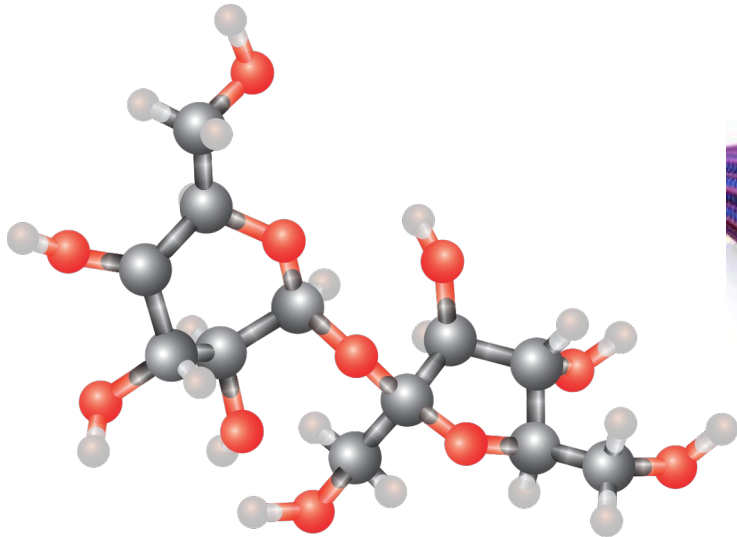
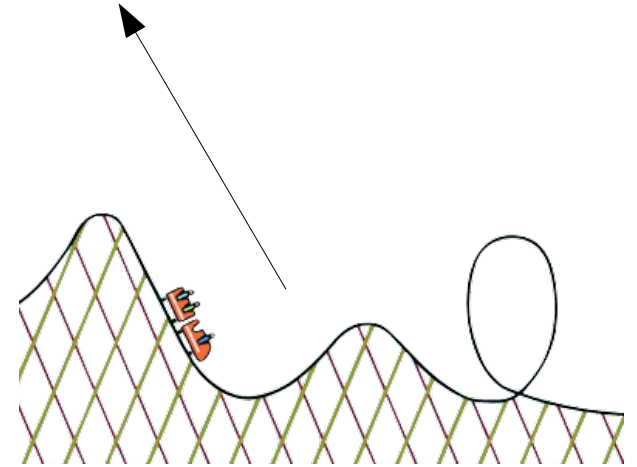
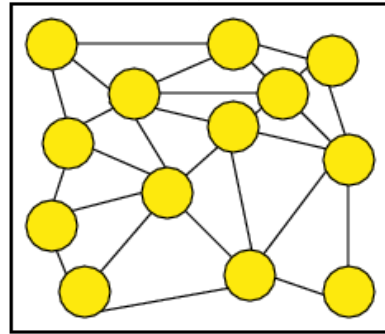


XC Energy functional (simple) approximations: pros and cons

The electronic structure problem

$$\hat{H} = \hat{T} + \hat{V}_{ee} + \sum_{i=1}^N V_{ext}(\hat{\vec{r}}_i)$$

GOAL: determine material properties directly from fundamental equations

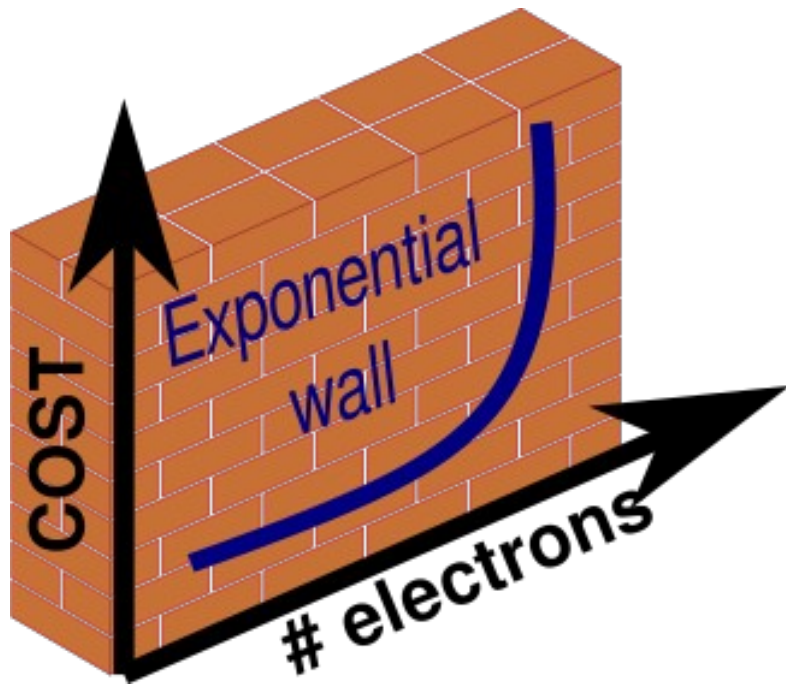


Challenge of the electronic structure problem

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$



$$\langle \vec{r}_1 \dots \vec{r}_N | \Psi \rangle = \Psi(\vec{r}_1 \dots \vec{r}_N)$$



PROBLEM: the time-to-solution of the Hamiltonian problem scales as the exponential of N

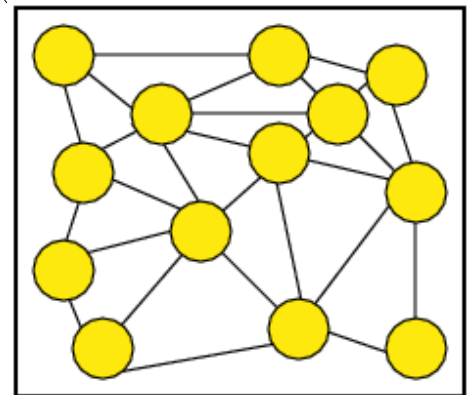
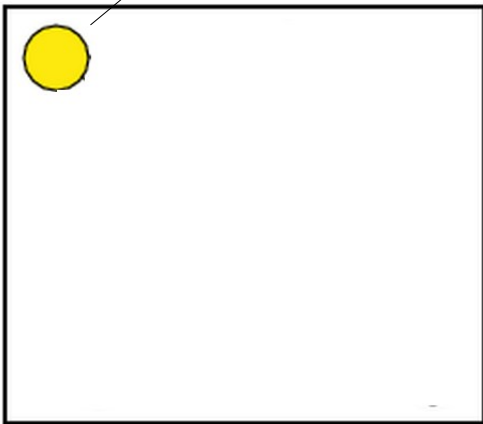
CHALLENGE: develop efficient and accurate methods

Breakdown of the exponential wall

$$\langle \vec{r}_1 \dots \vec{r}_N | \Psi \rangle = \Psi(\vec{r}_1 \dots \vec{r}_N)$$



$$n(\vec{r}) = 2N \int d\vec{r}_2 \dots \vec{r}_N \Psi(\vec{r}, \vec{r}_2, \dots, \vec{r}_N)$$

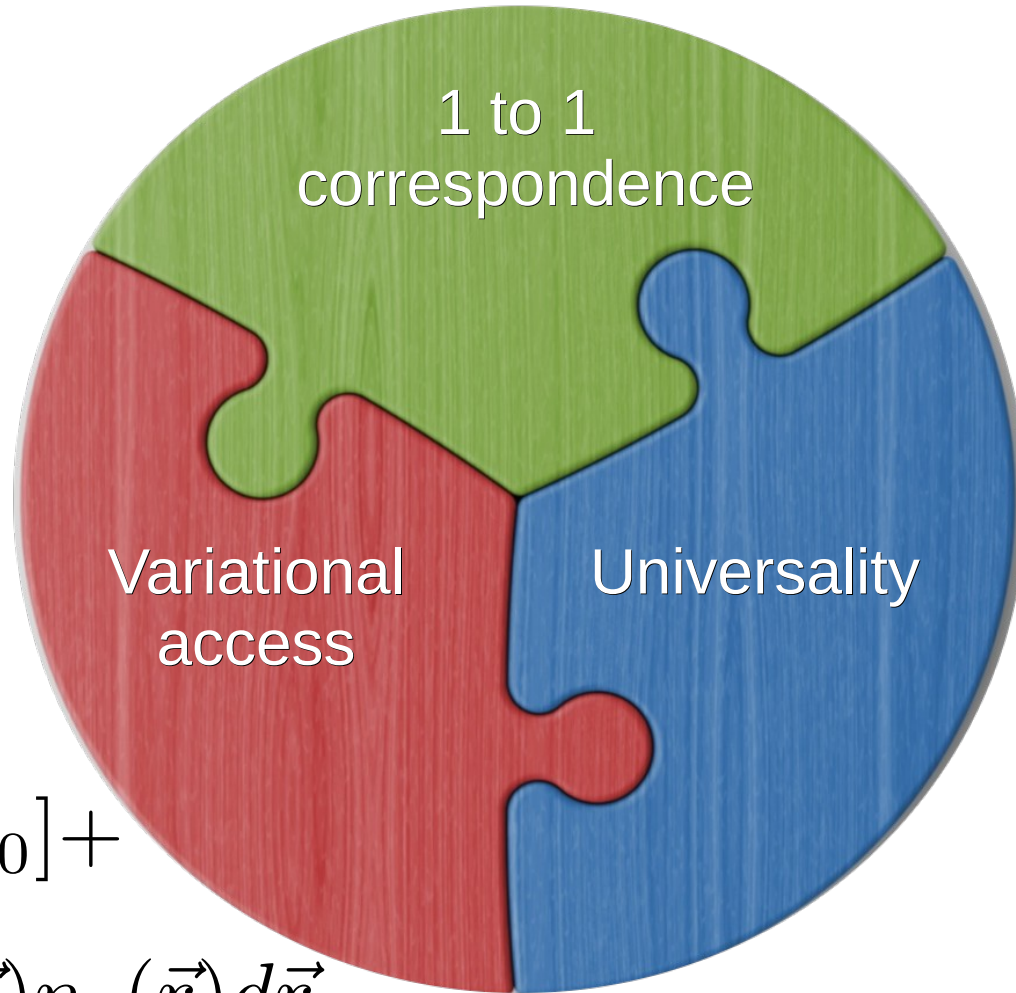


? Which information is contained in the density?

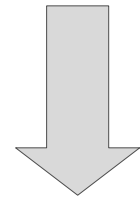
? Can we use the density to calculate materials properties?

The Hohenberg-Kohn theorem (1964)

$$V_{ext} \Leftrightarrow |\Psi_0\rangle \Leftrightarrow n_0(\vec{r})$$



$$|\Psi_0\rangle = |\Psi[n_0]\rangle$$



$$E_0 = F_{HK}[n_0] + \int V_{ext}(\vec{r})n_0(\vec{r})d\vec{r}$$

$$F_{HK}[n] \equiv \langle \Psi[n] | \hat{T} + \hat{V}_{ee} | \Psi[n] \rangle$$

HK density functional

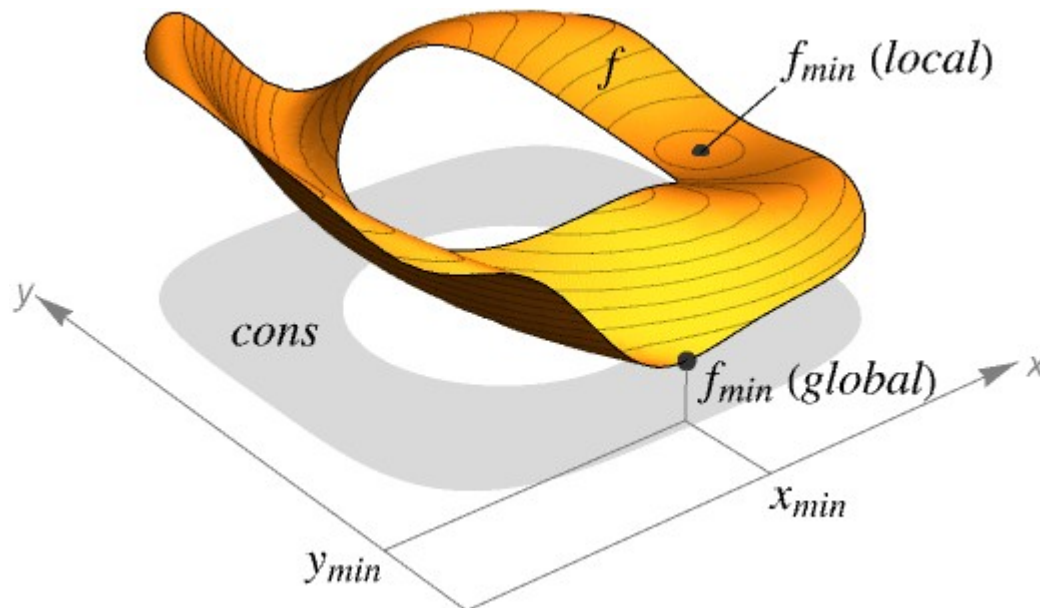
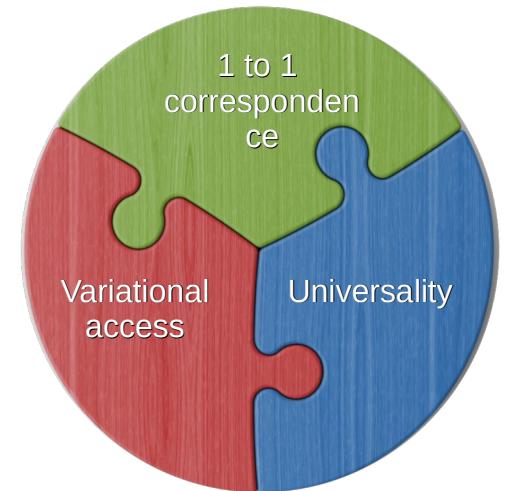
The Hohenberg-Kohn theorem (1964)

$$|\Psi_0 [n_0]\rangle \Leftrightarrow \langle \Psi_0 [n_0] | \hat{H} | \Psi_0 [n_0] \rangle = E_0 [n_0]$$

Ground state energy is
a density functional

$$E_0 [n_0] < E_0 [n'_0] \Leftrightarrow E_0 = \min_{m \in \mathcal{N}} E [n]$$

Ground state energy is
variational



With this minimum principle we
can develop a computational
method to calculate GS
properties of a system

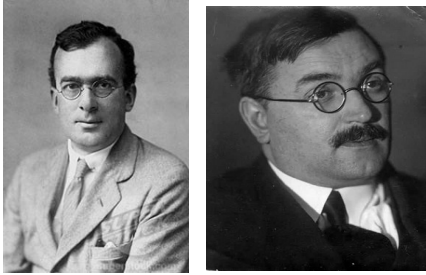
RECAP: Hartree-Fock



$$|\Psi_0 [n_0]\rangle \Leftrightarrow \langle \Psi_0 [n_0] | \hat{H} | \Psi_0 [n_0] \rangle = E_o [n_0]$$

$$E_o [n_0] < E_o [n'_0] \Leftrightarrow E_o = \min_{m \in \mathcal{N}} E [n]$$

DFT



$$\langle \Psi_0 | \hat{H} | \Psi_0 \rangle = E_o [\langle x_1, x_2, \dots | \Psi_0 \rangle]$$

$$\langle x_1, x_2, \dots | \Psi_0 \rangle \approx \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(x_1) & \varphi_2(x_1) & \dots & \varphi_N(x_1) \\ \varphi_1(x_2) & \varphi_2(x_2) & \dots & \varphi_N(x_2) \\ \dots & \dots & \dots & \dots \\ \varphi_1(x_N) & \varphi_2(x_N) & \dots & \varphi_N(x_N) \end{vmatrix}$$

HF

$$E_o^{HF} = \min_{\text{Single Determinants}} E_o [\langle x_1, x_2, \dots | \Psi_0 \rangle]$$

$$\left[h(x) + \sum_m (V_m^H - V_m^F) \right] \phi_k(x) = E_k^{HF} \phi_k(x)$$

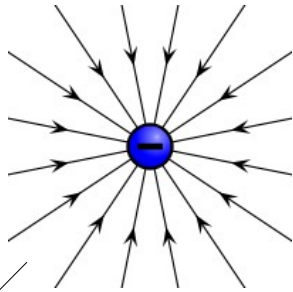
Hartree-Fock (HF) equation

RECAP: Hartree-Fock

Hartree-Fock (HF) equation

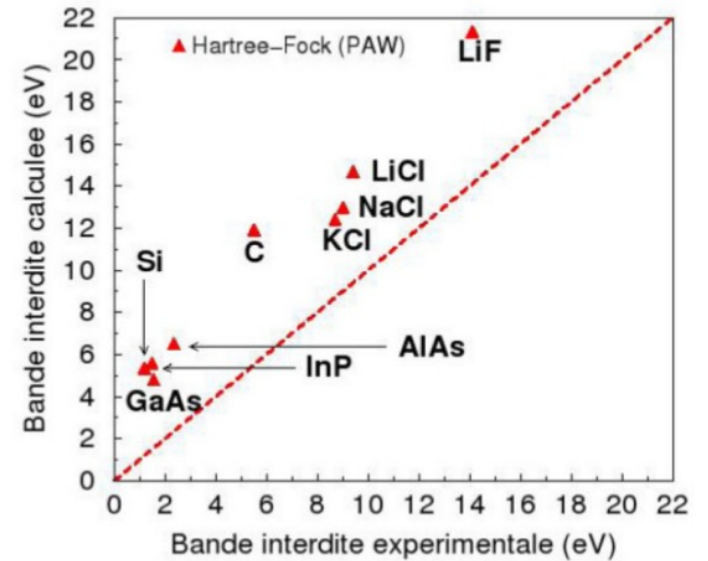
$$\left[h(x) + \sum_m (V_m^H - V_m^F) \right] \phi_k(x) = E_k^{HF} \phi_k(x)$$

Kinetic part Hartree Potential Fock Potential Hartree-Fock energies



$$V_m^H \varphi_k(x_1) = \int dx_2 \varphi_m^*(x_2) \varphi_m(x_2) \varphi_k(x_1) / r_{12}$$

$$V_m^F \varphi_k(x_1) = \int dx_2 \varphi_m^*(x_2) \varphi_k(x_2) \varphi_m(x_1) / r_{12}$$



The Kohn-Sham equation

$$E_0 = F_{HK}[n_0] + \int V_{ext}(\vec{r})n_0(\vec{r})d\vec{r}$$



KS states

$$n_0(\vec{r}) = \sum_i |\phi_i(\vec{r})|^2$$

KS energies

$$\left(-\frac{\nabla^2}{2} + V_s(n, \vec{r}) \right) \phi_i(\vec{r}) = \epsilon_i \phi_i(\vec{r})$$

KS potential

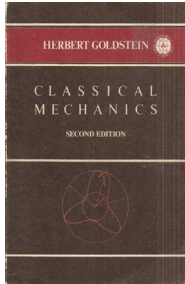
Kohn-Sham (KS) equation

The Exchange-Correlation Potential

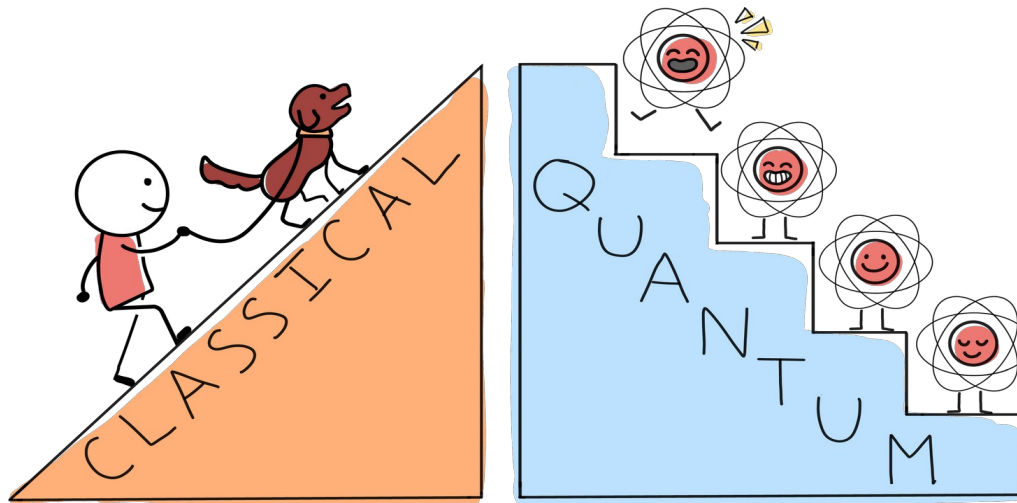
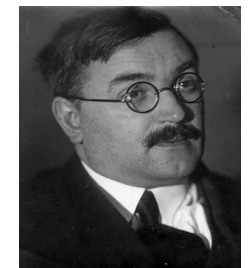
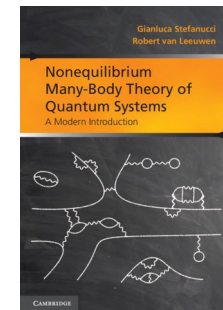
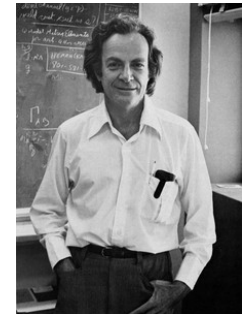
$$\left(-\frac{\nabla^2}{2} + V_s(n, \vec{r})\right)\phi_i(\vec{r}) = \epsilon_i\phi_i(\vec{r})$$

$$V_s(\vec{r}) = V_{ext}(\vec{r}) + \underbrace{\int d\vec{r}' \frac{n(\vec{r}')}{|\vec{r} - \vec{r}'|}}_{\text{Hartree potential}} + \underbrace{V_{xc}[n](\vec{r})}_{\text{Exchange-Correlation (xc) Potential}}$$

Hartree potential



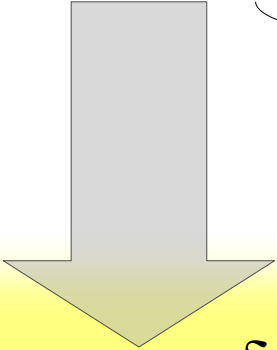
Exchange-Correlation (xc) Potential

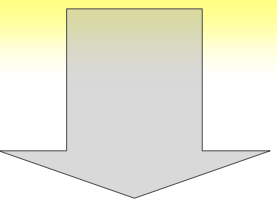


The Exchange-Correlation Energy functional

$$E_{xc}[n] = F_{HK}[n] - T_s[n] - \underbrace{\frac{1}{2} \int d\vec{r}_1 d\vec{r}_2 \frac{n(\vec{r}_1)n(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|}}_{E_H[n]}$$

Exchange-Correlation Functional



$$V_{xc}[n](\vec{r}) \equiv \frac{\delta E_{xc}[n]}{\delta n(\vec{r})}$$


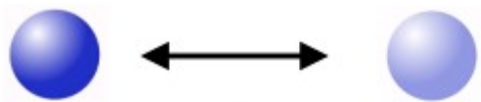
$$E[n] = T_s[n] + E_H[n] + E_{xc}[n] + \int d\vec{r} V_{ext}(\vec{r})n(\vec{r})$$

The Exchange-Correlation Hole

$$E_{xc}[n] = \frac{1}{2} \int d\vec{r}_1 d\vec{r}_2 \frac{n(\vec{r}_1) n_{xc}(\vec{r}_1, \vec{r}_2 - \vec{r}_1)}{|\vec{r}_1 - \vec{r}_2|}$$

Exchange-Correlation Hole

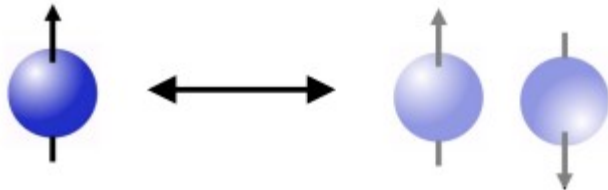
Spatial non-locality



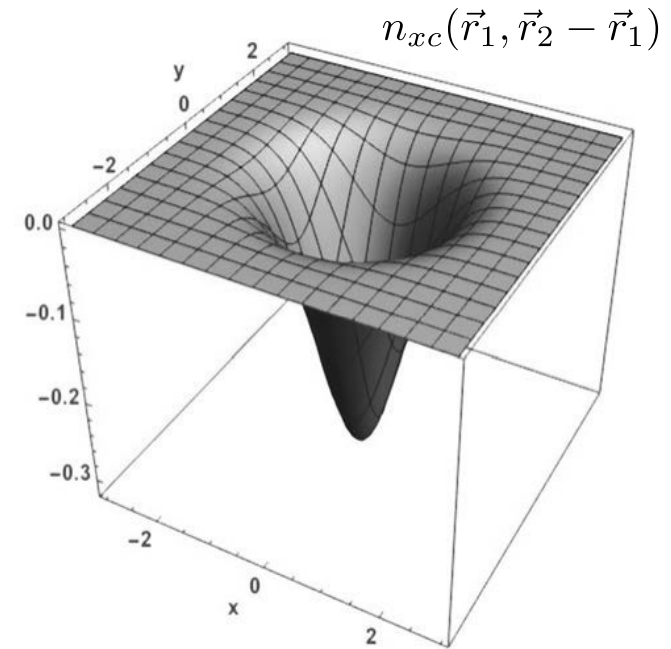
Classical Poisson's potential (Hartree)



Quantum statistical Exchange (Fock)



Correlation



Summary so far

- DFT is an exact ground state (GS) theory
- The GS density can be formally rewritten in terms of a gas of independent (KS) particles moving in an unknown mean-field KS potential.
- The KS potential is generated by an (still unknown) exchange-correlation functional.
- The exchange-correlation functional can be defined in terms of an exchange-correlation hole.



The marvelous world of ... Approximations

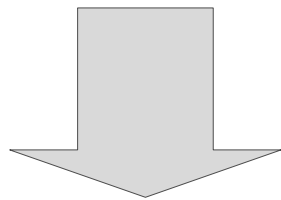
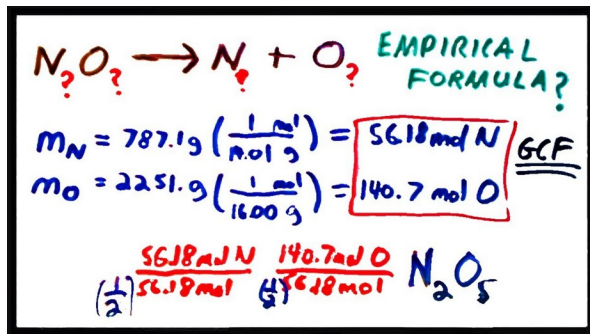


*If it is everything
UNKNOWN how
do I finish my PhD
calculations?!?!*

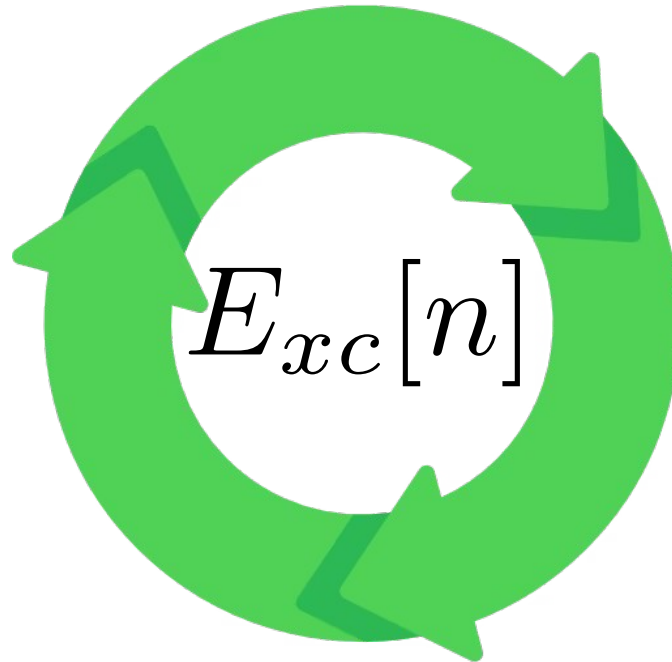
Strategies to approximate the xc functional

Exact expression would require the solution of the Many-Body problem. This can be done only for extremely simple toy models

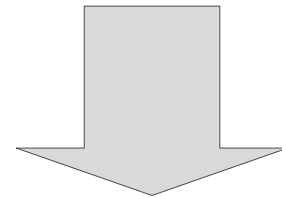
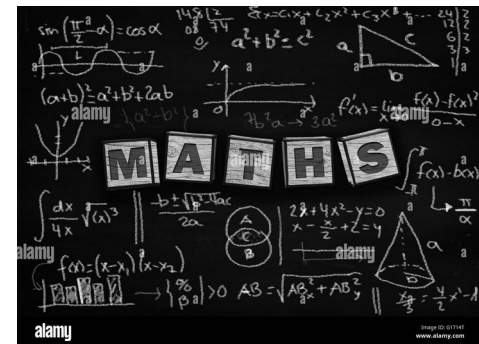
Empirical



Uses fitting parameters



Non-Empirical



Use exact constraints or alternative approaches (like MBPT)

Jacob's Ladder: from Earth to Heaven



EXACT Energy Functional

Approximated Forms

Hartree: no exchange-correlation

Jacob's Ladder: from Earth to Heaven



JACOBS LADDER™

Ultimate Fitness Experience

The marvelous world of ... Approximations



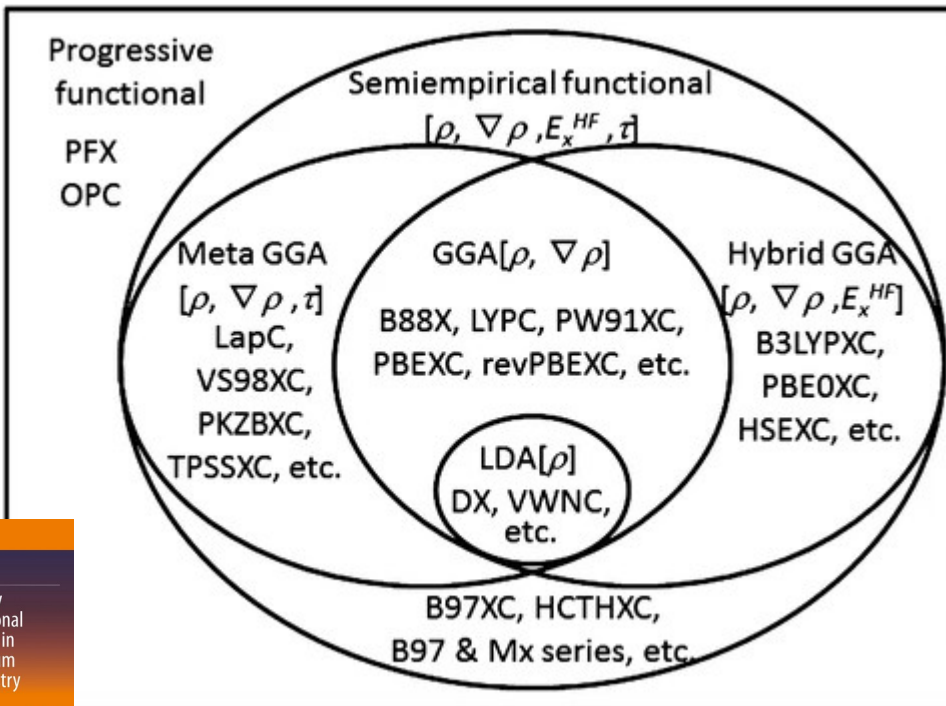
• Even just the next step up Jacob's ladder, the GGA, has no unique form.

• Purists like to use exact conditions of quantum mechanics to derive the parameters in their approximate functionals, and so claim to be non-empirical

• Pragmatists have allowed one or two parameters to be fit to specific systems, such as in B88 for exchange and LYP for correlation.

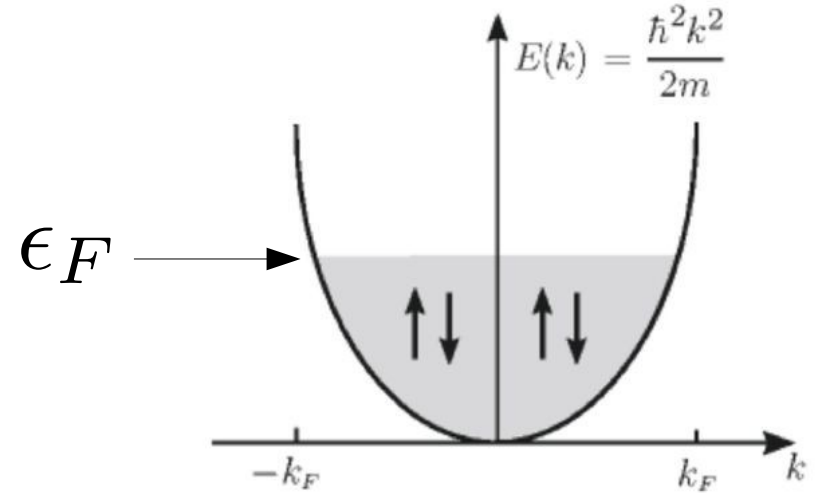
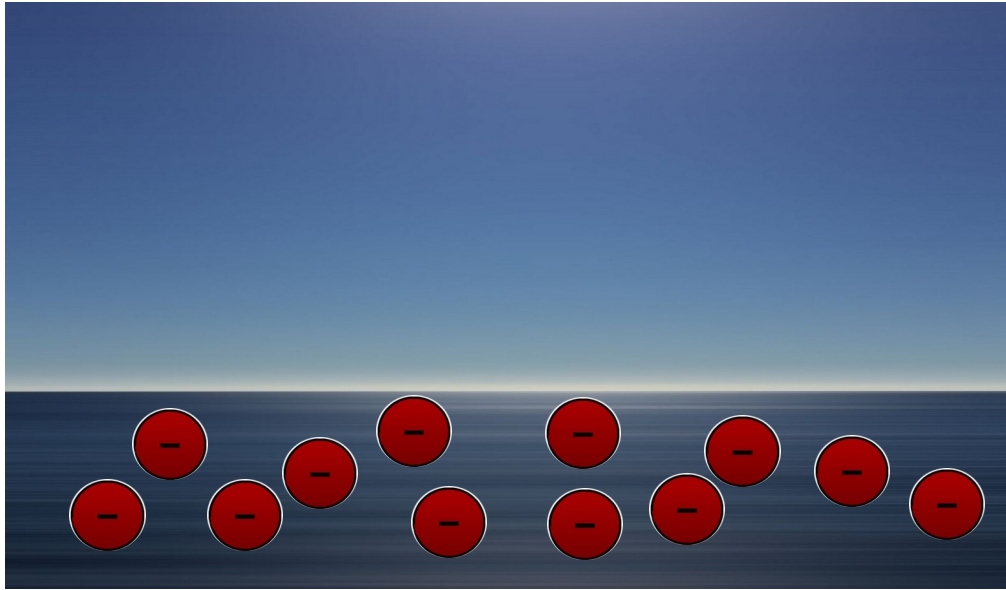
• By fitting, one usually finds higher accuracy for systems similar to those fitted, but greater inaccuracies far away.

J. Chem. Phys. 136, 150901 (2012)



J. Chem. Phys. 136, 150901 (2012)

Strategies to approximate the Exc: the HEG (High density limit)



$$e_{xc}^{HEG}[n] = \overbrace{e_x^{HEG}[n]}^{\text{Exact}} + \overbrace{e_c^{HEG}[n]}^{\text{Unknown}}$$

$$e_x^{HEG}[n] = -0.916n^{\frac{1}{3}}$$

$$e_c^{HEG}[n] \Big|_{GMB} = 0.0622 \ln(r_s) - 0.096 + O(r_s)$$

Wigner Radius $\left(\frac{1}{r_s} \sim n^{\frac{1}{3}}\right)$

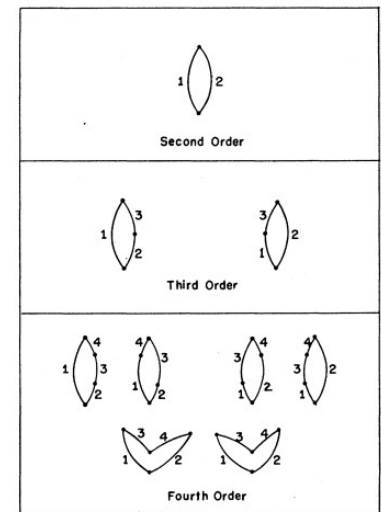
Correlation Energy of an Electron Gas at High Density*

MURRAY GELL-MANN, *Department of Physics, California Institute of Technology, Pasadena, California*

AND

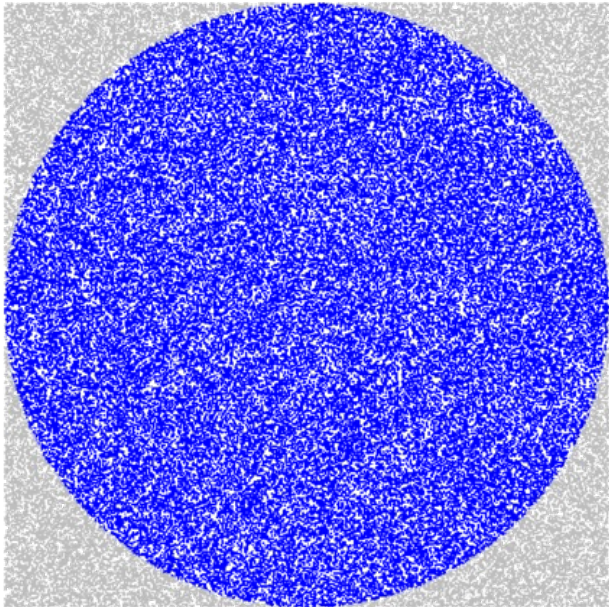
KEITH A. BRUECKNER, *Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania*

(Received December 14, 1956)



Strategies to approximate the Exc: the HEG (Low density limit)

$$e_{xc}^{HEG}[n] = \overbrace{e_x^{HEG}[n]}^{\text{Exact}} + \overbrace{e_c^{HEG}[n]}^{\text{DMC}}$$



VOLUME 45, NUMBER 7

PHYSICAL REVIEW LETTERS

18 AUGUST 1980

Ground State of the Electron Gas by a Stochastic Method

D. M. Ceperley

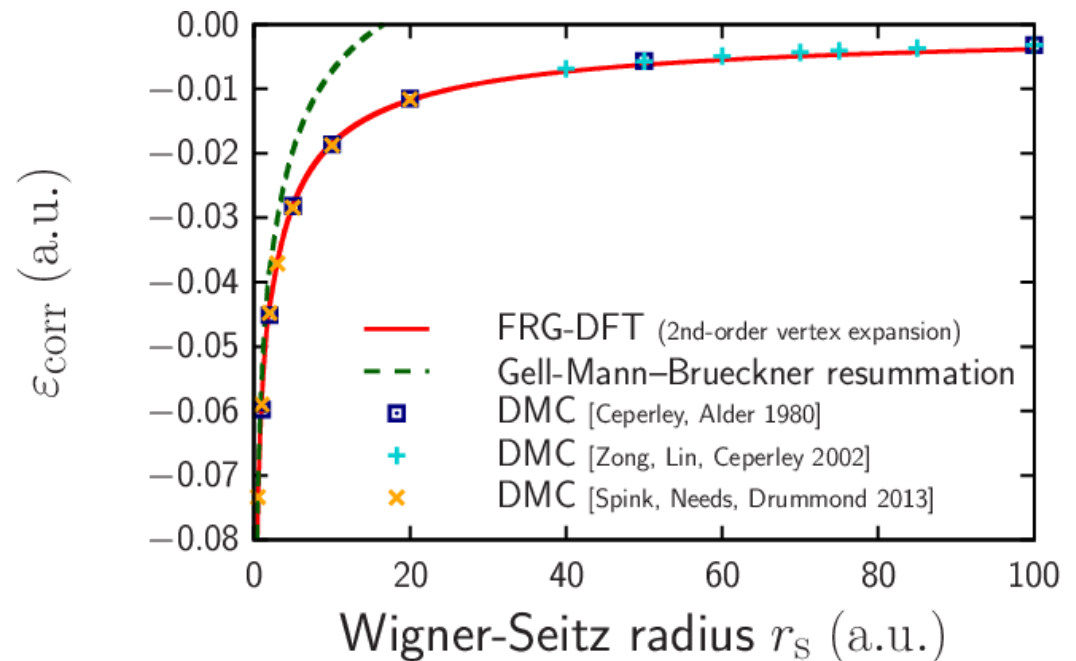
National Resource for Computation in Chemistry, Lawrence Berkeley Laboratory, Berkeley, California 94720

and

B. J. Alder

Lawrence Livermore Laboratory, University of California, Livermore, California 94550

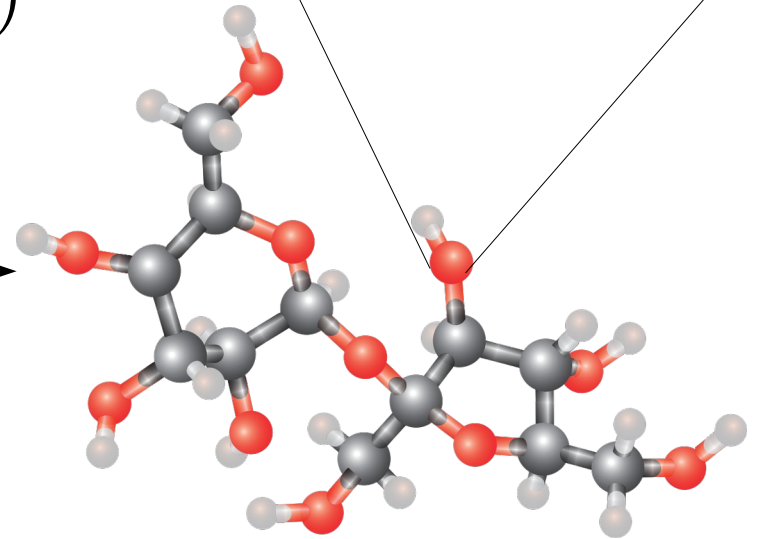
(Received 16 April 1980)



There are several expressions for the correlation energy which have been obtained by fitting to the results of accurate QMC calculations of the HEG. These expressions are rather complicated and they are usually referred to by their abbreviations such as *VWN*, *VWN5*, *CAPZ*, and others.

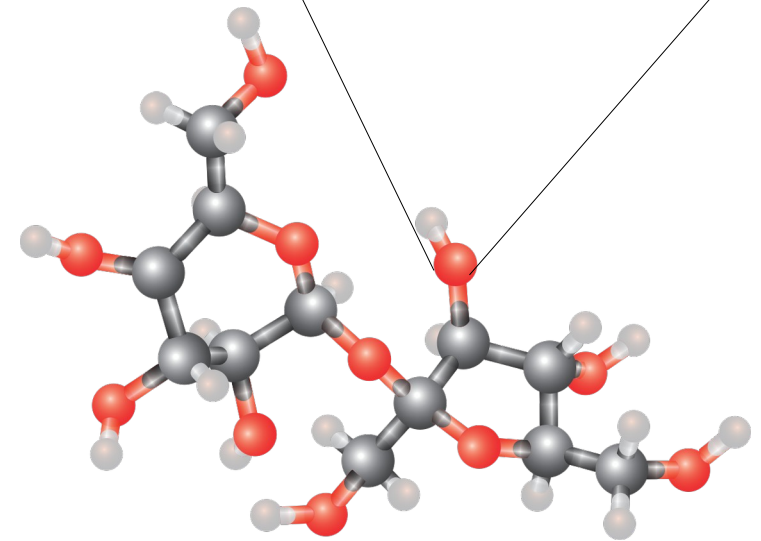
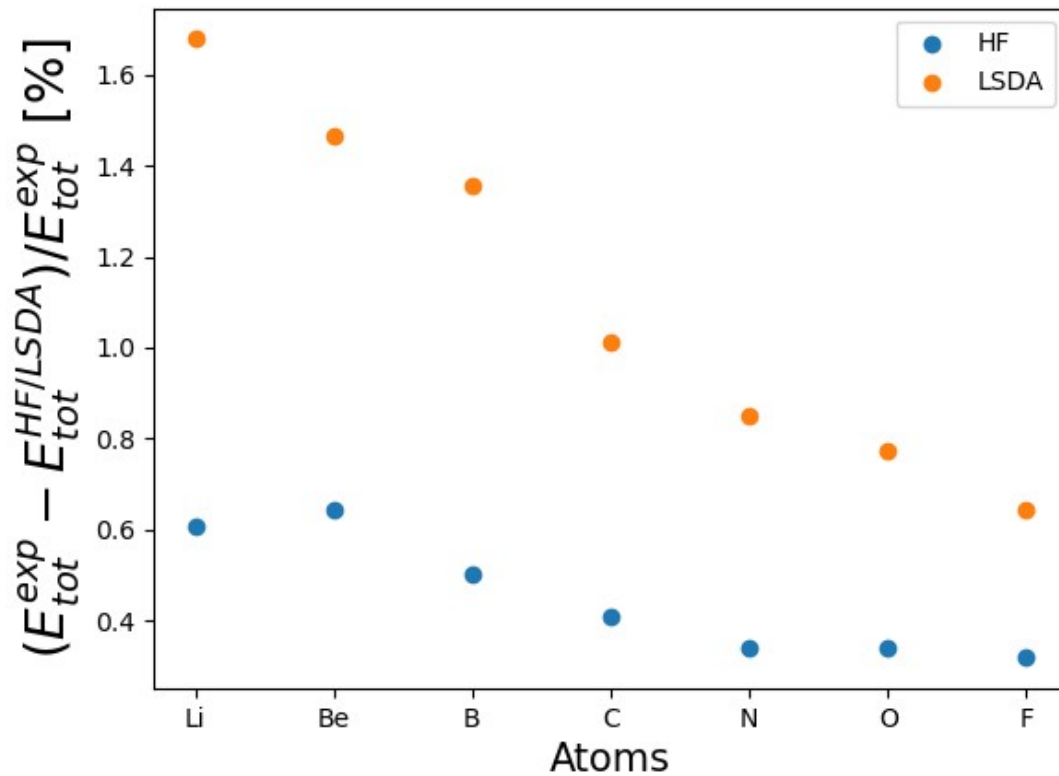
The Local Density Approximation

$$E_{xc}^{LDA}[n] \equiv \int d\vec{r} n(\vec{r}) e_{xc}^{HEG}(n(\vec{r}))$$



The Local Density Approximation (atoms)

Reviews of Modern Physics 61, 689 (1989)



Clearly arguments based on small departures from homogeneity cannot be applied.



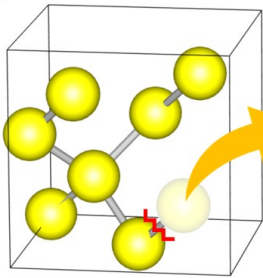
Both the HF and the LSDA methods lead to departures from experiment that are much greater than would be acceptable



$$\int d\vec{r}_1 n_{xc}(\vec{r}_1, \vec{r}_2 - \vec{r}_1) = -1$$

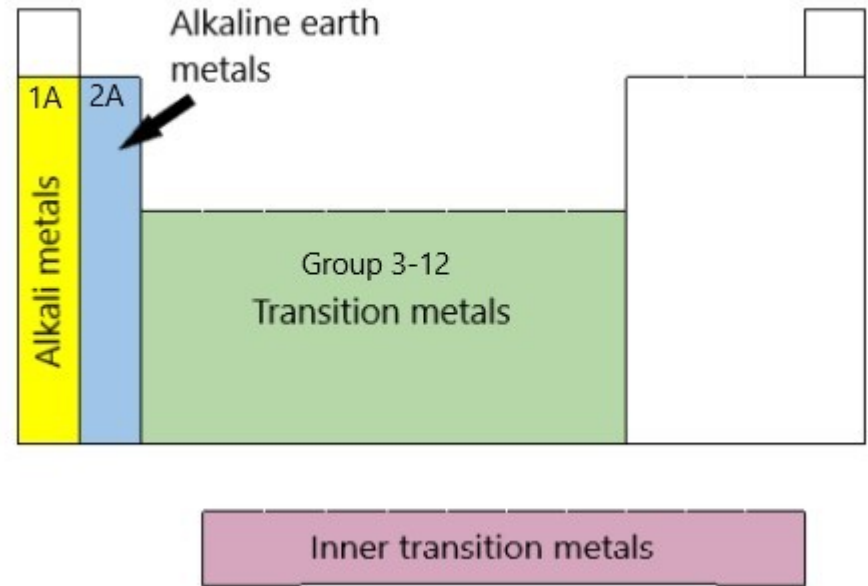
The Local Density Approximation (solids)

Cohesion is well described



$$E_{\text{cohesive}} = E_{\text{Bulk}} - E_{\text{Isolated atom}}$$

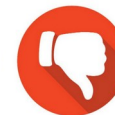
Trends in the lattice constants are described very well. In the case of the alkalis, the LSD calculations underestimate the bond lengths by a small amount



Period	group 1*	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1	H												B	C	N	O	F	Ne	
2	Li	Be											Al	Si	P	S	Cl	Ar	
3	Na	Mg											Ga	Ge	As	Se	Br	Kr	
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn		Ge	As	Se	Br	Kr	
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og	
Lanthanoid series			58	59	60	61	62	63	64	65	66	67	68	69	70	71			
Actinoid series			90	91	92	93	94	95	96	97	98	99	100	101	102	103			



Lattice constants and bulk moduli are given remarkably well



cohesive energies are overestimated by up to 1.0 eV.

The Local Density Approximation (failure)

PRL 101, 133002 (2008)

PHYSICAL REVIEW LETTERS

week ending
26 SEPTEMBER 2008

Optical Saturation Driven by Exciton Confinement in Molecular Chains: A Time-Dependent Density-Functional Theory Approach

Daniele Varsano

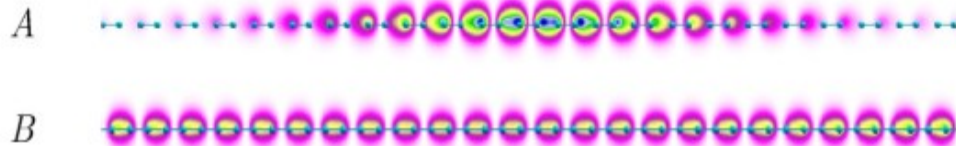
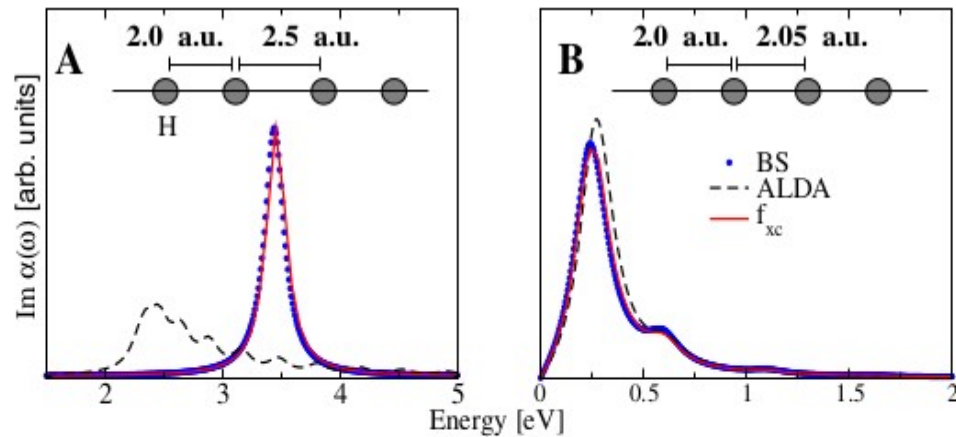
National Center on nanoStructures and Biosystems at Surfaces (S3) of INFN-CNR
and European Theoretical Spectroscopy Facility (ETSF), Via Campi 231/A, 41100 Modena, Italy

Andrea Marini

European Theoretical Spectroscopy Facility (ETSF), CNR-INFN Institute for Statistical Mechanics and Complexity, CNISM
and Dipartimento di Fisica, Università di Roma "Tor Vergata," via della Ricerca Scientifica 1, 00133 Roma, Italy

Angel Rubio

Nano-Bio Spectroscopy Group and Unidad de Física de Materiales Centro Mixto CSIC-UPV,
Universidad del País Vasco UPV/EHU and European Theoretical Spectroscopy Facility (ETSF),
Edificio Korta, Avenida de Tolosa 72, 20018 Donostia, Spain
(Received 10 October 2007; published 24 September 2008)



$$E_{xc}[n]$$

Total Energy

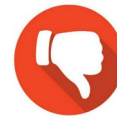
KS

$$V_{xc}[n](\vec{r}) \equiv \frac{\delta E_{xc}[n]}{\delta n(\vec{r})}$$

Ground state
Electrons

TDDFT

$$f_{xc}[n](\vec{r}, \vec{r}') \equiv \frac{\delta V_{xc}[n](\vec{r})}{\delta n(\vec{r}')} \quad \text{Excitations}$$

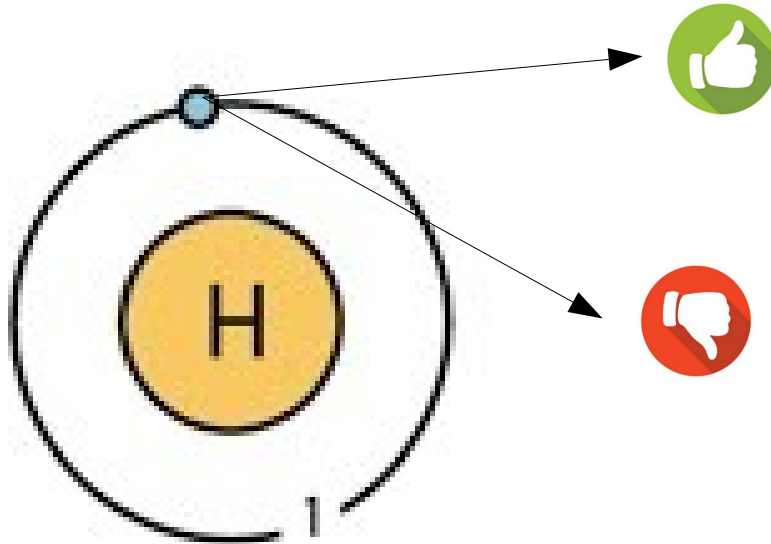


LDA fails dramatically in describing electronic localization due to correlation.

Self-Interaction Error

SI is an important source of error in LDA/GGA. This can lead to qualitatively wrong results

SI is caused by the approximate treatment of exchange



Only one electron → No CORRELATION

As Hartree (Exact) and Exchange (HEG) are calculated differently the electron has a residual interaction with itself (Self-Interaction)

PHYSICAL REVIEW B VOLUME 23, NUMBER 10 15 MAY 1981

Self-interaction correction to density-functional approximations for many-electron systems

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(Received 31 October 1980)

$$E_{SIC}[n] = E_{LDA}[n] - \sum_i \delta_i$$

Orbital dependence

PHYSICAL REVIEW A 75, 032505 (2007)

Self-interaction in Green's-function theory of the hydrogen atom

W. Nelson,^{1,*} P. Bokes,^{2,3} Patrick Rinke,^{3,4} and R. W. Godby^{1,3,†}

TABLE I. Quasiparticle energies (eV) for the 1s state of hydrogen (the ionization potential) obtained by diagonalizing the quasiparticle Hamiltonian (1). Two GW calculations are shown, starting from the LDA and from exact Kohn-Sham, respectively. For comparison, the Hartree-Fock (HF) and LDA eigenvalues are also shown.

Exact	HF	LDA	LDA+GW	Exact+GW
-13.61	-13.61	-6.36	-12.66	-13.40

The Generalized Gradient Approximation

"Even just the next step up Jacob's ladder, the GGA, has no unique form" (K. Burke)

$$E_{xc}^{GGA}[n] = \int d\vec{r} n(\vec{r}) e_{xc}(n(\vec{r}), |\nabla n(\vec{r})|)$$

$$E_x^{B88}[n_\sigma] = E_x^{LSDA}[n_\sigma] - \beta \sum_\sigma \int d\mathbf{r} n_\sigma^{4/3} \frac{x_\sigma^2}{1 + 6\beta \sinh^{-1}(x_\sigma)}$$

Exchange: Becke 1988

$$E_c^{LYP}[n] = -a \int \frac{d\mathbf{r}}{1 + dn} \left\{ n + bn^{-1/3} \left[C_F n^{5/3} - 2t_W + \frac{1}{9} (t_W + \frac{\nabla^2}{2} n) e^{-cn^{-1/3}} \right] \right\}$$

Correlation: Lee-Yang-Parr 1988

$$E_x^{PBE}[n] = \int d\mathbf{r} e_x^h(n) \left[1 + \kappa - \frac{\kappa}{1 + \beta \pi^2 s^2 / 3\kappa} \right]$$

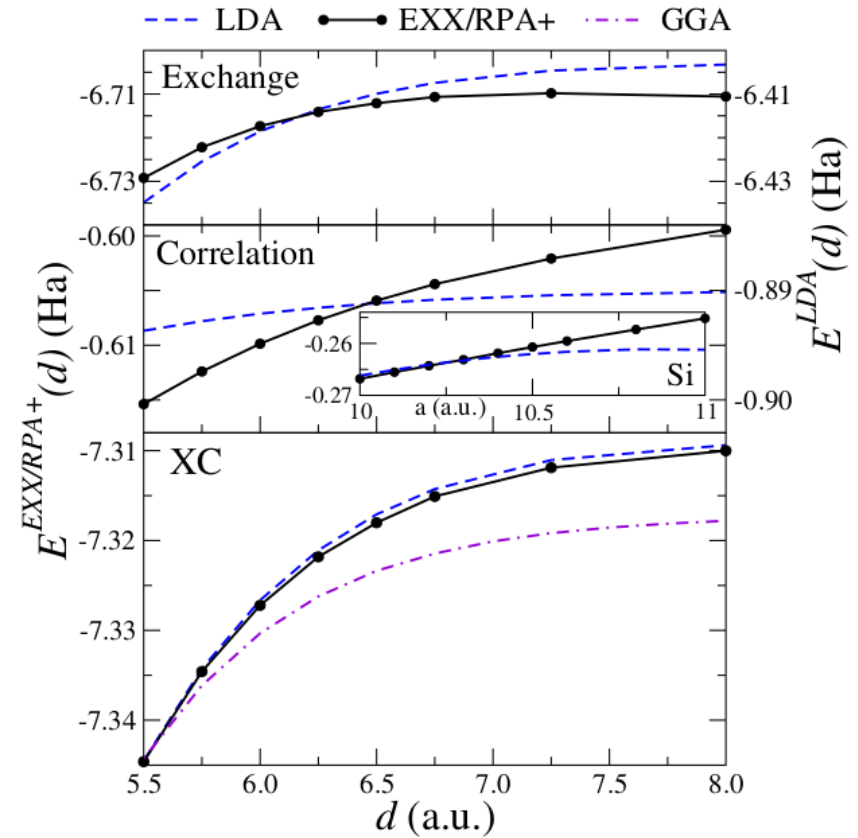
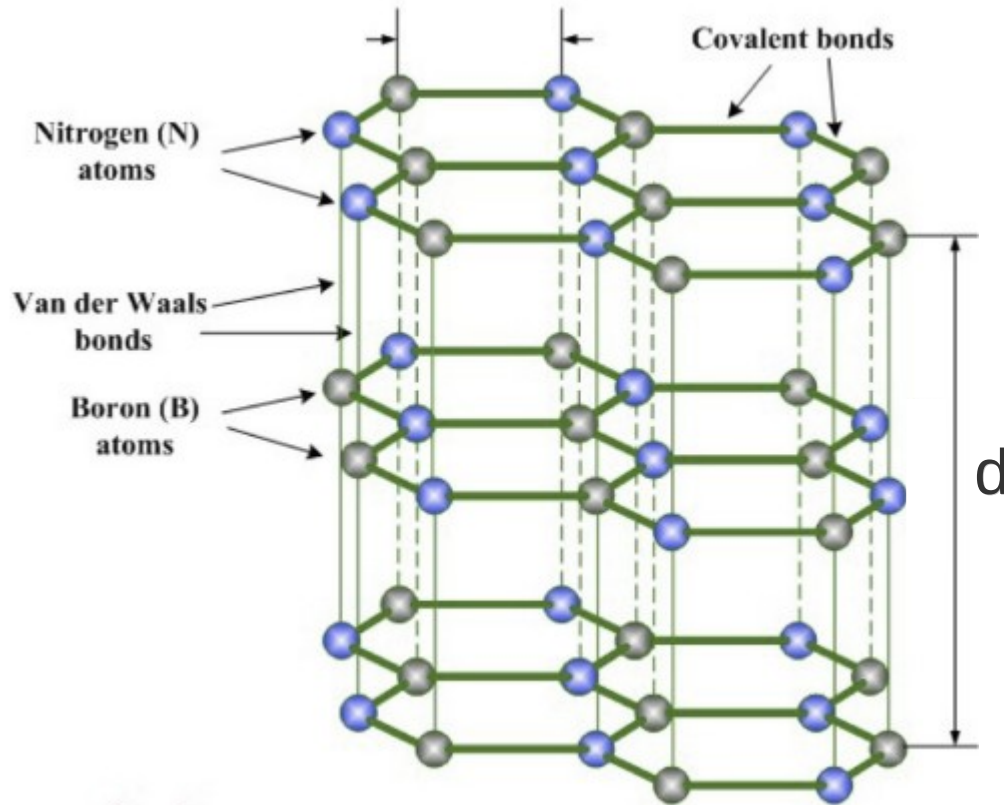
Perdew-Burke-Ernzerhof 1996

- LYP correlation works very well as part of B3LYP in chemistry, but fails badly for bulk metals.
- The PBE approximation works passably well for many materials purposes, but can be a factor of 2 or more worse than BLYP for dissociation energies.

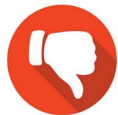


LDA vs GGA: the strange case of h-BN

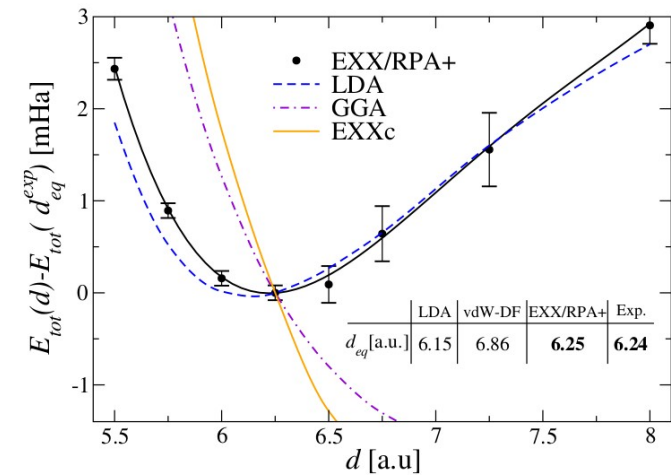
AM, P. García-González, and Angel Rubio Phys. Rev. Lett. 96, 136404 (2006)



LDA amazingly works due to drastic error cancellations.



GGA does not bind the layers.





RULES

1

Search the literature for calculations on similar materials and properties (many more properties than just the energy can be computed from DFT). Compare your "candidate" functionals by searching in the publications that describe their development for their strengths and weaknesses, especially with respect to the types of calculation you want to run.

2

Run some "calibration" calculations where you can compare the accuracy of possible functionals and basis sets to decide which combination is best for your "production" calculations.

3

Check, check and check again the literature! Computational simulations of materials consume a lot of computer time. It is a great disappointment if you discover that the calculations you have been running for 6 months are worthless!!!

The Many-Body approach



The exchange-correlation Energy can be formally derived from the Hamiltonian average by using Many-Body techniques

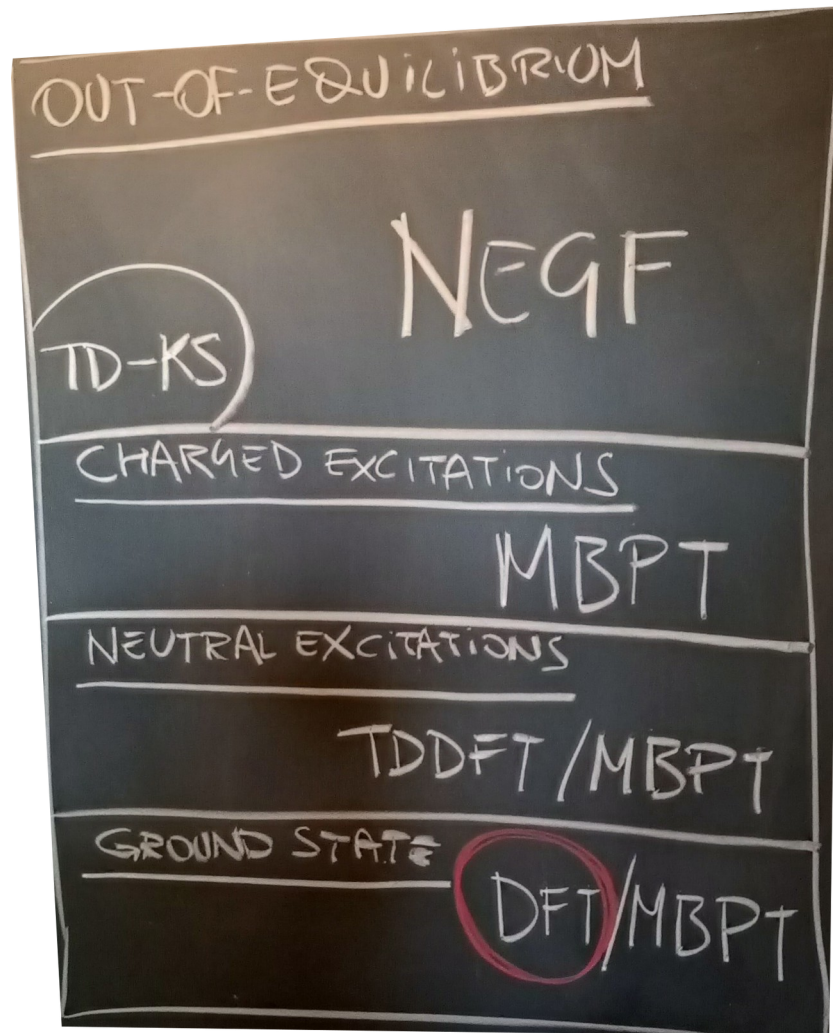
$$\hat{H} = \hat{T} + \hat{V}_{ee} + \sum_{i=1}^N V_{ext}(\hat{r}_i)$$



DFT

MBPT

Different physics, different approaches

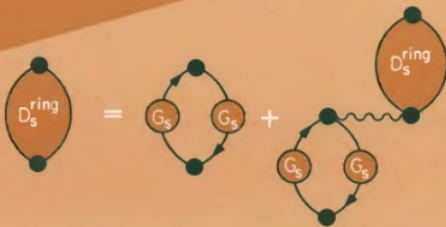


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R. M. Dreizler E. K. U. Gross

Density Functional Theory

An Approach to the Quantum Many-Body Problem



Springer-Verlag

The density functional formalism, its applications and prospects

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A scheme that reduces the calculations of ground-state properties of systems of interacting particles exactly to the solution of single-particle Hartree-type equations has obvious advantages. It is not surprising, then, that the density functional formalism, which provides a way of doing this, has received much attention in the past two decades. The quality of the energy surfaces calculated using a simple local-density approximation for exchange and correlation exceeds by far the original expectations. In this work, the authors survey the formalism and some of its applications (in particular to atoms and small molecules) and discuss the reasons for the successes and failures of the local-density approximation and some of its modifications.

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1. Total energies	702	The description of many-particle systems has been an important goal of physics during this century. Analytic solutions of the Schrödinger equation are possible for a few very simple systems, and numerically exact solutions can be found for a small number of atoms and molecules. However, most cases of interest, such as reaction surfaces in chemistry or electron-electron interactions in solids, require the use of model Hamiltonians or simplified computational schemes. The recent progress in the calculation of the electronic structure of atoms, molecules, and solids has emphasized, perhaps, how far we are from the goal of being able to predict the physical and chemical properties of many-particle systems with reliability and without excessive computation. In theoretical chemistry, for example, "tentative conclusions have been arrived at on the basis of theories which were such a patchwork of approximations that they appeared to have no right to work" (Hoffmann and Woodward, 1968). The development of schemes that provide useful information on real systems continues, and it is the purpose of this paper to describe one of them—the density functional (DF) formalism. We shall point out, in particular, the differences in perspective between this formalism and other methods used to discuss many-particle systems.	
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IN PHYSICS

C. Fiolhais
F. Nogueira
M. Marques
(Eds.)

A Primer in Density Functional Theory

Springer

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- [Theoretical spectroscopy](#) [□](#), M. Gatti
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- [PhD lectures: MBPT and Yambo](#) [□](#), L. Chiodo et al.
- [Introduction to Many Body Physics](#) [□](#), Piers Coleman
- [Pedagogical introduction to equilibrium Green's functions: condensed matter examples with](#)