

Foundations of density functional theory

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Course Outline

- Preliminaries
 - Many-electron wavefunctions
 - Rayleigh-Ritz variational principle
- Ground-state (static) density functional theory
 - Hohenberg-Kohn and Kohn-Sham theorems
 - Spin density functional theory
 - Formal aspects: N - and v -representability, derivative discontinuity, scaling
 - Functionals I: The local density approximation (LDA)
 - Functionals II: Gradient expansion and generalized gradient approximations (GGA's)
 - Functionals III: Orbital functionals and the optimized effective potential (OEP) method
 - Functionals IV: Hybrid functionals and meta-GGA's
- Time-dependent density functional theory
 - Runge-Gross theorem
 - Linear response theory: Excitation energies from TDDFT

Quote

“The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.”

Paul Dirac, in Proc. Roy. Soc. A **123**, 714 (1929)

Nobel prize in Chemistry 1998 for Walter Kohn

In 1998 the Nobel prize for Chemistry was awarded to Walter Kohn and John Pople. Walter Kohn received the prize “for his development of density functional theory”



Source: //nobelprize.org

Atomic units

Quantity	unit	physical meaning	value in SI units
mass	m_e or m	electron mass	9.1095×10^{-31} kg
charge	e	electron charge	1.602×10^{-19} C
angular momentum	\hbar		1.055×10^{-34} Js
length	a_0	Bohr radius of H atom	5.292×10^{-11} m
velocity	$v_0 = \alpha c$	electron velocity in first Bohr orbit	2.188×10^{-6} m/s
time	a_0/v_0		2.419×10^{-17} s
energy	$\frac{e^2}{4\pi\epsilon_0 a_0} = \alpha^2 m c^2$	twice the ionization potential of H atom	4.3598×10^{-18} J $\equiv 27.2116$ eV $\equiv 1$ Hartree $\equiv 2$ Rydberg