

ELECTRONIC DENSITY FUNCTIONAL THEORY

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[Density functional theory - Wikipedia](#)

Density functional theory (DFT) is a computational quantum mechanical modelling method used in physics, chemistry and materials science to investigate the electronic structure (principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases.

[Electronic Density Functional Theory: Recent Progress and ...](#)

This book is an outcome of the International Workshop on Electronic Density Functional Theory, held at Griffith University in Brisbane, Australia, in July 1996.

[Density Functional Theory of Electronic Structure](#)

Density Functional Theory of Electronic Structure W. Kohn,* A. D. Becke, and R. G. Parr Department of Physics, UniVersity of California, Santa Barbara, Santa Barbara, California 93106 ReceiVed: March 5, 1996X

Density functional theory (DFT) is a (in principle exact) theory of electronic structure, based on the electron density distribution $n(\mathbf{r})$, instead of the many-electron wave function $\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots)$. [Density Functional Theory for Beginners](#)

The purpose of this site is to explain in a non-mathematical way what density functional theory is and what it is used for. I hope to familiarise the reader with the syntax of solid state theory and give a basic understanding of the related topics.

[Structural, electronic and optical properties of cubic ...](#)

First-principles full-potential linearized augmented plane-wave method based on density functional theory is used to investigate the structural, electronic and optical properties of the cubic fluoroelpasolites Cs₂NaYF₆ within the local density approximation (LDA) and generalized gradient approximation (GGA) for potential exchange correlation.

[Density Functional Theory of Electronic Structure - The ...](#)

Density functional theory (DFT) is a (in principle exact) theory of electronic structure, based on the electron density distribution $n(\mathbf{r})$, instead of the many-electron wave function $\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots)$. Having been widely used for over 30 years by physicists working on the electronic structure of solids, surfaces, defects, etc., it has more

[Calculation of the electronic and optical properties of ...](#)

Density functional theory (DFT) was used to calculate the bulk electronic and optical properties of indium tin oxide (ITO). The ITO model was constructed replacing indium atoms with tin atoms in the cubic unit cell of indium oxide. [Density functional theory of structural, electronic and](#)

...

In this work, the structural, electronic structure and optical properties of $CuXY_2$ ($X=In, Ga$ and $Y=S, Se$) chalcopyrite semiconductors have been computed with density functional theory using

Electronic and optical properties of Y-doped Si_3N_4 by

...

Geometry structures, formation energies, electronic and optical properties of Y-doped $-Si_3N_4$ and $-Si_3N_4$ are investigated based on the density functional theory (DFT). **Density Functional Theory - pollux.chem.umn.edu**

Example: electronic structure of benzene (42 electrons) All the information is contained in the wave function, an antisymmetric function of 126 coordinates and 42 electronic spin components. Pierre Hohenberg and Walter Kohn, 1964 density functional theory All the information is contained in the density, a simple function of 3 coordinates.

Electronic Structure of Copper Phthalocyanine: a ...

Electronic Structure of Copper Phthalocyanine: a Comparative Density Functional Theory Study Noa Marom,¹ Oded Hod,² Gustavo E. Scuseria,² and Leor Kronik,^{1, 1} Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel ², Department of Chemistry, Rice University, Houston, Texas 77005 Abstract We present a systematic density functional theory study of the

Ab initio density functional theory investigation of the

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OSTI.GOV Journal Article: Ab initio density functional theory investigation of the structural, electronic and optical properties of Ca_3Sb_2 in hexagonal and cubic phases Title: Ab initio density functional theory investigation of the structural, electronic and optical properties of Ca_3Sb_2 in hexagonal and cubic phases

3.1 Density-functional theory - University of Cambridge

Density-functional theory, introduced in 1964 by Hohenberg and Kohn , makes two remarkable statements. The external potential is uniquely determined by the corresponding ground-state electronic density, to within an additive constant.

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