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Functional Theory  
Of Atoms And  
Molecules

# **Density Functional Theory Of Atoms And Molecules**

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## **Density Functional Theory Of Atoms**

This book is a rigorous, unified account of the fundamental principles of the density-functional theory of the

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Of Atoms And

Molecules  
electronic structure of  
matter and its  
applications to atoms  
and molecules.

Containing a detailed  
discussion of the  
chemical potential and  
its derivatives, it  
provides an  
understanding of the  
concepts of  
electronegativity,  
hardness and softness,  
and chemical  
reactivity.

**Density-Functional**

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**Theory of Atoms and  
Molecules ...**

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concepts of  
electronegativity,  
hardness and softness,  
and chemical  
reactivity.

## **Density-Functional Theory of Atoms and Molecules ...**

Density-functional  
theory ( DFT) is a  
computational  
quantum mechanical  
modelling method used  
in physics, chemistry  
and materials science  
to investigate the

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electronic structure (or nuclear structure) (principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases.

## **Density functional theory - Wikipedia**

The fundamental principles of the density-functional theory of the electronic structure of matter and its applications to atoms and molecules



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are covered in this book. It provides an understanding of the concepts of electronegativity, hardness and softness and chemical reactivity.

**Density-functional theory of atoms and molecules in ...**

Density-functional theory of atoms and molecules. R.G. Parr and W. Yang, Oxford University Press, New

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Functional Theory

York, Oxford, 1989. IX

+ 333 pp. Price £45.00

**Density-functional  
theory of atoms and  
molecules. R.G ...**

Current studies in density functional theory and density matrix functional theory are reviewed, with special attention to the possible applications within chemistry. Topics discussed include the concept of

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electronegativity, the  
concept of an atom in a  
molecule, calculation  
of electronegativities

from the  $X\alpha$  method,

the concept of

pressure, Gibbs-Duhem

equation, Maxwell

relations, stability

conditions, and local

density functional

theory.

**Density Functional  
Theory of Atoms and  
Molecules ...**

Density functional

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### Functional Theory

theory (DFT) is a quantum-mechanical (QM) method used in chemistry and physics to calculate the electronic structure of atoms, molecules and solids. It has been very popular in computational solid-state physics since the 1970s.

**Density functional theory across chemistry, physics and ...**

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### Functional Theory

Density functional theory (DFT) is one of the most widely used methods for ab initio calculations of the structure of atoms, molecules, crystals, surfaces, and their interactions.

Unfortunately, the customary introduction to DFT is often considered too lengthy to be included in various curricula.

## **Density functional**

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Functional Theory

**theory: An**

**introduction:**

**American ...**

This book is a rigorous, unified account of the fundamental principles of the density-functional theory of the electronic structure of matter and its applications to atoms and molecules.

Containing a detailed discussion of the chemical potential and its derivatives, it provides an

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understanding of the  
concepts of  
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reactivity.

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Ground State Energy  
Helium Atom Trial  
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keywords were added

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by machine and not by the authors. This process is experimental and the keywords may be updated as the learning algorithm improves.

## **Density Functional Theory of Atoms and Molecules ...**

This book is a rigorous, unified account of the fundamental principles of the density-functional theory of the



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Molecules.  
electronic structure of  
matter and its  
applications to atoms  
and molecules.

Containing...

## **Density-Functional Theory of Atoms and Molecules - Robert**

...

According to our recent  
study , a combination  
of density functional  
theory (DFT) [6,7] and  
Bader's quantum  
theory of atoms in  
molecules (QTAIM) [ , , ,

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], i.e. DFT + QTAIM,  
can provide a reliable  
ab initio approach to  
quantitatively shed  
light on the electronic  
structures and bonding  
properties of materials  
[5,, , , ].

### **Topological analysis of electron density in half-Heusler ...**

In this study, we  
evaluate the stable  
configurations of C  
and/or Sn atoms in Si  
(Ge) crystals with a

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focus on the formation  
of interstitial C ( $C_i$ )  
atoms by means of  
density functional  
theory calculations.

**Density functional  
theory study of  
stable  
configurations ...**

Current studies in  
density functional  
theory and density  
matrix functional  
theory are reviewed,  
with special attention  
to the possible

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applications within

chemistry. Topics

discussed include the  
concept of

electronegativity, the  
concept of an atom in a

molecule, calculation  
of electronegativities

from the  $X\alpha$  method,  
the concept of

pressure, Gibbs-Duhem  
equation, Maxwell

relations, stability ...

**Density-functional  
theory of atoms and  
molecules ...**

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The method Kohn introduced came to be known as the density-functional theory. It is now used in studies of numerous chemical problem areas, from calculating the geometrical structure of molecules (i.e. bonding distance and angles) to mapping chemical reactions.

**Press release: The  
1998 Nobel Prize in  
Chemistry ...**

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## Of Atoms And

## Molecules

Detailed density functional theory calculations performed herein indicate that Li/Mg adatoms evenly distributed on a borophene tend to transform the interaction between borophene and the Ag (111) substrate into van der Waals-like interaction and help to separate them, making the exfoliation of borophenes from substrates much

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easier.

Of Atoms And  
**Exfoliation of  
borophenes from  
silver substrates  
assisted ...**

We studied co-  
reactants for tungsten  
chloride precursors by  
density functional  
theory calculation to  
find the proper  
reducing agent.  
Tungsten chloride...

**Density Functional  
Theory Study on the**

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Of Atoms And

Molecules

## **Reducing Agents for**

## **...**

In this study, density functional theory (DFT) calculation was performed to evaluate whether Ti, Al, Zr and Ag atoms can act as active elements to solder SiC. Work of adhesion (Wad), charge density difference and density of states were used to study the interfaces without and with active elements.  $\beta$ -Sn(001)/ $\beta$ -



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**Composition design  
of Sn-based active  
solder for soldering**

...

Electronic and magnetic properties of substituted BN sheets: A density functional theory study . Abstract: Using density functional calculations, we investigate the geometries, electronic structures and

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magnetic properties of hexagonal BN sheets with 3d transition metal (TM) and nonmetal atoms embedded in three types of vacancies: VB, VN, and VB+N.

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