

Time Dependent Density Functional Theory: A Comprehensive Guide



Time-Dependent Density-Functional Theory: Concepts and Applications (Oxford Graduate Texts) by Herbert Meislich

★★★★☆ 4.7 out of 5

Language : English

File size : 18068 KB

Screen Reader: Supported

Print length : 544 pages

Lending : Enabled



Time Dependent Density Functional Theory (TDDFT) is a powerful tool for understanding the electronic structure and dynamics of molecules and materials. TDDFT is based on the density functional theory (DFT), which is a widely used method for calculating the electronic structure of atoms, molecules, and solids. DFT is based on the Hohenberg-Kohn theorem, which states that the ground state energy of a system is a unique functional of the electron density.

TDDFT extends DFT to time-dependent systems. This allows TDDFT to be used to study a wide range of phenomena, including the absorption and emission of light, the dynamics of chemical reactions, and the electronic properties of materials.

Theoretical Foundations of TDDFT

The theoretical foundations of TDDFT are based on the time-dependent Schrödinger equation:

$$i\hbar\partial\Psi/\partial t = H\Psi$$

where Ψ is the wavefunction of the system, \hbar is the reduced Planck constant, and H is the Hamiltonian.

The Hamiltonian for a system of electrons and nuclei can be written as:

$$H = -\sum_i^{(N_e)} \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_i^{(N_e)} \sum_A^{(N_A)} \frac{Z_A}{r_{iA}} + \sum_i^{(N_e)} \sum_{j>i}^{(N_e)} \frac{1}{r_{ij}} + \sum_A^{(N_A)} \sum_{B>A}^{(N_A)} \frac{Z_A Z_B}{R_{AB}}$$

where N_e is the number of electrons, N_A is the number of nuclei, Z_A is the atomic number of nucleus A , r_{iA} is the distance between electron i and nucleus A , r_{ij} is the distance between electrons i and j , and R_{AB} is the distance between nuclei A and B .

The time-dependent Schrödinger equation can be solved using a variety of numerical methods. The most common method is the finite difference time domain (FDTD) method. The FDTD method discretizes the time-dependent Schrödinger equation and solves it on a grid of points in space and time.

Applications of TDDFT

TDDFT has been used to study a wide range of phenomena, including:

- * The absorption and emission of light
- * The dynamics of chemical reactions
- * The electronic properties of materials
- * The design of new materials

TDDFT is a powerful tool for understanding the electronic structure and dynamics of molecules and materials. It is a valuable tool for scientists and engineers working in a variety of fields, including chemistry, physics, and materials science.

TDDFT is a powerful tool for understanding the electronic structure and dynamics of molecules and materials. It is a valuable tool for scientists and engineers working in a variety of fields, including chemistry, physics, and materials science.



Time-Dependent Density-Functional Theory: Concepts and Applications (Oxford Graduate Texts) by Herbert Meislich

★★★★☆ 4.7 out of 5

Language : English

File size : 18068 KB

Screen Reader: Supported

Print length : 544 pages

Lending : Enabled



Becoming Sports Agent Masters At Work: The Ultimate Guide

What is a Sports Agent? A sports agent is a person who represents athletes in their dealings with teams, leagues, and other businesses. Sports...



The Dead Girls: A Haunting and Unforgettable Literary Masterpiece

A Chilling and Captivating Tale Prepare to be captivated by Selva Almada's haunting and atmospheric novel, 'The Dead Girls.' This...