

Fundamentals Of Time Dependent Density Functional Theory Lecture Notes In Physics Vol 837

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Fundamentals Of Time Dependent Density

There have been many significant advances in time-dependent density functional theory over recent years, both in enlightening the fundamental theoretical basis of the theory, as well as in computational algorithms and applications.

Fundamentals of Time-Dependent Density Functional Theory ...

Fundamentals of Time-Dependent Density Functional Theory (Lecture Notes in Physics, Vol. 837) 1st Edition. by Miguel A.L. Marques (Editor), Neepa T. Maitra (Editor), Fernando M.S. Nogueira (Editor), E.K.U. Gross (Editor), Angel Rubio (Editor) & 2 more. 4.5 out of 5 stars 2 ratings. ISBN-13: 978-3642235177.

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Fundamentals of Time-Dependent Density Functional Theory ...

The Runge-Gross theorem (Runge and Gross, Phys Rev Lett, 52:997-1000, 1984) states that for a given initial state the time-dependent density is a unique functional of the external potential. Let us...

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Fundamentals of Time-Dependent Density Functional TheoryII. Neepa T. Maitra. Hunter College and the Graduate Center of the City University of New York

Fundamentals of Time-Dependent Density Functional Theory II

time-dependent case, yielding the exact time-dependent potential acting on an electron. This led to the birth of the foundational theorem of TDDFT, the Runge-Gross theorem [2]. What Runge and Gross considered, were non-equilibrium systems of electrons treated non-relativistically, described by the following universal Hamiltonian: $H^{\wedge}(t) = \sum_i \left[\frac{p_i^2}{2} + v_{\text{ext}}(r_i) \right]$

Perspective: Fundamental Aspects of Time-Dependent Density ...

Quantum chemical calculations are important for elucidating light-capturing mechanisms in photobiological systems. The time-dependent density functional theory (TDDFT) has become a popular methodology because of its balance between accuracy and computational scaling, despite its problems in describing, for example, charge transfer states.

Benchmarking the Performance of Time-Dependent Density ...

Fundamentals of Time-Dependent Density Functional Theory. Summary: This book offers systematic coverage of recent developments in time-dependent density functional theory, including basic concepts, and contemporary applications from real-time coupled-electron-ion dynamics, to excited-state dynamics and molecular transport.

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