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Titolo	Density-Functional Theory for Electrons : Basic Theory and New Formalism / / by Hideaki Takahashi
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Descrizione fisica	1 online resource (421 pages)
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Nota di contenuto	Wave-function theory vs Density-functional theory -- Static Correlation -- Foundation of the Density-Functional Theory on the Energy Electron Density -- Functional Development for Static Correlation -- Functional Development for Kinetic Energy -- Summary and Perspective.
Sommario/riassunto	In this book, the author provides a detailed review and discussion on new density-functional theory (DFT) for electrons, where electron distribution on the energy coordinate, instead of the electron density, plays a fundamental role. The book also includes a review of the currently prevailing DFT to make comparisons with the new theory. A particular emphasis is placed on the discussion on the advantage of the new theory in solving the toughest problems in the current DFT. Explicitly, it is suggested in the book that the new theory has a potential to solve the static correlation errors which arise in the description of chemical bonds through the current DFT. Some prototypes of the functionals are presented in the book. The theory is also utilized to make a contribution to the development of the kinetic

energy functional known as the most difficult issue in DFT. The book offers a lot of helpful explanations of the new theory for the researchers and students to understand and utilize the theory for their future developments.