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Titolo	Theoretical Chemistry for Experimental Chemists [[electronic resource]] : Pragmatics and Fundamentals / / by Kazuyoshi Tanaka
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ISBN	981-15-7195-3
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Descrizione fisica	1 online resource (201 pages)
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Soggetti	Chemistry, Physical and theoretical Chemoinformatics Nanochemistry Physical chemistry Catalysis Theoretical and Computational Chemistry Computer Applications in Chemistry Physical Chemistry
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Nota di contenuto	1. Introduction -- 2. Actual Potentials of Theoretical Chemistry: What Can Be Obtained -- 2-1 Molecular Structure -- 2-2 Chemical Bonds -- 2-3 Electronic Structures -- 2-4 Electronic Properties -- 2-5 Optical Properties -- 2-6 Mechanical Properties -- 2-7 Chemical Reaction -- 2-8 Molecular Design -- 3. Fundamentals of the Analysis Tools -- 3-1 Molecular Orbital Calculations -- 3-2 Density Functional Theory (DFT) Calculations -- 3-3 ONIOM Calculations -- 3-4 Crystal Orbital Calculations -- 3-5 Molecular Mechanics and Molecular Dynamics Calculations -- 3-6 Hints for Selection of Appropriate Calculation Methods -- 4. Toward More Sophisticated (Further) Problems -- 4-1 General Nanoscience -- 4-2 Electrochemistry -- 4-3 Catalytic Chemistry -- 4-4 Biological Themes.
Sommario/riassunto	This book presents active application aspects of theoretical chemistry, and is particularly intended for experimental chemists, ranging from graduate students to more professional researchers, who are developing new materials or searching for novel properties of the

materials they work with. It not only addresses the fundamental aspects of theoretical chemistry but also provides abundant examples of applications based on the electronic structure analyses of actual systems. As the book demonstrates, these analyses can deepen our understanding of a variety of chemical phenomena, including the chemical reactivities and electronic properties of substances, in a bottom-up manner. By illustrating how electronic structure analyses can be effectively applied, the book introduces readers to the impressive potential of theoretical chemistry, which they can adapt for their own purposes, and without having to suffer through a parade of complex formulae.