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Nota di contenuto	The DV-Xa Molecular Orbital Calculation Method and Recent Development -- Algebraic Molecular Orbital Theory -- Analytical Expression of Molecular Integrals over Slater-Type Functions for Generating their Polynomial Expressions -- Atom-Atom Interaction Potential from the Gaussian Quadrature Method and Classical Molecular Dynamics -- Comparison of Contributions to Interatomic Interactions between Covalent and Ionic Bonds from Total Energy Calculations -- Total Energy Calculation by DV-Xa Method and Its Accuracy -- Energy Expression of the Chemical Bond between Atoms in Hydrides and Oxides and Its Application to Materials Design -- Comparative Study on Optical Properties of YPO4: Mn, Zr Phosphor by Experiment and Calculation -- Applications of DV-Xa Method for New Material Design in Dye-Sensitized Solar Cell -- Microscopic Approach to Water by Using the DV-Xa Method, and Some Innovative Applications -- Electronic Structure and Chemical Bonding of Li1.1Nb0.9O2-y as a Negative

Electrode Material for Lithium Secondary Batteries -- Chemical Bonding, Point Defects and Positron Lifetimes in FeSi2 from First-Principles Calculations -- Structural Analysis of Al2TiO5 at Room Temperature and at 600 ºC by DV-Xa Approach (II) -- Wavelength of Luminescence and Energy Level Structure of Binuclear Copper(I) Complex. .

Sommario/riassunto

This multi-author contributed volume contains chapters featuring the development of the DV-X method and its application to a variety of problems in Materials Science and Spectroscopy written by leaders of the respective fields. The volume contains a Foreword written by the Chairs of Japanese and Korea DV-X Societies. This book is aimed at individuals working in Quantum Chemistry.