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Descrizione fisica	1 online resource (514 p.)
Altri autori (Persone)	NollerPatricia KarantzasGery C
Disciplina	158.24 306.87
Soggetti	Families - Psychological aspects Couples - Psychology Interpersonal relations Família Parella Aspectes psicològics Relacions humanes Llibres electrònics
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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	pt. 1. Trends in couple and family relationships -- pt. 2. Families across the lifespan -- pt. 3. Communication and conflict processes in couples and families -- pt. 4. Individual differences perspectives on intimacy, love, and caregiving -- pt. 5. Cognitive and affective processes in couple relationships -- pt. 6. Education and intervention

in couple and family relationships -- pt. 7. Interpersonal processes, families, and mental health -- pt. 8. Implications for policy -- pt. 9. Integration and conclusion.

Sommario/riassunto

The Wiley-Blackwell Handbook of Couples and Family Relationships presents original articles from leading experts that link research, policy, and practice together to reflect the most current knowledge of contemporary relationships. Offers interesting new perspectives on a range of relationship issues facing twenty-first century Western societyHelps those who work with couples and families facing with relationship issuesIncludes practical suggestions for dealing with relationship problemsExplores diverse issues, including family structure versus functioning;

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Titolo

A chemist's guide to valence bond theory // Sason Shaik, Philippe C. Hiberty

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Soggetti

Valence (Theoretical chemistry)

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Nota di contenuto

A CHEMIST'S GUIDE TO VALENCE BOND THEORY; CONTENTS; PREFACE; 1 A Brief Story of Valence Bond Theory, Its Rivalry with Molecular Orbital Theory, Its Demise, and Resurgence; 1.1 Roots of VB Theory;

1.2 Origins of MO Theory and the Roots of VB-MO Rivalry; 1.3 One Theory is Up the Other is Down; 1.4 Mythical Failures of VB Theory: More Ground is Gained by MO Theory; 1.5 Are the Failures of VB Theory Real?; 1.5.1 The O(2) Failure; 1.5.2 The C(4)H(4) Failure; 1.5.3 The C(5)H(5)(+) Failure; 1.5.4 The Failure Associated with the Photoelectron Spectroscopy of CH(4)

1.6 Valence Bond is a Legitimate Theory Alongside Molecular Orbital Theory

1.7 Modern VB Theory: Valence Bond Theory is Coming of Age; 2 A Brief Tour Through Some Valence Bond Outputs and Terminology;

2.1 Valence Bond Output for the H(2) Molecule; 2.2 Valence Bond Mixing Diagrams; 2.3 Valence Bond Output for the HF Molecule; 3 Basic Valence Bond Theory; 3.1 Writing and Representing Valence Bond Wave Functions; 3.1.1 VB Wave Functions with Localized Atomic Orbitals; 3.1.2 Valence Bond Wave Functions with Semilocalized AOs; 3.1.3 Valence Bond Wave Functions with Fragment Orbitals

3.1.4 Writing Valence Bond Wave Functions Beyond the 2e/2c Case

3.1.5 Pictorial Representation of Valence Bond Wave Functions by Bond Diagrams; 3.2 Overlaps between Determinants; 3.3 Valence Bond Formalism Using the Exact Hamiltonian; 3.3.1 Purely Covalent Singlet and Triplet Repulsive States; 3.3.2 Configuration Interaction Involving Ionic Terms; 3.4 Valence Bond Formalism Using an Effective Hamiltonian; 3.5 Some Simple Formulas for Elementary Interactions; 3.5.1 The Two-Electron Bond; 3.5.2 Repulsive Interactions in Valence Bond Theory; 3.5.3 Mixing of Degenerate Valence Bond Structures

3.5.4 Nonbonding Interactions in Valence Bond Theory

3.6 Structural Coefficients and Weights of Valence Bond Wave Functions; 3.7 Bridges between Molecular Orbital and Valence Bond Theories; 3.7.1 Comparison of Qualitative Valence Bond and Molecular Orbital Theories; 3.7.2 The Relationship between Molecular Orbital and Valence Bond Wave Functions; 3.7.3 Localized Bond Orbitals: A Pictorial Bridge between Molecular Orbital and Valence Bond Wave Functions;

Appendix; 3.A.1 Normalization Constants, Energies, Overlaps, and Matrix Elements of Valence Bond Wave Functions

3.A.1.1 Energy and Self-Overlap of an Atomic Orbital-Based Determinant

3.A.1.2 Hamiltonian Matrix Elements and Overlaps between Atomic Orbital-Based Determinants; 3.A.2 Simple Guidelines for Valence Bond Mixing; Exercises; Answers; 4 Mapping Molecular Orbital-Configuration Interaction to Valence Bond Wave Functions; 4.1 Generating a Set of Valence Bond Structures; 4.2 Mapping a Molecular Orbital-Configuration Interaction Wave Function into a Valence Bond Wave Function; 4.2.1 Expansion of Molecular Orbital Determinants in Terms of Atomic Orbital Determinants

4.2.2 Projecting the Molecular Orbital-Configuration Interaction Wave Function Onto the Rumer Basis of Valence Bond Structures

Sommario/riassunto

This reference on current VB theory and applications presents a practical system that can be applied to a variety of chemical problems in a uniform manner. After explaining basic VB theory, it discusses VB applications to bonding problems, aromaticity and antiaromaticity, the dioxygen molecule, polyradicals, excited states, organic reactions, inorganic/organometallic reactions, photochemical reactions, and catalytic reactions. With a guide for performing VB calculations, exercises and answers, and numerous solved problems, this is the premier reference for practitioners and upper-level student