1. Record Nr. UNISALENTO991001304129707536

Autore	Squarotti, Giorgio Bàrberi
Titolo	Le maschere dell'eroe : dall'Alfieri a Pasolini / Giorgio Bàrberi Squarotti
Pubbl/distr/stampa	Lecce : Milella, 1990
ISBN	8870481875
Descrizione fisica	377 p. ; 18 cm.
Collana	La scrittura possibile. Letteratura, critica, teoria
Soggetti	Eroe nella letteratura
Lingua di pubblicazione	Italiano
Formato	Materiale a stampa
Livello bibliografico	Monografia

2. Record Nr. UNINA9910780377503321

Autore	Gallup Gordon A (Gordon Alban), <1927->
Titolo	Valence bond methods : theory and applications / / Gordon A. Gallup [[electronic resource]]
Pubbl/distr/stampa	Cambridge : , : Cambridge University Press, , 2002
ISBN	1-107-12354-2 0-511-17713-5 0-511-30484-6 0-521-02127-8 1-280-43336-1 0-511-53538-4 0-511-15805-X 9786610433360 0-511-04387-2
Descrizione fisica	1 online resource (xv, 238 pages) : digital, PDF file(s)
Disciplina	541.2/24
Soggetti	Valence (Theoretical chemistry)
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia

Note generali	Title from publisher's bibliographic system (viewed on 05 Oct 2015).
Nota di bibliografia	Includes bibliographical references (p. 231-233) and index.
Nota di contenuto	; Part I. Theory and Two-Electron Systems: -- . Introduction -- H2 and localised orbitals -- H2 and delocalised orbitals -- Three electrons in doublet states -- Advanced methods for larger molecules -- Spatial symmetry -- Varieties of valence bond treatments -- Physics of ionic structures -- ; Part II. Examples and Interpretations: -- Selection of structures and arrangement of bases -- Four simple three-electron systems -- Second row homonuclear diatomics -- Second row heteronuclear diatomics -- Methane, ethane and hybridization -- Rings of hydrogen atoms -- Aromatic compounds -- Interaction of molecular fragments -- Appendix.
Sommario/riassunto	Valence bond theory is one of two commonly used methods in molecular quantum mechanics, the other is molecular orbital theory. This book focuses on the first of these methods, ab initio valence bond theory. The book is split into two parts. Part I gives simple examples of two-electron calculations and the necessary theory to extend these to larger systems. Part II gives a set of case studies of related molecule sets designed to show the nature of the valence bond description of molecular structure. It also highlights the stability of this description to varying basis sets. There are references to the CRUNCH computer program for molecular structure calculations which is currently available in the public domain. The book will be of primary interest to researchers and students working on electronic theory and computation in chemistry and chemical physics.