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| Descrizione fisica | 1 online resource (XXII, 407 p. 173 illus., 141 illus. in color.) |
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| Soggetti | Chemical bonds Quantum chemistry |
| Lingua di pubblicazione | Inglese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| Nota di bibliografia | Includes bibliographical references and index. |
| Nota di contenuto | Introduction -- Topological spaces -- Part I Descriptors -- The electron density -- Electron pairing descriptors -- Weak interactions -- Part II Applications -- Molecules -- Solid state -- Part III Exercises -- Algorithms & software -- Exercises -- Solutions. |
| Sommario/riassunto | This graduate textbook provides comprehensive information on topological analysis in real space of the electronic structure. Application of the topological tools is becoming routine for understanding the outcome of quantum chemical calculations. This title thoroughly reviews a selection of currently available topological tools, their use and spectrum of applications and provides graduate students and researchers with information not easily obtained from the available textbooks. The book is accompanied by worked examples, exercises and solutions and is a great tool for any quantum chemistry or computational chemistry course at the graduate and advanced undergraduate levels. |