1. Record Nr. UNISA996297331803316

Titolo	Country review Burkina Faso
Pubbl/distr/stampa	Houston, TX, : Commercial Data International
Descrizione fisica	1 online resource
Soggetti	Ecology Economic history Politics and government Social conditions Periodicals. Burkina Faso Economic conditions 1987- Periodicals Burkina Faso Environmental conditions Periodicals Burkina Faso Politics and government 1987-2014 Periodicals Burkina Faso Social conditions Periodicals Burkina Faso
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Periodico

2. Record Nr. UNINA9910485602903321

Autore	Kato Tatsuhisa
Titolo	Vibronic Coupling Density : Understanding Molecular Deformation / / by Tatsuhisa Kato, Naoki Haruta, Tohru Sato
Pubbl/distr/stampa	Singapore : , : Springer Nature Singapore : , : Imprint : Springer, , 2021
ISBN	981-16-1796-1
Edizione	[1st ed. 2021.]
Descrizione fisica	1 online resource (122 pages)
Collana	SpringerBriefs in Molecular Science, , 2191-5415
Disciplina	541.22
Soggetti	Quantum chemistry Atomic structure Molecular structure Chemical structure Quantum Chemistry Atomic and Molecular Structure and Properties Structure And Bonding
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	1. Introduction: What is understanding chemistry? -- 2. How the chemical processes are qualitatively explained by the simple molecular orbital theory -- 3. How the chemical processes are visualized and quantified by VCD and VCC -- 4. Relationship between Fukui function and VCD -- 5. Transition dipole moment density -- 6. Outlooks for new chemical systems by VCD and VCC -- 7. Appendix.
Sommario/riassunto	This book introduces vibronic coupling density and vibronic coupling constant analyses as a way to understand molecular structure and chemical reactions. After quantum study, the behavior of electrons circulating around nuclei led to the principal concept that underlies all explanations in chemistry. Many textbooks have given plausible explanations to clarify molecular structure—for example, the bond elongation of ethylene under anionization and the nonplanar structure of ammonia. Frontier molecular orbital concepts were proposed to visualize the path of chemical reactions, and conventional explanations gave students a familiarity with molecular structures in terms of the electronic state. By contrast, this book offers a more rational and more

convincing path to understanding. It starts from the ab initio molecular Hamiltonian and provides systematic, rational approaches to comprehend chemical phenomena. In this way, the book leads the reader to a grasp of the quantitative evaluation of the force applied under the molecular deformation process. As well, guidelines are offered for integrating the traditional “hand-waving” approach of chemistry with more rational and general VCD and VCC alternatives along with the outlook for newly functionalized chemical systems.