

1. Record Nr.	UNINA990001106010403321
Autore	Ginzburg, Vitalij Lazarevi <1916-2009>
Titolo	High Temperature Superconductivity / Edited by V.L. Ginzburg and D.A. Kirzhnits ; Translated from russian by A.K. Agyei ; Translation edited by Joseph L. Birman
Pubbl/distr/stampa	New York : Consultants Bureau, 1982
ISBN	0-306-10970-0
Disciplina	537.623
Locazione	FI1
Collocazione	32A-056
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
2. Record Nr.	UNISA996205516503316
Titolo	Byzantion
Pubbl/distr/stampa	Bruxelles, : Fondation Byzantine Boston, : Byzantine Institute of America Louvain, : Peeters
ISSN	2294-6209
Descrizione fisica	1 online resource
Disciplina	949.5
Soggetti	Education Byzantinistiek Byzantijnse kunst Periodicals. Byzantine Empire Study and teaching Periodicals Empire byzantin Étude et enseignement Périodiques Byzantine Empire
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Periodico

Note generali	Refereed/Peer-reviewed Editors: 1924- P. Graindor, H. Grégoire.
Nota di bibliografia	Includes section "Comptes rendus."
Sommario/riassunto	"Revue internationale des études byzantines."
3. Record Nr.	UNINA9910734857503321
Autore	Jenkins Samantha
Titolo	Next Generation Quantum Theory of Atoms in Molecules : From Stereochemistry to Photochemistry and Molecular Devices / / by Samantha Jenkins, Steven Robert Kirk
Pubbl/distr/stampa	Singapore : , : Springer Nature Singapore : , : Imprint : Springer, , 2023
ISBN	981-9903-29-7
Edizione	[1st ed. 2023.]
Descrizione fisica	1 online resource (237 pages)
Collana	Lecture Notes in Chemistry, , 2192-6603 ; ; 110
Disciplina	050
Soggetti	Quantum chemistry Chemistry, Physical and theoretical Chemistry - Data processing Chemical structure Photochemistry Quantum Chemistry Theoretical Chemistry Computational Chemistry Structure And Bonding
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Introduction to Computational Quantum Chemistry -- Exploring the Topological Origins of QTAIM -- Bridging Scalar QTAIM and Vector-Based Next Generation QTAIM -- The NG-QTAIM Interpretation of the Chemical Bond.
Sommario/riassunto	This book begins by providing a simplified version of the computational quantum chemistry sufficient to calculate the

wavefunctions that are the basic input of NG-QTAIM. Enough basic (scalar) QTAIM theory is provided to understand the later chapters. In addition, our developments of scalar QTAIM are presented and activities at various levels of difficulty are provided for the readership to facilitate understanding. The topological origins of Quantum Theory of Atoms in Molecules (QTAIM) before explaining the highlights and consequences of the developments of Next-Generation QTAIM (NG-QTAIM) that is a 3-D vector-based realization of QTAIM. The book compiles all developments and extensions of Next-Generation QTAIM in one place for easy reference for those engaged in theoretical/computational chemistry. Essential insights into molecular switch functioning not available from the energy barrier or any scalar measures are presented along with a new measure to assess the efficiency of rotary molecular motors. The book also discusses how the treatment of external forces such as electric fields and laser irradiation is included in NG-QTAIM. This book benefits theoretical/computational chemists/physics/engineers, students (graduate and undergraduate) and chemical/pharmaceutical industry researchers who carry out chemical computations in universities and industries. Where appropriate, Target Learning Outcomes and Further Reading are provided along with a list of the scientific goals to be addressed in addition to a glossary table in the summary sections. Where applicable each chapter concludes by outlining benefits, limitations and suggestions for further investigations. All our NG-QTAIM publications are available as pre-prints in the form of .pdf files along with the corresponding supplementary materials at our BEACON website www.beaconresearch.org.
