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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 toassess 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.