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Titolo	The quantum theory of atoms in molecules [[electronic resource]] : from solid state to DNA and drug design / / edited by Cherif F. Matta and Russell J. Boyd
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Altri autori (Persone)	MattaCherif F BoydRussell J
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Nota di contenuto	The Quantum Theory of Atoms in Molecules; Foreword; Contents; Preface; List of Abbreviations Appearing in this Volume; List of Contributors; 1 An Introduction to the Quantum Theory of Atoms in Molecules; 1.1 Introduction; 1.2 The Topology of the Electron Density; 1.3 The Topology of the Electron Density Dictates the Form of Atoms in Molecules; 1.4 The Bond and Virial Paths, and the Molecular and Virial Graphs; 1.5 The Atomic Partitioning of Molecular Properties; 1.6 The Nodal Surface in the Laplacian as the Reactive Surface of a Molecule; 1.7 Bond Properties 1.7.1 The Electron Density at the BCP ((b))1.7.2 The Bonded Radius of an Atom ($r(b)$), and the Bond Path Length; 1.7.3 The Laplacian of the Electron Density at the BCP ((2)(b)); 1.7.4 The Bond Ellipticity (); 1.7.5

Energy Densities at the BCP; 1.7.6 Electron Delocalization between Bonded Atoms: A Direct Measure of Bond Order; 1.8 Atomic Properties; 1.8.1 Atomic Electron Population [N()] and Charge [q()]; 1.8.2 Atomic Volume [Vol.()]; 1.8.3 Kinetic Energy [T()]; 1.8.4 Laplacian [L()]; 1.8.5 Total Atomic Energy [E(e())]; 1.8.6 Atomic Dipolar Polarization [()]

1.8.7 Atomic Quadrupolar Polarization [Q()]

1.9 ""Practical"" Uses and Utility of QTAIM Bond and Atomic Properties; 1.9.1 The Use of QTAIM Bond Critical Point Properties; 1.9.2 The Use of QTAIM Atomic Properties; 1.10 Steps of a Typical QTAIM Calculation; References; Part I Advances in Theory; 2 The Lagrangian Approach to Chemistry; 2.1 Introduction; 2.1.1 From Observation, to Physics, to QTAIM; 2.2 The Lagrangian Approach; 2.2.1 What is The Lagrangian Approach and What Does it Do?; 2.2.2 The Lagrangian and the Action Principle - A Return to the Beginnings; 2.2.3 Minimization of the Action

2.2.4 Steps in Minimizing the Action

2.3 The Action Principle in Quantum Mechanics; 2.3.1 Schrodinger's Appeal to the Action; 2.3.2 Schrodinger's Minimization; 2.3.2.1 Two Ways of Expressing the Kinetic Energy; 2.3.3 Obtaining an Atom from Schrodinger's Variation; 2.3.3.1 The Role of Laplacian in the Definition of an Atom; 2.3.4 Getting Chemistry from $G(,;)$; 2.4 From Schrodinger to Schwinger; 2.4.1 From Dirac to Feynman and Schwinger; 2.4.2 From Schwinger to an Atom in a Molecule; 2.5 Molecular Structure and Structural Stability; 2.5.1 Definition of Molecular Structure

2.5.2 Prediction of Structural Stability

2.6 Reflections and the Future; 2.6.1 Reflections; 2.6.2 The Future; References and Notes; 3 Atomic Response Properties; 3.1 Introduction; 3.2 Apparent Origin-dependence of Some Atomic Response Properties; 3.3 Bond Contributions to ""Null"" Molecular Properties; 3.4 Bond Contributions to Atomic Charges in Neutral Molecules; 3.5 Atomic Contributions to Electric Dipole Moments of Neutral Molecules; 3.6 Atomic Contributions to Electric Polarizabilities; 3.7 Atomic Contributions to Vibrational Infrared Absorption Intensities

3.8 Atomic Nuclear Virial Energies

Sommario/riassunto

This book distills the knowledge gained from research into atoms in molecules over the last 10 years into a unique, handy reference. Throughout, the authors address a wide audience, such that this volume may equally be used as a textbook without compromising its research-oriented character. Clearly structured, the text begins with advances in theory before moving on to theoretical studies of chemical bonding and reactivity. There follow separate sections on solid state and surfaces as well as experimental electron densities, before finishing with applications in biological sciences and drug-de

2. Record Nr.	UNINA9910797861603321
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Titolo	A colourful presence : the evolution of women's representation in Iranian cinema / / by Maryam Ghorbankarimi
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Descrizione fisica	1 online resource (221 p.)
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Soggetti	Women in motion pictures Motion pictures - Iran
Lingua di pubblicazione	Inglese
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Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and filmographies.
Sommario/riassunto	This book analyzes the changes in the representation of women in Iranian cinema since the 1960's, and investigates the reasons and motives for this. Iranian cinema, both before and after the Islamic Revolution, has been closely monitored by the ruling power, and has been utilized to relay messages and information that comply with the ruling ideology. However, it was only after the 1979 Revolution and the subsequent legitimization of cinema by the Islamic rule that cinema became widely accessible to the general public. Within this context, this book explores the changing roles of women in film pr