

1. Record Nr.	UNINA9910830885103321
Titolo	Reduced-density-matrix mechanics : with applications to many-electron atoms and molecules / / edited by David A. Mazziotti
Pubbl/distr/stampa	Hoboken, N.J., : Wiley, c2007
ISBN	1-280-82702-5 9786610827022 0-470-10660-3 0-470-10659-X
Descrizione fisica	1 online resource (596 p.)
Collana	Advances in chemical physics ; ; v. 134
Altri autori (Persone)	MazziottiDavid A
Disciplina	541.3 541.305 541/.08
Soggetti	Matrix mechanics Electronic structure
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.es.
Nota di contenuto	REDUCED-DENSITY-MATRIX MECHANICS: WITH APPLICATION TO MANY-ELECTRON ATOMS AND MOLECULES A SPECIAL VOLUME OF ADVANCES IN CHEMICAL PHYSICS VOLUME 134; CONTRIBUTORS TO VOLUME 134; PREFACE; INTRODUCTION; CONTENTS; Part I; CHAPTER 1 N-REPRESENTABILITY; CHAPTER 2 HISTORICAL INTRODUCTION; Part II; CHAPTER 3 VARIATIONAL TWO-ELECTRON REDUCED-DENSITY-MATRIX THEORY; CHAPTER 4 THE LOWER BOUND METHOD FOR DENSITY MATRICES AND SEMIDEFINITE PROGRAMMING; CHAPTER 5 THE T1 AND T2 REPRESENTABILITY CONDITIONS; CHAPTER 6 SEMIDEFINITE PROGRAMMING: FORMULATIONS AND PRIMAL-DUAL INTERIOR-POINT METHODS; Part III CHAPTER 7 THEORY AND METHODOLOGY OF THE CONTRACTED SCHRÖDINGER EQUATIONCHAPTER 8 CONTRACTED SCHRÖDINGER EQUATION; CHAPTER 9 PURIFICATION OF CORRELATED REDUCED DENSITY MATRICES: REVIEW AND APPLICATIONS; CHAPTER 10 CUMULANTS, EXTENSIVITY, AND THE CONNECTED FORMULATION OF THE CONTRACTED SCHRÖDINGER EQUATION; CHAPTER 11

GENERALIZED NORMAL ORDERING, IRREDUCIBLE BRILLOUIN CONDITIONS, AND CONTRACTED SCHRÖDINGER EQUATIONS; CHAPTER 12 ANTI-HERMITIAN FORMULATION OF THE CONTRACTED SCHRÖDINGER THEORY; CHAPTER 13 CANONICAL TRANSFORMATION THEORY FOR DYNAMIC CORRELATIONS IN MULTIREFERENCE PROBLEMS; Part IV
CHAPTER 14 NATURAL ORBITAL FUNCTIONAL THEORYCHAPTER 15 GEMINAL FUNCTIONAL THEORY; CHAPTER 16 LINEAR INEQUALITIES FOR DIAGONAL ELEMENTS OF DENSITY MATRICES; Part V; CHAPTER 17 PARAMETERIZATION OF THE 2-RDM; CHAPTER 18 ENTANGLEMENT, ELECTRON CORRELATION, AND DENSITY MATRICES; AUTHOR INDEX; SUBJECT INDEX

Sommario/riassunto

An up-to-date account of this cutting-edge research in a consistent and understandable framework, of special interest to experts in other areas of electronic structure and/or quantum many-body theory. It will serve equally well as a self-contained guide to learning about reduced density matrices either through self-study or in a classroom as well as an invaluable resource for understanding the critical advancements in the field.
