Record Nr. UNINA9910136542403321 **Titolo** Reviews in computational chemistry . Volume 29 / / edited by Abby L. Parrill and Kenny B. Lipkowitz Pubbl/distr/stampa Hoboken, New Jersey:,: Wiley,, 2016 ©2016 **ISBN** 1-119-15756-0 1-119-15755-2 Descrizione fisica 1 online resource (607 p.) Collana Reviews in Computational Chemistry, , 1069-3599; ; Volume 29 Disciplina 542/.8 Soggetti Chemistry - Data processing Chemistry - Mathematics Electronic books. 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 at the end of each chapters and index. Title Page; Table of Contents; CONTRIBUTORS; PREFACE; Nota di contenuto CONTRIBUTORS TO PREVIOUS VOLUMES; 1 NONCOVALENT INTERACTIONS IN DENSITY FUNCTIONAL THEORY; INTRODUCTION; THEORY BACKGROUND; NONCOVALENT INTERACTIONS IN DFT; PERFORMANCE OF DENSITY FUNCTIONALS FOR NONCOVALENT INTERACTIONS: NONCOVALENT INTERACTIONS IN PERSPECTIVE: ACKNOWLEDGMENTS: REFERENCES: 2 LONG-RANGE INTERPARTICLE INTERACTIONS; INTRODUCTION; THE INTERACTION ENERGY AT LONG RANGE: MOLECULAR QED THEORY: ELECTROSTATIC INTERACTION IN MULTIPOLAR QED; ENERGY TRANSFER; MEDIATION OF RET BY A THIRD **BODY** DISPERSION POTENTIAL BETWEEN A PAIR OF ATOMS OR MOLECULESTRIPLE-DIPOLE DISPERSION POTENTIAL; DISPERSION FORCE INDUCED BY EXTERNAL RADIATION; MACROSCOPIC QED; SUMMARY; REFERENCES; 3 EFFICIENT TRANSITION STATE MODELING USING MOLECULAR MECHANICS FORCE FIELDS FOR THE EVERYDAY CHEMIST: INTRODUCTION: MOLECULAR MECHANICS AND TRANSITION STATE BASICS; GROUND STATE FORCE FIELD TECHNIQUES; TSFF TECHNIQUES; CONCLUSION AND PROSPECTS; REFERENCES; 4 MACHINE LEARNING IN

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