Record Nr. UNINA9910785152103321 Accurate condensed-phase quantum chemistry / / editor, Frederick R. **Titolo** Manby Pubbl/distr/stampa Boca Raton:,: Taylor & Francis,, 2011 **ISBN** 0-429-13424-X 1-4398-0837-6 Descrizione fisica 1 online resource (214 p.) Collana Computation in chemistry Altri autori (Persone) ManbyFrederick R Disciplina 541/.28 Soggetti Quantum chemistry Condensed matter 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. Nota di contenuto Front cover: Contents: Series Preface: Preface: Editor: Contributors: chapter one. Laplace transform second-order Møller-Plesset methods in the atomic orbital basis for periodic systems; chapter two. Density fitting for correlated calculations in periodic systems; chapter three. The method of increments-a wavefunction-based correlation method for extended systems; chapter four. The hierarchical scheme for electron correlation in crystalline solids; chapter five. Electrostatically embedded many-body expansion for large systems chapter six. Electron correlation in solids: Delocalized and localized orbital approacheschapter seven. Ab initio Monte Carlo simulations of liquid water; Back cover The theoretical methods of quantum chemistry have matured to the Sommario/riassunto point that accurate predictions can be made and experiments can be understood for a wide range of important gas-phase phenomena. A large part of this success can be attributed to the maturation of hierarchies of approximation, which allow one to approach very high accuracy, provided that sufficient computational resources are available. Until recently, these hierarchies have not been available in condensed-phase chemistry, but recent advances in the field have now

led to a group of methods that are capable of reaching this goa