1. Record Nr. UNISA990000335250203316

Titolo	Journal of physics. A, Mathematical and general / Institute of Physics
Pubbl/distr/stampa	London : Institute of Physics, 1975-2006
ISSN	0305-4470
Descrizione fisica	v. : ill. ; 25 cm
Disciplina	530.5
Soggetti	Fisica -- Periodici
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Periodico

2. Record Nr. UNINA9910785152103321

Titolo	Accurate condensed-phase quantum chemistry / / editor, Frederick R. 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
Sommario/riassunto	The theoretical methods of quantum chemistry have matured to the 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