

1. Record Nr.	UNINA9910483746803321
Titolo	Basis sets in computational chemistry // Eva Perlt, editor
Pubbl/distr/stampa	Cham, Switzerland : , : Springer, , [2021] ©2021
ISBN	3-030-67262-X
Edizione	[1st ed. 2021.]
Descrizione fisica	1 online resource (VII, 255 p. 86 illus., 64 illus. in color.)
Collana	Lecture notes in chemistry ; ; 107
Disciplina	542.85
Soggetti	Cheminformatics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes index.
Nota di contenuto	An Introduction and Overview of Basis Sets for Molecular and Solid-state Calculations -- Slater-type Orbitals -- Local Orbitals in Quantum Chemistry -- An introduction to discretization error analysis for computational chemists -- Basis Sets for Correlated Methods -- Gaussian Basis Sets for Solid State Calculations -- Basis Sets for Heavy Atoms -- Adaptable Gaussian Bases for Quantum Dynamics of the Nuclei.
Sommario/riassunto	This book addresses the construction and application of the major types of basis sets for computational chemistry calculations. In addition to a general introduction, it includes mathematical basics and a discussion of errors arising from incomplete or inappropriate basis sets. The different chapters introduce local orbitals and orbital localization as well as Slater-type orbitals and review basis sets for special applications, such as those for correlated methods, solid-state calculations, heavy atoms and time-dependent adaptable Gaussian bases for quantum dynamics simulations. This detailed review of the purpose of basis sets, their design, applications, possible problems and available solutions provides graduate students and beginning researchers with information not easily obtained from the available textbooks and offers valuable supporting material for any quantum chemistry or computational chemistry course at the graduate and/or undergraduate level. This book is also useful as a guide for researchers who are new to computational chemistry but are willing to extend their

research tools by applying such methods. .

2. Record Nr.	UNIORUON00383526
Autore	Mengaldo, Pier Vincenzo
Titolo	Attraverso la poesia italiana : analisi di testi esemplari / Pier Vincenzo Mengaldo
Pubbl/distr/stampa	Roma, : Carocci, 2008
ISBN	978-88-430-4630-0
Descrizione fisica	207 p. ; 22 cm.
Disciplina	851.09
Soggetti	POESIA ITALIANA
Lingua di pubblicazione	Italiano
Formato	Materiale a stampa
Livello bibliografico	Monografia