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Autore	Lewars Errol G
Titolo	Computational Chemistry : Introduction to the Theory and Applications of Molecular and Quantum Mechanics // by Errol G. Lewars
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Descrizione fisica	1 online resource (XVI, 728 p. 211 illus., 7 illus. in color.)
Disciplina	541.2
Soggetti	Chemistry, Physical and theoretical Chemometrics Chemical engineering Theoretical and Computational Chemistry Math. Applications in Chemistry Industrial Chemistry/Chemical Engineering
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	1. An Outline of What Computational Chemistry is All About -- 2. The Concept of the Potential Energy Surface -- 3. Molecular Mechanics -- 4. Introduction to Quantum Mechanics in Computational Chemistry -- 5. Ab Initio Calculations -- 6. Semiempirical Calculations -- 7. Density Functional Calculations -- 8. Some "Special" Topics -- 9. Selected Literature Highlights, Books, Websites, Software and Hardware -- Suggested Answers to Harder Questions -- Index.
Sommario/riassunto	This is the third edition of the successful text-reference book that covers computational chemistry. It features changes to the presentation of key concepts and includes revised and new material with several expanded exercises at various levels such as 'harder questions' for those ready to be tested in greater depth - this aspect is absent from other textbooks in the field. Although introductory and assuming no prior knowledge of computational chemistry, it covers the essential aspects of the subject. There are several introductory textbooks on computational chemistry; this one is (as in its previous editions) a unique textbook in the field with copious exercises (and questions) and

solutions with discussions. Noteworthy is the fact that it is the only book at the introductory level that shows in detail yet clearly how matrices are used in one important aspect of computational chemistry. It also serves as an essential guide for researchers, and as a reference book.

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