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Altri autori (Persone)	ReimersJeffrey R
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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	A. DFT : the basic workhorse -- B. Higher-accuracy methods -- C. More-economical methods -- D. Advanced applications.
Sommario/riassunto	"While its results normally complement the information obtained by chemical experiments, computer computations can in some cases predict unobserved chemical phenomena Electronic-Structure Computational Methods for Large Systems gives readers a simple description of modern electronic-structure techniques. It shows what techniques are pertinent for particular problems in biotechnology and nanotechnology and provides a balanced treatment of topics that teach strengths and weaknesses, appropriate and inappropriate methods. It's a book that will enhance the your calculating confidence and improve your ability to predict new effects and solve new problems"-- "Provides a simple description of modern electronic-structure techniques. Shows what techniques are pertinent for particular problems in biotechnology and nanotechnology. Provides a balanced treatment of the topics that teaches strengths and weaknesses,

appropriate and inappropriate methods. Provides confidence to calculators that their results are useful for predicting new effects and for interpreting newly presented problem scenarios - reference tool for industrial scientists who develop applications as well as a teaching aid for new graduate students in computational chemistry, physics, biochemistry, biotechnology, materials science and nanoscience"--
