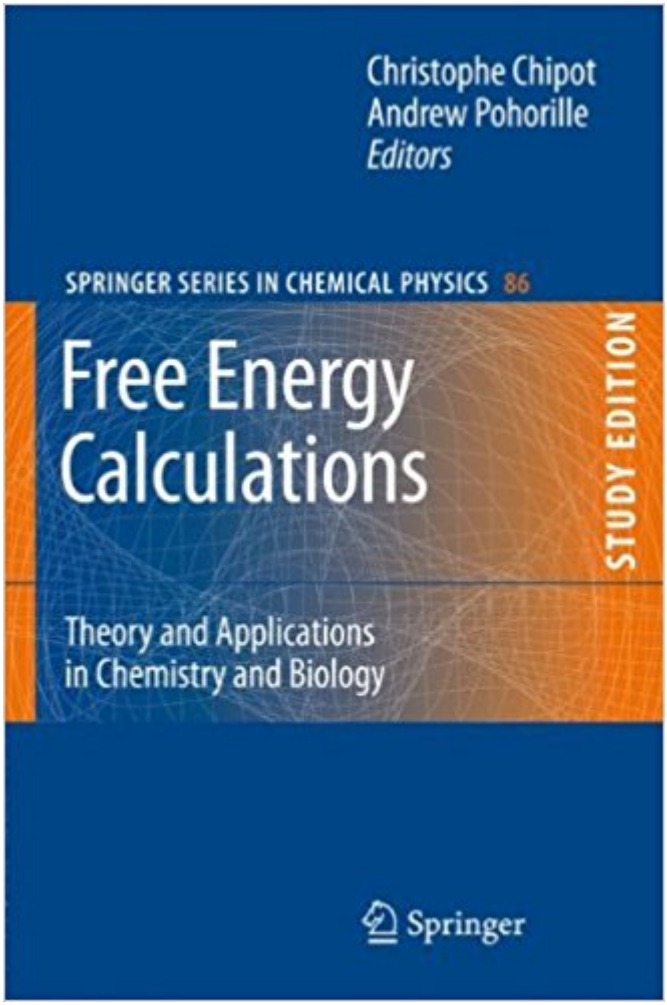
Free Energy Calculations: Theory And Applications In Chemistry And Biology (Springer Series In Chemical Physics)



Synopsis

This volume offers a coherent account of the concepts that underlie different approaches devised for the determination of free energies. It provides insight into the theoretical and computational foundations of the subject and presents relevant applications from molecular-level modeling and simulations of chemical and biological systems. The book is aimed at a broad readership of graduate students and researchers.

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Customer Reviews

From the reviews: "This is a welcome book for computational chemists. Ã¢â ¬Â¦ the book assumes an advanced knowledge of graduate and research-level statistical mechanics. Ã¢â ¬Â¦ The book can be highly recommended to serious practitioners who carry out or plan to carry out, proper liquid-phase simulations of free energy changes or equilibrium constants by the molecular dynamics method." (Donald G. Truhlar, Theoretical Chemistry Accounts, Vol. 121, 2008)

Free energy constitutes the most important thermodynamic quantity to understand how chemical species recognize each other, associate or react. Examples of problems in which knowledge of the underlying free energy behaviour is required, include conformational equilibria and molecular association, partitioning between immiscible liquids, receptor-drug interaction, protein-protein and protein-DNA association, and protein stability. This volume sets out to present a coherent and

comprehensive account of the concepts that underlie different approaches devised for the determination of free energies. The reader will gain the necessary insight into the theoretical and computational foundations of the subject and will be presented with relevant applications from molecular-level modelling and simulations of chemical and biological systems. Both formally accurate and approximate methods are covered using both classical and quantum mechanical descriptions. A central theme of the book is that the wide variety of free energy calculation techniques available today can be understood as different implementations of a few basic principles. The book is aimed at a broad readership of graduate students and researchers having a background in chemistry, physics, engineering and physical biology.

I really enjoyed reading this book---it's a very nice reference on free energy calculation in general, and at the mean time, provides in-depth explanations of specific methods that are commonly used in computational chemistry, i.e., TI, FEP, ABF, Jarzynski.. The one thing I like the most is that the text is very well written. Even though it has quite a lot of statistical mechanics content (and many many equations), it doesn't feel hard to read at all. Overall, I'd highly recommend this book to anyone who wants to learn more about the theory of free energy calculations and the various methods out there.

Free energy calculations have been around for several decades, and are now a field of their own, with its massive literature and a thick jungle of algorithms and implementations. Experienced researchers have to invest a lot of time to keep up to date (not everyone does), and to newcomers, it can be very confusing. Young researchers still use introductory material from the famous books of Allen and Tildesley, and Frenkel and Smit. While very precious, those are now old (especially Allen and Tildesley) and cover many other subjects, so they give little detail about classic techniques and virtually nothing about more recent ones, such as nonequilibrium methods or Wang-Landau sampling.This book brings together a handful of recognized experts from around the globe, who try to sum up the state of the art in free energy calculations in a concise, yet in-depth manner. Newcomers to the field will appreciate the first chapter, which gives an overview and an introduction to essential concepts. The following chapters present the main families of methods in a systematic way, from transition path sampling to simplified methods designed to treat large biological systems efficiently. Depending on each author's style, the chapters have different balances of raw theory and real-world applications. Even authors writing mostly about theory try to keep an eye on practical implications. Beyond the formally exact equations, many chapters put an emphasis on finite

sampling errors and methods to minimize them: in real life, that often makes the difference between free energy calculations that work and those that don't.

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