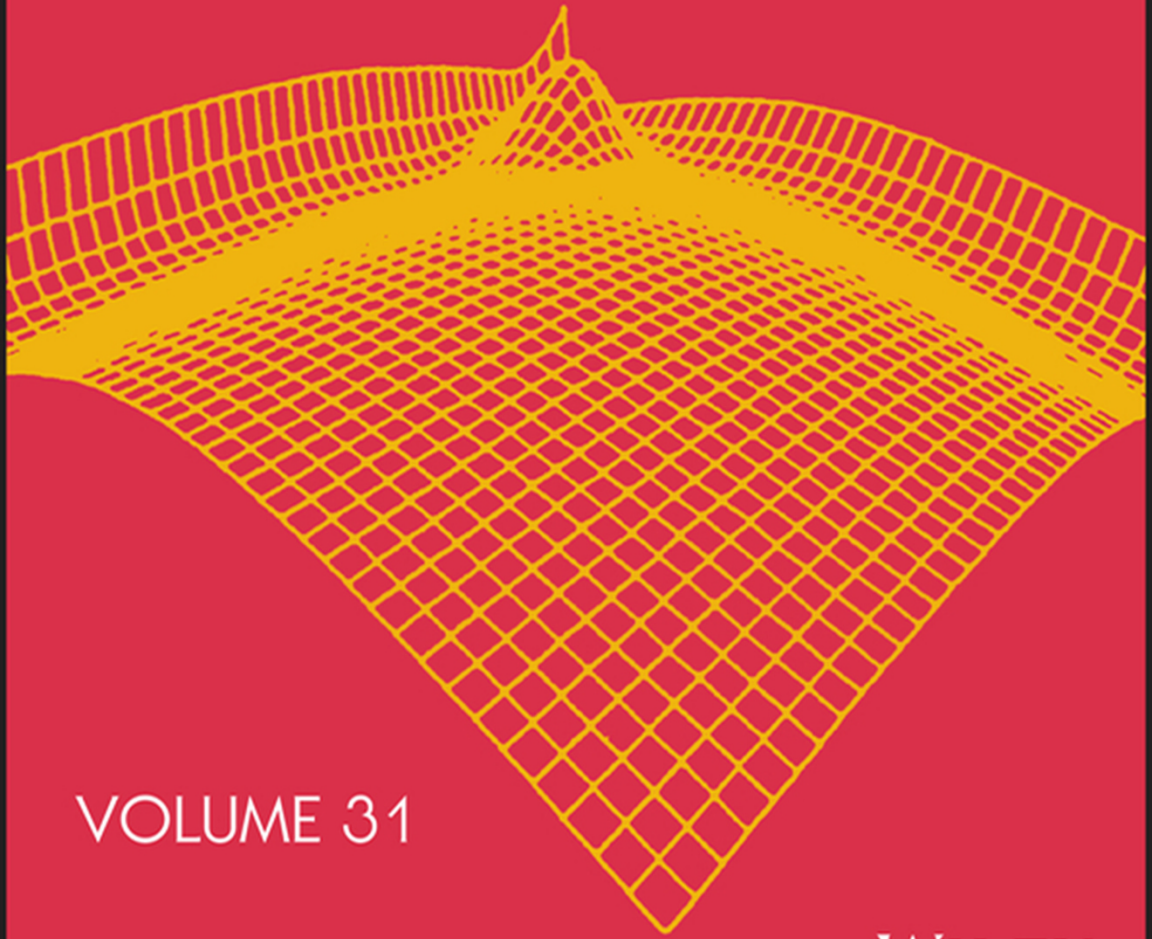
REVIEWS IN COMPUTATIONAL CHEMISTRY

Edited by Abby L. Parrill and Kenny B. Lipkowitz



VOLUME 31

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REVIEWS IN COMPUTATIONAL CHEMISTRY, VOLUME 31

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PREFACE

This book series seeks to aid researchers in selecting and applying new computational chemistry methods to their own research problems. This aim is achieved through tutorial-style chapters that provide both minitutorials for novices and with critical literature reviews highlighting advanced applications. Volume 31 continues this longstanding tradition. While each chapter has a unique focus, two themes connect many of the chapters in this volume, including modeling of soft matter systems such as polymers and proteins in Chapters 1–3, and first-principles methods necessary for modeling chemical reactions in Chapters 4–6.

The focus of the first chapter is on modeling soft matter systems using Lattice Boltzmann Simulations. Soft matter systems include colloidal suspensions, biomaterials, liquid crystals, polymer suspensions, and gels. Such systems are readily deformed by thermal stresses at room temperature, are often liquid systems that show nonlinear flow behavior due to multiple length scales, and therefore offer substantial challenges for theory. The exorbitant number of degrees of freedom in such systems makes atomistic simulations intractable, requiring application of mesoscale modeling methods in order to gain insights into the behaviors of soft matter systems. Ulf Schiller and Olga Kuksenok provide an introduction to the Lattice Boltzmann equation and commonly used Lattice Boltzmann models. This introduction includes advice on parameter choices that must be made when setting up Lattice Boltzmann simulations. Examples of shear flow simulations of colloidal suspensions and nanoparticles as well as simulations of liquid droplets bouncing on a structured surface are used to illustrate applications of the Lattice Boltzmann methods. Recent advances in simulating electrokinetic phenomena and current

challenges for method development, such as modeling fluids with high density ratios, are also identified.

Proteins exhibit complex dynamics and allostery, properties influenced by the highly anisotropic and long-range internal energy transport networks. Chapter 2, by David M. Leitner and Takahisa Yamato, introduces energy flow in macromolecules and how energy transport networks are reflected in low-frequency normal modes and time-correlation functions. Both normal modes and time-correlation functions can be derived from molecular dynamics simulations, thus energy transport networks can be identified from methods already broadly applied to proteins. Two methods for locating energy transport networks in proteins, communication maps and CURrent calculations for Proteins (CURP), are presented with an informative set of example applications. Differences in the nonbonded networks identified using communication maps in a liganded and unliganded example of a homodimeric hemoglobin from Scapharca inaequivalvis (HbI) highlight two regions important in allostery, and allowed modeling of energy dynamics within the protein. The use of CURP to study long-range intramolecular signaling within the photoactive yellow protein (PYP) illustrates the energy transport network that couples ultrafast photoisomerization of a chromophore to initiate partial unfolding at the distant N-terminal cap. Rich areas for additional method development, including practical approaches to quantify energy transport via nonbonded interactions and the need to identify patterns between structure, dynamics, and energy transport close out the chapter.

In any field of science, it is important to design experiments in such a way that the validity and reliability of the results can be assessed. Controls, replicates, repetitions, and other aspects of experimental design provide mechanisms to assess the validity and reliability of experimental results. In Chapter 3, Paul N. Patrone and Andrew Dienstfrey provide a thorough and informative review on uncertainty quantification (UQ) for molecular dynamics simulations, a modeling technique that is most often applied in the study of soft matter systems. Importantly, UQ is presented in the practical sense of providing information on which decisions can be made, not only consisting of confidence intervals for a simulated prediction but also consistency checks to ensure the desired physics are modeled. Methods for uncertainty quantification by inference techniques are presented from the context of the underlying probability theory and statistics. A series of tutorials allow readers to perform uncertainty quantification as part of trajectory analysis, ensemble verification, and glass-transition temperature prediction. These tutorials expose readers to the cost–benefit analysis inherent in committing time and resources appropriate to the importance of the decision to be made. The importance of integrating uncertainty quantification with the specifics of the molecular dynamics simulation is also clearly emphasized.

Chapter 4 begins with an introduction to the properties that must be optimized in the search for better catalysts, extending far past just promotion of the highest reaction rate, but balancing that against additional factors that contribute to overall cost, such as resistance to poisoning, catalyst lifetime, ability to separate

products, heat management, and mass transfer. Horia Metiu, Vishal Agarwal, and Henrik H. Kristoffersen then outline the experimental catalyst screening process with an illustrative example. The chapter continues with a summary of principles, scaling relations, and connections between kinetics and thermodynamics that can dramatically reduce the number of time-consuming first-principles computations that must be performed in order to integrate computational methods into the optimization of catalysts. The factors important to consider in the catalyst development process are then illustrated using a series of industrial catalyst examples. The chapter closes with an important take-home message: computational methods are increasingly important contributors to the catalyst development process, but are not likely to produce ideal catalysts *in silico*, an integrated computational/experimental approach will be required for the foreseeable future.

Richard Dawes and Ernesto Quintas-Sánchez focus on the use of *ab initio* methods to construct potential energy surfaces (PES) that characterize energy variations as a function of geometry for small- to medium-sized molecules (3–10 atoms). PES for such systems will have between 3 and 24 degrees of freedom, and serve as powerful tools to describe chemical phenomena, provided that a representation of the PES with appropriate reduction of dimensionality and requisite accuracy and preservation of symmetry can be constructed and examined. This tutorial/review provides an informative introduction to both the quantum chemistry methods that are used to determine energies for a set of geometric configurations, as well as the fitting process that produces a multidimensional PES from this limited set of configurations. Fitting methods appropriate to the task of PES construction, both interpolative and non-interpolative, are discussed. The use of automated PES construction methods is illustrated with examples. The authors close by reiterating the desirable properties of PES representations, which include high accuracy, correct symmetry properties, rapid evaluations, tailoring to dynamics, and ease of applicability and how these properties should be weighted to match the target use of the resulting PES.

The final chapter in this volume, by Heather Kulik, focuses on modeling mechanochemistry, or the application of mechanical force to induce covalent bond cleavage. Emerging techniques that enable selective mechanochemistry are stimulating the development of computational approaches suitable to better understand the interplay between mechanical force and chemical reactions. Such methods may lead to the design of stress-sensing or self-healing responsive materials. Two theoretical models of mechanochemical bond cleavage are introduced, and the limitations of such models to situations in which the force is applied in a single dimension to a reaction that can be described by a single reaction coordinate are discussed. The first-principles models for mechanochemical bond cleavage that constitute the focus of this chapter have been motivated to address these limitations. The author provides not only the theoretical background for these models, but also provides a set of representative case studies to illustrate their applications, and delineates best practices for mechanochemical simulation.

The value of Reviews in Computational Chemistry stems from the pedagogically-driven reviews that have made this ongoing book series so popular. We are grateful to the authors featured in this volume for continuing the tradition of providing not only comprehensive reviews, but also highlighting best practices and factors to consider in performing similar modeling studies.

Volumes of Reviews in Computational Chemistry are available in an online form through Wiley InterScience. Please consult Wiley Online Library (https://onlinelibrary.wiley.com) or visit www.wiley.com for the latest information.

We thank the authors of this and previous volumes for their excellent chapters.

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