Preface

Calculus of variations is a branch of mathematical analysis that deals with functionals, i.e., algebraic relations mapping functions into real numbers. The original ideas were established by Leonhard Euler in 1733, and since then, variational methods have found widespread applications in science and engineering. A key objective in the calculus of variations is to identify a specific function that minimizes (or maximizes) a given functional. The mathematical procedure is naturally applicable to statistical thermodynamics as demonstrated in the groundbreaking works of J. Willard Gibbs. Today, the maximum entropy principle (MaxEnt), a cornerstone of the so-called Bayesian statistics, is broadly used not only in equilibrium as well as non-equilibrium statistical mechanics but also in pattern recognition and image processing, risk analysis, urban and regional planning, and business financing, just to name a few from a large class of probabilistic problems. Calculus of variations is also useful in both classical and quantum mechanics as shown in the pioneering works of Joseph-Louis Lagrange and in the variational principle for determining the ground states of quantum systems.

This monograph is an exposition of recent applications of variational methods in molecular modeling for thermodynamic systems. While variational principles have been routinely used in both Lagrangian mechanics and the Kohn–Sham density functional theory, their applications to complex molecular systems are rarely discussed in the conventional texts of molecular modeling and statistical mechanics. Instead of describing molecular motions and electronic structures, this book is mostly concerned with the formulation and application of free-energy functionals that connect thermodynamic variables with potential fields or the ensemble averaged atomic, molecular, or particle distributions. Prime examples include classical density functional theory for simple as well as complex fluids, self-consistent-field theories for ionic mixtures and polymer blends, phase-field methods for phase separations and interfacial phenomena, and the Ginzburg-Landau-type theories for molecular self-assembly and order-disorder transitions. In addition, this book covers the applications of variational methods to describing time-dependent phenomena and to solving quantum many-body problems.

To introduce these fascinating topics to a broad audience, each chapter in this book provides a pedagogical overview of variational methods for specific subjects, with the key theoretical results illustrated with tutorial examples. With emphasis placed on physical understanding rather than on rigorous mathematical derivations, this monograph should be accessible to graduate students and researchers in the broad areas of applied mathematics, condensed matter physics, materials science and engineering, chemistry, and chemical and biomolecular engineering without specific training in the calculus of variations.

I am tremendously grateful to all contributors of this monograph for their dedicated work and cooperation in finishing their writings in a timely manner. Preparation of pedagogical materials is not most rewarding in today's academic environment, yet it is very time-consuming to summarize the previous research in particular publications from others. Therefore, I feel especially lucky to have contributions to this book from a cohort of very distinguished authors. I also want to thank all reviewers of this monograph for their careful examination of individual chapters and professional services: Jaydeep P. Bardhan, Northeastern University; Daniel Borgis, École Normale Supérieure; Joachim Dzubiella, Humboldt University; Jian Jiang, California Institute of Technology; Isamu Kusaka, Ohio State University; Yu Liu, East China University of Science and Technology; Umberto M.B. Marconi, University of Camerino; Friederike Schmid, University of Mainz; Cyrus Umrigar, Cornell University; Qiang (David) Wang, Colorado State University; Rik Wensink, University of Paris-Sud XI; Zhenli Xu, Shanghai Jiao Tong University; and Pingwen Zhang, Peking University. Last, but not least, I would like to thank Prof. Edward Maginn, the Chief Editor of this book series, for inviting me to prepare this monograph and Mr. Praveen Kumar, the Springer Project Coordinator, for his considerable help and patience to put things together.

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