

Prelude

Every sentence I utter must be understood not as an affirmation but as a question.

Niels Bohr (1885–1962).

Only rarely does science undergo a dramatic transformation that can be likened to a tectonic rumble, as its character is transfigured under the weights of changing forces. *We are now in such an exciting time.* The discovery of the DNA double helix in the early 1950s prefigured the rise of molecular biology and its many offspring in the next half century, just as the rise of Internet technology in the 1980s and 1990s has molded, and is still reshaping, nearly every aspect of contemporary life. With completion of the first draft of the human genome sequence trumpeting the beginning of the twenty-first century, triumphs in the biological sciences are competing with geopolitics and the economy for prominent-newspaper headlines. The genomic sciences now occupy the center stage, linking basic to applied (medical) research, applied research to commercial success and economic growth, and the biological sciences to the chemical, physical, mathematical and computer sciences.

The subject of this text, molecular modeling, represents a subfield of this successful marriage. In this text, I attempt to draw to the field newcomers from other disciplines and to share basic knowledge in a modern context and interdisciplinary perspective. Though many details on current investigations and projects will undoubtedly become obsolete as soon as this book goes to press, the basic foundations of modeling will remain similar. Over the next decades, we will

surely witness a rapid growth in the field of molecular modeling, as well as many success stories in its application.