Appendix C

Supplementary Course Texts

1. M. P. Allen and D. J. Tildesley. *Computer Simulation of Liquids.* Oxford University Press, New York, NY, 1990.

   [Good advanced reference book for molecular simulations.]

2. A. D. Bates and A. Maxwell. *DNA Topology*, second edition. Oxford University Press, New York, NY, 2005.

   [Beautiful paperback on the higher organizational forms of DNA.]

3. O. M. Becker, A. D. Mackerell Jr., B. Roux, and M. Watanabe, Editors. *Computational Biochemistry and Biophysics*. Marcel Dekker Inc, New York, NY, 2001.

   [Useful resource to computational chemists on various modeling techniques such as molecular mechanics and dynamics, conformational analysis, long-range interactions, implicit solvation, and free energy methods.]

4. J. M. Berg, J. L. Tymoczko, and L. Stryer, *Biochemistry.* W. H. Freeman, New York, NY, latest edition (sixth in May 2006).

   [Wonderful biochemistry textbook, up to date.]

5. H. J. C. Berendsen. *Simulating the Physical World: Hierarchical Modeling from Quantum Mechanics to Fluid Dynamics*. Cambridge University Press, Cambridge, UK, 2007.

   [Introduction to fundamental theory and applications of computer modeling and simulation, from quantum mechanics to fluid dynamics, with practical recommendations and sample Python programs.]

6. V. A. Bloomfield, D. M. Crothers, and I. Tinoco, Jr. *Nucleic Acids: Structures, Properties, and Functions.* University Science Books, Sausalito, CA, 2000.

[Comprehensive account of nucleic acids at an advanced level, with emphasis on biological function and experimental techniques. The first part describes nucleic acid properties on the atomic and molecular levels as deduced by various experimental techniques. The second part presents macromolecular features of nucleic acids in solution (e.g., dynamics behavior, DNA supercoiling). The third part covers noncovalent interactions of nucleic acids and other molecules (ions, drugs, proteins) and higher-order structures due to cellular packing.]

7. C. Branden and J. Tooze. *Introduction to Protein Structure*, second edition. Garland Publishing Inc., New York, NY, 1999. (www.proteinstructure.com/).

    [A modern and nicely illustrated protein structure textbook dealing with basic structural principles (part 1) and other topics (part 2, broadly grouped under the heading of relationships among structure, function, and engineering). Part 2 includes chapters on transcription regulation, signal transduction, immune regulation, membrane and fibrous proteins, and virus structures.]

8. P. Bratley, B. L. Fox, and L. E. Schrage. *A Guide to Simulation*, second edition. Springer, New York, NY, 1987.

    [Good introduction to Monte Carlo simulations.]

9. C. L. Brooks, III, M. Karplus, and B. M. Pettitt. *Proteins: A Theoretical Perspective of Dynamics, Structure, and Thermodynamics.* John Wiley & Sons Inc., New York, NY, 1988.

    [Nice collection on protein simulations.]

10. U. Burkert and N. L. Allinger. *Molecular Mechanics*. American Chemical Society, Washington D.C., 1982.

    [Excellent introduction to molecular mechanics.]

11. C. R. Cantor and P. R. Schimmel. *Biophysical Chemistry.* Parts 1,2,3. W. H. Freeman, San Francisco, CA, 1980.

    [Classic text and reference to many aspects of biophysical chemistry.]

12. D. Chandler. *Introduction to Modern Statistical Mechanics*. Oxford University Press, New York, NY, 1987.

    [Good introduction to Monte Carlo methods.]

13. N. C. Cohen, Editor. *Guidebook on Molecular Modeling in Drug Design.* Academic Press Inc., San Diego, CA, 1996.

    [Reference for molecular modeling as applied to drug design problems, containing contributed chapters by industrial and academic scientists, on problem formulation (database analysis, docking), modeling tools, and medicinal chemistry applications.]

14. C. J. Cramer. *Essentials of Computational Chemistry: Theories and Models*, second edition. John Wiley & Sons Inc., Hoboken, NJ, 2004.

    [Good introduction to quantum mechanical and classical/quantum mechanical modeling and theory.]

15. P. Deuflhard, J. Hermans, B. Leimkuhler, A. E. Mark, S. Reich,. R. D. Skeel, Editors. *Computational Molecular Dynamics: Challenges, Methods, Ideas – Proceedings of the 2nd International Symposium on Algorithms for Macromolecular Modelling, Berlin, May 21-24, 1997*, Lecture Notes in Computational Science and Engineering, Vol. 4 (Series Editors M. Griebel, D. E. Keyes, R. M. Nieminen, D. Roose, and T. Schlick), Springer-Verlag, Berlin, 1999.

    [Collection of articles from invited presentations to the May 1997 Berlin workshop on methods for macromolecular modeling. The book contains sections on the following topics: conformational dynamics, thermodynamic modeling, enhanced time-stepping algorithms, quantum-classical simulations, and parallel force field evaluation.]

16. T. E. Creighton, Editor. *Protein Folding*. W. H. Freeman, New York, NY, 1992.

    [Nice collection on general topics regarding protein structure and folding.]

17. D. Eisenberg and D. Crothers. *Physical Chemistry with Applications to the Life Sciences*. The Benjamin/Cummings Publishing Company Inc., Menlo Park, CA, 1979.

    [Wonderful physical chemistry textbook, with useful biomolecular information.]

18. R. Elber, Editor. *Recent Developments in Theoretical Studies of Proteins*. World Scientific Publishing Company Inc., Singapore, 1996.

    [Six chapters on important topics in protein structure and modeling (e.g., reaction path studies, analytical theories of protein folding, ion channels, and protein structure prediction) by the groups of K. Kuczera, R. Elber, J. Straub, D. Thirumalai, R.S. Eisenberg, and P.G. Wolynes.]

19. A. Fersht. *Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding*. W. H. Freeman, New York, NY, 1999.

    [Comprehensive perspective on both enzyme catalysis and protein folding by a pioneer researcher, an updated version of the author's 1995 text on Enzyme Structure and Mechanism; the text reviews protein structure, emphasizing general principles, as well as mentioning recent advances and insights from theoretical approaches.]

20. M. J. Field. *A Practical Introduction to the Simulation of Molecular Systems*, second edition. Cambridge University Press, Cambridge, UK, 2007.

    [Introduction to simulation techniques, including potential energy calculations, conformational/dynamic/thermodynamic sampling, with program modules in Python.]

21. D. Frenkel and B. Smit. *Understanding Molecular Simulations: From Algorithms to Applications*, second edition. Academic Press, San Diego, CA, 2002.

    [Excellent introduction to computer simulation of molecular systems, containing a nice mix of mathematical details and more informal, descriptive text. The focus is on Monte Carlo and molecular dynamics methodologies, including simple algorithms and numerical illustrations. Some important recent methodological advances are also included.]

22. L. M. Gierasch and J. King, Editors. *Protein Folding: Deciphering the Second Half of the Genetic Code.* AAAS, Washington D.C., 1990.

[Interesting and beautifully illustrated collection of articles; best bet: Jane Richardson's origami analogues of protein folding motifs!]

23. H. Gould, J. Tobochnik, and W. Christian. *An Introduction to Computer Simulation Methods: Applications to Physical Systems,* third edition. Addison Wesley, San Francisco, CA, 2007.

[Good introduction to computer simulations, with a focus on classical mechanics in Part 1 and statistical physics in Part 2. The material is made highly accessible to undergraduates by the inclusion of many simple numerical examples, useful illustrations, and programming segments.]

24. A. Y. Grosberg and A. R. Khokhlov. *Giant Molecules: Here, There, and Everywhere* . . ., second edition. World Scientific Publishing Company, Mountain View, CA, 2009.

[Lively introduction to polymer physics, with nice illustrations and enticing color plates, aptly fitting a beautiful subject. In the format of a coffee-table book, the authors cover important subjects like the wide range of polymeric subjects, ideal chain models and their properties, Brownian motion, biological polymers, and polymer dynamics. An accompanying CD-ROM animates polymer motion, including reptation and coil collapse.]

25. J. M. Haile. *Molecular Dynamics Simulation: Elementary Methods.* John Wiley & Sons, Inc., New York, NY, 1992.

[Elementary text on molecular dynamics.]

26. M. H. Kalos and P. A. Whitlock. *Monte Carlo Methods*, second edition. Wiley-VCH, Weinheim, Germany, 2008.

[Good introduction to Monte Carlo techniques.]

27. A. R. Leach. *Molecular Modelling. Principles and Applications*, second edition. Prentice Hall, Reading, MA, 2001.

[Broad introduction to many aspects of molecular modeling and computational chemistry techniques, covering basic concepts, quantum and molecular mechanics models, techniques for energy minimization, molecular dynamics, Monte Carlo sampling, protein structure prediction, free energies, solvation, and drug design applications.]

28. B. Leimkuhler, C. Chipot, R. Elber, A. Laaksonen, A. Mark, T. Schlick, C. Schütte, R. Skeel, Editors. *New Algorithms for Macromolecular Simulation – Proceedings of the 4th International Workshop on Algorithms for Macromolecular Modeling, Leicester, UK August 2004*, Lecture Notes in Computational Science and Engineering, Vol. 49 (Series Editors T. J. Barth, M. Griebel, D. E. Keyes, R. M. Nieminen, D. Roose, and T. Schlick), Springer-Verlag, Berlin, 2006.

[Collection of articles from presentations at the 2004 international workshop on macromolecular modeling, covering biomolecular simulation methods and applications. The contributions are grouped under the following subjects: macromolecular models: from theories to effective algorithms,

minimization of complex molecular landscapes, dynamical and stochastic-dynamical foundations, free energy computation, fast electrostatics and enhanced solvation models, and quantum-chemical models for macro-molecular simulation.]

29. B. Leimkuhler and S. Reich. *Simulating Hamiltonian Dynamics*. Cambridge Monographs on Applied and Computational Mathematics, Cambridge University Press, Cambridge, UK, 2004.

[Clear exposition of numerical techniques for simulating the dynamics of conservative systems from a mathematical perspective, including various integration methods, with simple molecular applications and good exercises.]

30. K. B. Lipkowitz and D. B. Boyd, Editors *Reviews in Computational Chemistry*. John Wiley & Sons, Inc., New York, NY, 1990 – present.

[Nice series of books, with volumes appearing annually with comprehensive reviews and tutorials on many aspects of computational chemistry.]

31. D. Marx and J. Hutter. *Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods*. Cambridge University Press, Cambridge, UK, 2009.

[Introduction to various ab initio molecular dynamics techniques, including pseudo-code segments and program design.]

32. J. A. McCammon and S. C. Harvey. *Dynamics of Proteins and Nucleic Acids*. Cambridge University Press, Cambridge, UK, 1987.

[First book on biomolecular dynamics simulations. Excellent overview of field.]

33. D. A. McQuarrie. *Statistical Mechanics,* second edition. University Science Books, Sausalito, CA, 2000.

[Good reference text to statistical mechanics.]

34. National Research Council Report. *Mathematical Challenges from Theoretical / Computational Chemistry*. National Academies Press, Washington D.C., 1995. (www.nap.edu/readingroom/books/mctcc/).

[Panel report on the opportunities for collaboration, past achievements, and future possibilities between mathematical and chemical scientists.]

35. P. A. Pevzner. *Computational Molecular Biology: An Algorithmic Approach*. MIT Press, Cambridge, MA, 2000.

[Modern text in computational molecular biology mainly addressed to computer scientists and mathematicians interested in discrete algorithms but accessible to biologists with mathematical grounding. Topics covered include gene hunting, sequencing and mapping, DNA microarray analysis, sequence comparison and alignment, genome evolution, and proteomics.]

36. P. von Ragué Schleyer, Editor-in-Chief, and N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, H. F. Schaefer, III, and P. R. Schreiner, Editors. *Encyclopedia of Computational Chemistry*. John Wiley & Sons Inc., West Sussex, UK, 1998.

[Comprehensive reference series (five large volumes) written by experts in the field.]

37. D. C. Rapaport. *The Art of Molecular Dynamics Simulation*, second edition. Cambridge University Press, Cambridge, UK, 2004.

[Elementary text on molecular dynamics focusing on software details.]

38. W. Saenger. *Principles of Nucleic Acid Structure.* Springer Advanced Texts in Chemistry, Springer-Verlag, New York, NY, 1984.

[Wonderful guide to the richness of DNA structure, with an amazing breadth of topics.]

39. T. Schlick and H. H. Gan, Editors. *Computational Methods for Macromolecules: Challenges and Applications – Proceedings of the 3rd International Workshop on Algorithms for Macromolecular Modeling, New York, October 12–14, 2000*, Lecture Notes in Computational Science and Engineering, Vol. 24 (Series Editors T. J. Barth, M. Griebel, D. E. Keyes, R. M. Nieminen, D. Roose, and T. Schlick), Springer-Verlag, Berlin, 2002.

[Collection of articles from presentations at the 2000 international workshop on macromolecular modeling, covering biomolecular simulation methods and applications. The contributions are grouped under the following subjects: field perspective (preface), biomolecular dynamics applications, molecular dynamics methods, Monte Carlo methods, other conformational sampling approaches, free energy methods, long-range interactions and fast electrostatics, and statistical approaches to protein structures.]

40. R. R. Sinden. *DNA Structure and Function.* Academic Press, San Diego, CA, 1994.

[Nice modern textbook on DNA structure.]

41. T. Schwede and M. Peitsch, Editors. *Computational Structural Biology: Methods and Applications*. World Scientific, Hackensack, NJ, 2008.

[A collection of 27 chapters on structure prediction methods, protein design, drug discovery, new experimental methods, databases, and molecular graphics.]

42. G. E. Schulz and R. H. Schirmer. *Principles of Protein Structure.* Springer Advanced Texts in Chemistry, Springer-Verlag, New York, NY, 1979.

[Nice advanced text on the rapidly-changing field of protein folding.]

43. J. Šponer and F. Lankaš, Editors. *Computational Studies of RNA and DNA*. Challenges and Advances in Computational Chemistry and Physics. Springer, Dordrecht, The Netherlands, 2006.

[A collection of 24 chapters on various aspects of modeling DNA, RNA, and complexes by various computational approaches.]

44. W. R. Taylor and A. Aszódi. *Protein Geometry, Classification, Topology and Symmetry: A Computational Analysis of Structure.* Taylor & Francis Group, New York, NY, 2005.

[Nice introduction to protein structure from a geometric perspective.]

45. W. F. Van Gunsteren and P. K. Weiner, Editors (1989) and W. F. Van Gunsteren, P. K. Weiner, and A. J. Wilkinson, Editors (1993, 1996): *Computer Simulation of Biomolecular Systems: Theoretical and Experimental Applications.* Vol. 1,2,3. Springer-Verlag, New York, NY, 1989, 1993, 1996.

   [Good series on biomolecular simulations, covering both algorithms and applications.]

46. G. A. Voth, Editor. *Coarse-Graining of Condensed Phase and Biomolecular Systems*. Taylor & Francis Group, Boca Raton, FL, 2009.

   [Recent developments in coarse graining modeling of and applications to complex molecular systems, with examples for peptides and proteins at various levels of resolution.]

47. D. Wales. *Energy Landscapes*. Cambridge University Press, Cambridge, UK, 2004.

   [Introduction to energy landscape theory, with applications to clusters, biomolecules and glasses.]

48. A. Warshel. *Computer Simulation of Chemical Reactions in Enzymes and Solutions*. John Wiley & Sons, New York, NY, 1991.

   [Excellent reference text in the field of computational biological chemistry, particularly studies of enzymatic reactions. From basic principles of chemical bonding and enzyme mechanisms, the authors describe the governing force fields for molecular simulations, associated algorithms, various approaches to modeling chemical reactions, and examples of different mechanisms.]

49. Ahmed H. Zewail, Editor. *Physical Biology. From Atoms to Medicine*. Imperial College Press (2008).

   [A collection of 20 chapters that provide a beautiful broad overview into the challenges in our 21st-century biology, including instrumentation and computational advances, protein folding, computer-aided drug discovery, and sampling approaches for biomolecules.]