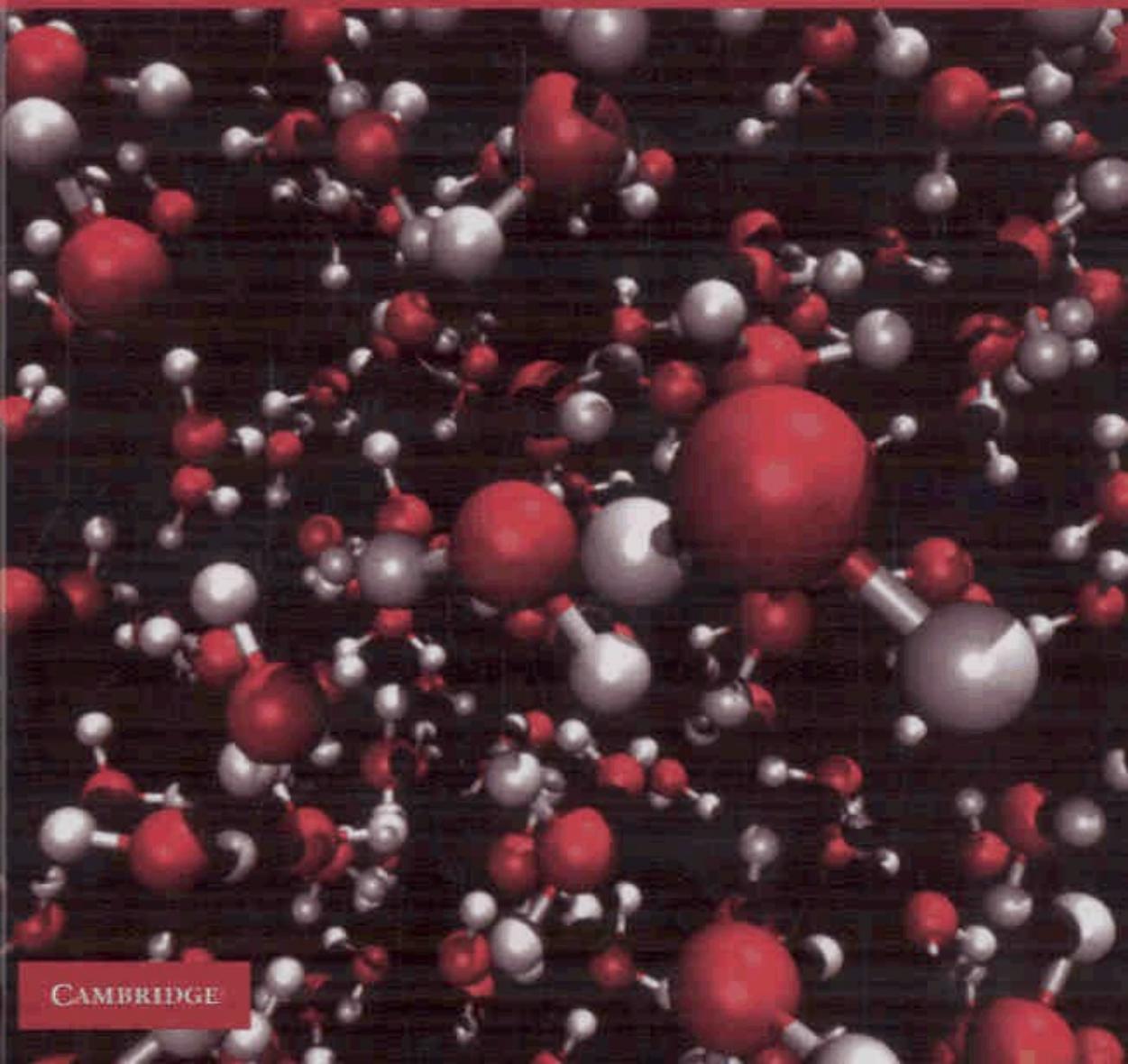


MARTIN J. FIELD

A Practical Introduction to the Simulation of Molecular Systems

SECOND EDITION



CAMBRIDGE

Contents

<i>Preface to the first edition</i>	<i>page</i> ix
<i>Preface to the second edition</i>	xi
1 Preliminaries	1
1.1 Introduction	1
1.2 Python	2
1.3 Object-oriented programming	5
1.4 The pDynamo library	8
1.5 Notation and units	9
2 Chemical models and representations	14
2.1 Introduction	14
2.2 The System class	14
2.3 Example 1	17
2.4 Common molecular representations	18
2.5 Example 2	27
3 Coordinates and coordinate manipulations	31
3.1 Introduction	31
3.2 Connectivity	31
3.3 Internal coordinates	35
3.4 Example 3	38
3.5 Miscellaneous transformations	41
3.6 Superimposing structures	45
3.7 Example 4	47
4 Quantum chemical models	51
4.1 Introduction	51
4.2 The Born–Oppenheimer approximation	51
4.3 Strategies for obtaining energies on a potential energy surface	53

4.4	Molecular orbital methods	54
4.5	The Hartree–Fock approximation	56
4.6	Analysis of the charge density	67
4.7	Example 5	70
4.8	Derivatives of the potential energy	74
4.9	Example 6	78
5	Molecular mechanics	81
5.1	Introduction	81
5.2	Typical empirical energy functions	81
5.3	Calculating a molecular mechanics energy	93
5.4	Example 7	101
5.5	Parametrizing potential energy functions	103
5.6	Soft constraints	105
6	Hybrid potentials	110
6.1	Introduction	110
6.2	Combining QC and MM potentials	110
6.3	Example 8	114
6.4	Covalent bonds between QC and MM atoms	116
6.5	Example 9	120
7	Finding stationary points and reaction paths on potential energy surfaces	122
7.1	Introduction	122
7.2	Exploring potential energy surfaces	122
7.3	Locating minima	126
7.4	Example 10	129
7.5	Locating saddle points	130
7.6	Example 11	134
7.7	Following reaction paths	136
7.8	Example 12	139
7.9	Determining complete reaction paths	140
7.10	Example 13	144
8	Normal mode analysis	148
8.1	Introduction	148
8.2	Calculation of the normal modes	148
8.3	Rotational and translational modes	153
8.4	Generating normal mode trajectories	156
8.5	Example 14	158
8.6	Calculation of thermodynamic quantities	161
8.7	Example 15	165

9 Molecular dynamics simulations I	170
9.1 Introduction	170
9.2 Molecular dynamics	170
9.3 Example 16	178
9.4 Trajectory analysis	182
9.5 Example 17	184
9.6 Simulated annealing	186
9.7 Example 18	189
10 More on non-bonding interactions	195
10.1 Introduction	195
10.2 Cutoff methods for the calculation of non-bonding interactions	195
10.3 Example 19	205
10.4 Including an environment	209
10.5 Periodic boundary conditions	212
10.6 Example 20	215
10.7 Ewald summation techniques	217
10.8 Fast methods for the evaluation of non-bonding interactions	223
11 Molecular dynamics simulations II	225
11.1 Introduction	225
11.2 Analysis of molecular dynamics trajectories	225
11.3 Example 21	233
11.4 Temperature and pressure control in molecular dynamics simulations	235
11.5 Example 22	244
11.6 Calculating free energies: umbrella sampling	246
11.7 Examples 23 and 24	252
11.8 Speeding up simulations	258
12 Monte Carlo simulations	262
12.1 Introduction	262
12.2 The Metropolis Monte Carlo method	262
12.3 Monte Carlo simulations of molecules	266
12.4 Example 25	277
12.5 Calculating free energies: statistical perturbation theory	280
12.6 Example 26	286
Appendix 1 The pDynamo library	294
Appendix 2 Mathematical appendix	298
A2.1 The eigenvalues and eigenvectors of a matrix	298
A2.2 The method of Lagrange multipliers	300

Appendix 3 Solvent boxes and solvated molecules	302
A3.1 Example 27	302
A3.2 Example 28	305
<i>Bibliography</i>	307
<i>Author index</i>	326
<i>Subject index</i>	330