

# Contents

<b>1 Computer Simulation Studies in Condensed Matter Physics: An Introduction</b> <i>D.P. Landau, S.P. Lewis, H.-B. Schüttler</i> .....	1
<hr/>	
<b>Part I Systems out of Equilibrium</b>	
<hr/>	
<b>2 Shake, Rattle or Roll: Things to do with a Granular Mixture on a Computer</b> <i>D.C. Rapaport</i> .....	7
<b>3 A New Method of Investigating Equilibrium Properties from Nonequilibrium Work</b> <i>S. Yukawa</i> .....	19
<b>4 Numerical Simulations of Critical Dynamics far from Equilibrium</b> <i>B. Zheng</i> .....	25
<hr/>	
<b>Part II Soft and Disordered Materials</b>	
<hr/>	
<b>5 Entropy Driven Phase Separation</b> <i>R. Vink</i> .....	45
<b>6 Supercooled Liquids under Shear: Computational Approach</b> <i>R. Yamamoto, R. Temam, J. Dean, D. Grove, C. Chambers, K.B. Bruce, E. Bertino</i> .....	61
<b>7 Optimizing Glasses with Extremal Dynamics</b> <i>S. Boettcher, A.G. Percus</i> .....	74
<b>8 Stochastic Collision Molecular Dynamics Simulations for Ion Transfer Across Liquid–Liquid Interfaces</b> <i>S. Frank, W. Schmickler</i> .....	80

---

**Part III Biological Systems**


---

<b>9 Generalized-Ensemble Simulations of Small Proteins</b>	
<i>U.H.E. Hansmann</i> .....	87
<b>10 A Biological Coevolution Model with Correlated Individual-Based Dynamics</b>	
<i>V. Sevim, P.A. Rikvold</i> .....	90
<b>11 An Image Recognition Algorithm for Automatic Counting of Brain Cells of Fruit Fly</b>	
<i>T. Shimada, K. Kato, K. Ito</i> .....	95
<b>12 Preferred Binding Sites of Gene-Regulatory Proteins Based on the Deterministic Dead-End Elimination Algorithm</b>	
<i>R.G. Endres, T.C. Schulthess, N.S. Wingreen</i> .....	100

---

**Part IV Algorithms and Methods**


---

<b>13 Geometric Cluster Algorithm for Interacting Fluids</b>	
<i>E. Luijten, J. Liu</i> .....	109
<b>14 Polymer Simulations with a Flat Histogram Stochastic Growth Algorithm</b>	
<i>T. Prellberg, J. Krawczyk, A. Rechnitzer</i> .....	122
<b>15 Convergence of the Wang–Landau Algorithm and Statistical Error</b>	
<i>C. Zhou, R.N. Bhatt</i> .....	136
<b>16 Wang–Landau Sampling with Cluster Updates</b>	
<i>M. Körner, M. Troyer</i> .....	142
<b>17 Multibarc-Multithermal Simulations for Lennard–Jones Fluids</b>	
<i>H. Okumura, Y. Okamoto</i> .....	146
<b>18 A Successive Umbrella Sampling Algorithm to Sample and Overcome Free Energy Barriers</b>	
<i>P. Virnau, M. Müller</i> .....	151

---

**Part V Computer Tools**


---

<b>19 C++ and Generic Programming for Rapid Development of Monte Carlo Simulations</b>	
<i>G. Brown, H.K. Lee, T.C. Schulthess</i> .....	157
<b>20 Visualization of Vector Spin Configurations</b>	
<i>R. Hihinashvili, J. Adler, S.-H. Tsai, D.P. Landau</i> .....	169
<b>21 The BlueGene/L Project</b>	
<i>D. Chen</i> .....	174

---

**Part VI Molecules, Clusters and Nanoparticles**


---

<b>22 All-Electron Path Integral Monte Carlo Simulations of Small Atoms and Molecules</b>	
<i>J. Shumway</i> .....	181
<b>23 Projective Dynamics in Realistic Models of Nanomagnets</b>	
<i>S.H. Thompson, G. Brown, P.A. Rikvold</i> .....	196
<b>24 Cumulants for an Ising Model for Folded 1-d Small-World Materials</b>	
<i>M.A. Novotny</i> .....	201
<b>25 Embryonic Forms of Nickel and Palladium: A Molecular Dynamics Computer Simulation</b>	
<i>Z. El-bayyari</i> .....	205

---

**Part VII Surfaces and Alloys**


---

<b>26 Usage of Pattern Recognition Scheme in Kinetic Monte Carlo Simulations: Application to Cluster Diffusion on Cu(111)</b>	
<i>C. Ghosh, A. Kara, T.S. Rahman</i> .....	215
<b>27 Including Long-Range Interactions in Atomistic Modelling of Diffusional Phase Changes</b>	
<i>D.R. Mason, R.E. Rudd, A.P. Sutton</i> .....	241
<b>28 Br Electrodeposition on Au(100): From DFT to Experiment</b>	
<i>S.J. Mitchell, M.T.M. Koper</i> .....	258

<b>29 Simulation of ZnSe, ZnS Coating on CdSe Substrate: The Electronic Structure and Absorption Spectra</b>	
<i>J.S. Kim, S.J. Yun, G.S. Lee</i> .....	265
<b>30 Simulation of Islands and Vacancy Structures for Si/Ge-covered Si(001) Using a Hybrid MC-MD Algorithm</b>	
<i>L. Nurminen, F. Tavazza, D.P. Landau, A. Kuronen, K. Kaski</i> .....	270
<b>31 Spin-Polarons in the FM Kondo Model</b>	
<i>M. Daghofer, W. Koller, A. Prüll, H.G. Evertz, W. von der Linden</i> ...	276
<b>List of Contributors</b> .....	283

Computer Simulation Studies in Condensed-Matter

Physics XVII

Proceedings of the Seventeenth Workshop, Athens, GA,

USA, February 16-20, 2004

Landau, D.P.; Lewis, S.P.; Schüttler, H.-B. (Eds.)

2006, XI, 277 p., Hardcover

ISBN: 978-3-540-26564-1