

## Publication List

1. B. Dünweg and K. Binder, *Model calculations of phase diagrams of magnetic alloys on the body-centered cubic lattice*, Physical Review **B 36**, 6935 (1987).
2. B. Dünweg and K. Binder, *Monte Carlo calculations of phase diagrams of magnetic alloys on the body-centered cubic lattice*, in *Alloy Phase Stability* (G. M. Stocks and A. Gonis, eds.), NATO ASI series E, vol. **163**, Kluwer Academic Publishers, Dordrecht / Boston / London 1989, p. 263.
3. G. S. Grest, B. Dünweg, and K. Kremer, *Vectorized link cell FORTRAN code for molecular dynamics simulations for a large number of particles*, Computer Physics Communications **55**, 269 (1989).
4. B. Dünweg and K. Kremer, *Application of molecular dynamics on polymer systems*, lecture on the 1989 spring school at the Institut für Festkörperforschung, Forschungszentrum Jülich, on “Computer Simulations in Physics” (lecture notes edited by Forschungszentrum Jülich; in German).
5. W. Helbing, B. Dünweg, K. Binder, and D. P. Landau, *Surface-induced disordering at first-order transitions in body-centered cubic binary alloys: A Monte Carlo simulation*, Zeitschrift für Physik **B 80**, 401 (1990).
6. B. Minchau, B. Dünweg, and K. Binder, *Microphase separation transition in block copolymers: A test of Leibler’s theory by Monte Carlo simulation*, Polymer Communications **31**, 348 (1990).
7. K. Kremer, G. S. Grest, and B. Dünweg, *Computer simulations for polymer dynamics*, in *Computer Simulation Studies in Condensed Matter Physics III* (D. P. Landau, K. K. Mon, H.-B. Schüttler, eds.), Springer Proceedings in Physics **53**, Springer-Verlag 1991, p. 85.
8. B. Dünweg, A. Milchev, and P. A. Rikvold, *A model for adsorption of O on Mo(110): Phase transitions with non-universal behavior*, Journal of Chemical Physics **94**, 3958 (1991).
9. B. Dünweg and K. Kremer, *Microscopic verification of dynamic scaling in dilute polymer solutions: A molecular-dynamics simulation*, Physical Review Letters **66**, 2996 (1991).
10. B. Dünweg and W. Paul, *Brownian dynamics simulations without Gaussian random numbers*, International Journal of Modern Physics C (Physics and Computers) **2**, 817 (1991).

11. B. Dünweg and K. Kremer, *Microscopic verification of dynamic scaling in dilute polymer solutions: A molecular-dynamics simulation*, Polymer Preprints **33**, no. 1 (April 1992), p. 675.
12. N. Georgiev, A. Milchev, M. Paunov, and B. Dünweg, *A grand ensemble Monte Carlo study of metal adsorption on a (110) bcc substrate*, Surface Science **264**, 455 (1992); Erratum **275**, 493 (1992).
13. S. Puri and B. Dünweg, *Temporally linear domain growth in the segregation of binary fluids*, Physical Review **A 45**, R6977 (1992).
14. K. Kremer, B. Dünweg, and M. J. Stevens, *Computer simulations for polymer solutions*, Physica **A 194**, 321 (1993).
15. B. Dünweg, *Molecular dynamics algorithms and hydrodynamic screening*, Journal of Chemical Physics **99**, 6977 (1993).
16. B. Dünweg and K. Kremer, *Molecular dynamics simulation of a polymer chain in solution*, Journal of Chemical Physics **99**, 6983 (1993).
17. B. Dünweg and D. P. Landau, *Monte Carlo studies of compositional ordering in binary semiconductors*, in *Computer Aided Innovation of New Materials II* (M. Doyama, J. Kihara, M. Tanaka, and R. Yamamoto, eds.), Elsevier Science Publishers 1993, p. 433.
18. B. Dünweg and D. P. Landau, *Phase diagram and critical behavior of the Si-Ge unmixing transition: A Monte Carlo Study of a model with elastic degrees of freedom*, Physical Review **B 48**, 14182 (1993).
19. B. Dünweg and D. P. Landau, *Monte Carlo studies of unmixing in semiconductor alloys: Effects of elastic degrees of freedom*, in *Alloy Modeling and Design* (G. M. Stocks and P. E. A. Turchi, eds.), TMS Society, Warrendale, PA, 1994, p. 175.
20. B. Dünweg, M. J. Stevens, and K. Kremer, *Structure and dynamics of neutral and charged polymer solutions: Effects of long-range interactions*, in *Monte Carlo and Molecular Dynamics Simulations in Polymer Science* (K. Binder, ed.), Oxford University Press, New York / Oxford 1995, p. 125.
21. B. Dünweg, *Fourier-accelerated polymer dynamics*, in *Computer Simulation Studies in Condensed Matter Physics VII* (D. P. Landau, K. K. Mon, H.-B. Schüttler, eds.), Springer Proceedings in Physics **78**, Springer-Verlag 1994, p. 177.

22. M. Laradji, D. P. Landau, and B. Dünweg, *Structural properties of  $Si_{1-x}Ge_x$  alloys: A Monte Carlo simulation with the Stillinger–Weber potential*, Physical Review **B 51**, 4894 (1995).
23. M. Laradji, D. P. Landau, and B. Dünweg, *A Monte Carlo Simulation of the Stillinger–Weber Model for Si–Ge Alloys*, Material Research Society Symposium Proceedings, Vol. 358, 67–72 (1995).
24. S. Kämmerer, B. Dünweg, K. Binder, and M. d’Onorio De Meo, *Nearest-neighbor Ising antiferromagnet on the fcc lattice: Evidence for multicritical behavior*, Physical Review **B 53**, 2345 (1996).
25. Y. Rouault, B. Dünweg, J. Baschnagel, and K. Binder, *Concentration profile near the surface of polymer mixtures: A Monte Carlo study*, Polymer **37**, 297 (1996).
26. B. O. Peters, B. Dünweg, K. Binder, M. d’Onorio de Meo, and K. Vollmayr, *Finite size scaling in the  $p$ -state mean field Potts glass: Exact statistical mechanics for small samples*, Journal of Physics A: Math. Gen. **29**, 3503 (1996).
27. T. Flebbe, B. Dünweg, and K. Binder, *Phase separation versus wetting: A mean field theory for symmetrical polymer mixtures confined between selectively attractive walls*, Journal de Physique II France **6**, 667 (1996).
28. B. Dünweg, *Simulation of phase transitions: Critical phenomena*, invited lecture at the Euroconference on “Monte Carlo and Molecular Dynamics of Condensed Matter Systems”, Como, July 3–28, 1995, Conference proceedings Vol. 49, edited by K. Binder and G. Ciccotti, Societa Italiana Fisica, Bologna, 1996, p. 215.
29. B. Dünweg, S. Kämmerer, and M. Presber, *Phase diagrams of alloys and adsorbed monolayers: Some recent results*, in *Computer Simulation Studies in Condensed Matter Physics IX* (D. P. Landau, K. K. Mon, H.–B. Schüttler, eds.), Springer Proceedings in Physics **82**, Springer–Verlag 1997, p. 5.
30. B. Dünweg, G. S. Grest, and K. Kremer, *Molecular Dynamics simulations of polymer systems*, in *Numerical Methods for Polymeric Systems* (S. G. Whittington, ed.), IMA Volumes in Mathematics and its Applications **102**, Springer–Verlag 1998, p. 159.
31. A. Kopf, W. Paul, and B. Dünweg, *Multiple time step integrators and momentum conservation*, Computer Physics Communications **101**, 1 (1997).

32. A. Heuer, B. Dünweg, and A. M. Ferrenberg, *Considerations on correlations in shift-register pseudorandom number generators and their removal*, Computer Physics Communications **103**, 1 (1997).
33. A. Kopf, B. Dünweg, and W. Paul, *Dynamics of polymer “isotope” mixtures: Molecular Dynamics simulation and Rouse model analysis*, Journal of Chemical Physics **107**, 6945 (1997).
34. M. Pütz, A. Kolb, and B. Dünweg, *Parallel simulation of polymers on the Cray T3E*, in *Supercomputer 1997* (H.-W. Meuer, ed.), K. G. Saur Verlag München, 1997, p. 94.
35. Ch. Bennemann, W. Paul, K. Binder, and B. Dünweg, *Molecular-dynamics simulations of the thermal glass transition in polymer melts:  $\alpha$ -relaxation behavior*, Physical Review E **57**, 843 (1998).
36. M. Presber, B. Dünweg, and D. P. Landau, *Monte Carlo studies of adsorbed monolayers: Lattice-gas models with translational degrees of freedom*, Physical Review E **58**, 2616 (1998).
37. P. Ahlrichs and B. Dünweg, *Lattice Boltzmann simulation of polymer-solvent systems*, proceedings of the 7th international conference on discrete simulations of fluids, Oxford, July 1998, International Journal of Modern Physics C **9**, 1429 (1998).
38. A. V. Lyulin, B. Dünweg, O. V. Borisov and A. A. Darinskii, *Computer simulation studies of a single polyelectrolyte chain in poor solvent*, Macromolecules **32**, 3264 (1999).
39. A. Kolb and B. Dünweg, *Optimized constant pressure stochastic dynamics*, Journal of Chemical Physics **111**, 4453 (1999).
40. P. Ahlrichs and B. Dünweg, *Simulation of a single polymer chain in solution by combining lattice Boltzmann and Molecular Dynamics*, Journal of Chemical Physics **111**, 8225 (1999).
41. V. Yamakov, A. Milchev, O. V. Borisov and B. Dünweg, *Adsorption of a polyelectrolyte chain on a charged surface: A Monte Carlo simulation of scaling behavior*, Journal of Physics: Condensed Matter **11**, 9907 (1999).
42. V. Yamakov, A. Milchev, H.-J. Limbach, B. Dünweg and R. Everaers, *Conformations of random polyampholytes*, Physical Review Letters **85**, 4305 (2000).

43. A. Bunker and B. Dünweg, *Parallel excluded volume tempering for polymer melts*, Physical Review E **63**, 016701 (2001).
44. P. Ahlrichs, R. Everaers and B. Dünweg, *Screening of hydrodynamic interactions in semidilute polymer solutions: A computer simulation study*, Physical Review E **64**, 040501(R) (2001).
45. B. Dünweg, P. Ahlrichs, and R. Everaers, *Simulation of the dynamics of polymers in solution via a hybrid Molecular Dynamics – lattice Boltzmann scheme*, in *Computer Simulation Studies in Condensed Matter Physics XIV* (D. P. Landau, S. P. Lewis, H.–B. Schüttler, eds.), Springer–Verlag 2001.
46. Th. J. H. Vlugt and B. Dünweg, *Computing phase equilibria by parallel excluded volume tempering*, Journal of Chemical Physics **115**, 8731 (2001).
47. T. Soddemann, B. Dünweg, and K. Kremer, *A generic computer model for amphiphilic systems*, European Physical Journal E **6**, 409 (2001).
48. B. Dünweg, D. Reith, M. Steinhauser, and K. Kremer, *Corrections to scaling in the hydrodynamic properties of dilute polymer solutions*, Journal of Chemical Physics **117**, 914 (2002).
49. B. Liu and B. Dünweg, *Translational diffusion of polymer chains with excluded volume and hydrodynamic interactions by Brownian dynamics simulation*, Journal of Chemical Physics **118**, 8061 (2003).
50. T. Soddemann, B. Dünweg, and K. Kremer, *Dissipative Particle Dynamics: A useful thermostat for equilibrium and nonequilibrium Molecular Dynamics simulations*, Physical Review E **68**, 046702 (2003).
51. B. Dünweg, D. P. Landau, A. Milchev (eds.), *Computer simulations of surfaces and interfaces*, proceedings of the NATO Advanced Study Institute / Euroconference, Albena, Bulgaria, September 2002, Kluwer Academic Publishers, Dordrecht / Boston / London (2003), ISBN 1–4020–1463–5.
52. B. Dünweg, *Langevin methods*, contribution in entry 51, pp. 77–92.
53. B. Dünweg, *Accelerated algorithms 2*, contribution in entry 51, pp. 209–222.
54. D. Andrienko, B. Dünweg, and O. I. Vinogradova, *Boundary slip as a result of a prewetting transition*, Journal of Chemical Physics **119**, 13106 (2003).

55. T. Soddemann, G. K. Auernhammer, H. X. Guo, B. Dünweg, and K. Kremer, *Shear-induced undulations of smectic-A: Molecular Dynamics simulations vs. analytical theory*, European Physical Journal E e2004-00045-0 (2004).
56. V. Lobaskin and B. Dünweg, *A new model for simulating colloidal dynamics*, New Journal of Physics **6**, 54 (2004).
57. B. Dünweg, *Advanced simulations for hydrodynamic problems: Lattice Boltzmann and Dissipative Particle Dynamics*, in *Computational soft matter: From synthetic polymers to proteins*, edited by N. Attig, K. Binder, H. Grubmüller, and K. Kremer, NIC Series Volume 23, ISBN 3-00-012641-4, Jülich 2004.
58. I. Pasichnyk and B. Dünweg, *Coulomb interactions via local dynamics: A molecular-dynamics algorithm*, Journal of Physics: Condensed Matter **16**, S3999 (2004).
59. V. Lobaskin, B. Dünweg, and C. Holm, *Electrophoretic mobility of a charged colloidal particle: A computer simulation study*, Journal of Physics: Condensed Matter **16**, S4063 (2004).
60. J. Yaneva, B. Dünweg, and A. Milchev, *Non-Fickian interdiffusion of dynamically asymmetric species: A molecular dynamics study*, Journal of Chemical Physics **122**, 204105 (2005).
61. B. J. Schulz, B. Dünweg, K. Binder, and M. Müller, *Suppression of capillary wave broadening of interfaces in binary alloys due to elastic interactions*, Physical Review Letters **95**, 096101 (2005).
62. X. L. Zhu, F. Tavazza, D. P. Landau and B. Dünweg, *Critical behavior of an elastic Ising antiferromagnet at constant pressure*, Physical Review B **72**, 104102 (2005).
63. D. P. Landau, B. Dünweg, M. Laradji, F. Tavazza, J. Adler, L. Cannavacciuolo and X. Zhu, *Monte Carlo simulations of compressible Ising models: Do we understand them?*, in “Computer simulations in condensed matter: From materials to chemical biology”, Lecture Notes in Physics **704**, 127 (2006), edited by M. Ferrario, G. Ciccotti and K. Binder, Springer-Verlag 2006.
64. B. Dünweg, *Mesosopic simulations for problems with hydrodynamics, with emphasis on polymer dynamics*, in “Computer simulations in condensed matter: From materials to chemical biology”, Lecture Notes in Physics **704**, 309 (2006), edited by M. Ferrario, G. Ciccotti and K. Binder, Springer-Verlag 2006 (extended and updated version of entry 57).

65. B. Dünweg, *Computer simulations of the dynamics of polymer solutions*, in the proceedings of the conference “Multiscale materials modeling”, P. Gumbsch (ed.), Fraunhofer IRB Verlag, 2006.
66. V. Lobaskin, B. Dünweg, M. Medebach, T. Palberg, and C. Holm, *Electrophoresis of colloidal dispersions in the low-salt regime*, Physical Review Letters **98**, 176105 (2007).
67. B. Dünweg, U. D. Schiller, and A. J. C. Ladd, *Statistical mechanics of the fluctuating lattice Boltzmann equation*, Physical Review E **76**, 036704 (2007).
68. B. Dünweg and A. J. C. Ladd, *Lattice Boltzmann simulations of soft matter systems*, Advances in Polymer Science **221**, 89 (2009).
69. B. Dünweg, V. Lobaskin, K. Seethalakshmy-Hariharan, and C. Holm, *Colloidal electrophoresis: Scaling analysis, Green-Kubo relation, and numerical results*, Journal of Physics: Condensed Matter **20**, 404214 (2008).
70. B. Dünweg, *Computer simulations of the dynamics of polymer solutions*, Journal of Computer–Aided Materials Design **14**, 259 (2007), “official” version of entry 65.
71. B. Dünweg, *Book review on “Elements of Nonequilibrium Statistical Mechanics” by V. Balakrishnan*, Soft Materials **6**, 157 (2008).
72. B. Dünweg, U. D. Schiller, and A. J. C. Ladd, *Progress in the understanding of the fluctuating lattice Boltzmann equation*, Computer Physics Communications **180**, 605 (2009).
73. J. Lee, B. Dünweg, and J. Schumacher, *Multiscale modelling strategy using the lattice Boltzmann method for polymer dynamics in a turbulent flow*, Computers & Mathematics with Applications **59**, 2374 (2010).
74. M. Baptista, R. Schmitz, and B. Dünweg, *Simple and robust solver for the Poisson–Boltzmann equation*, Physical Review E **80**, 016705 (2009).
75. B. Dünweg, *Computer simulations of systems with hydrodynamic interactions: The coupled Molecular Dynamics — lattice Boltzmann approach*, in *Multiscale Simulation Methods in Molecular Sciences*, edited by J. Grotendorst, N. Attig, S. Blügel and D. Marx, NIC Series Volume 42, ISBN 978-3-9810843-8-2, Jülich 2009.

76. Tri T. Pham, Ulf D. Schiller, J. Ravi Prakash, and B. Dünweg, *Implicit and explicit solvent models for the simulation of a single polymer chain in solution: Lattice Boltzmann vs Brownian dynamics*, Journal of Chemical Physics **131**, 164114 (2009).
77. Tri T. Pham, B. Dünweg, and J. Ravi Prakash, *Collapse dynamics of copolymers in a poor solvent: Influence of hydrodynamic interactions and chain sequence*, Macromolecules **43**, 10084 (2010).
78. R. Schmitz, S. Yordanov, H.-J. Butt, K. Koynov, and B. Dünweg, *Studying flow close to an interface by total internal reflection fluorescence cross-correlation spectroscopy: Quantitative data analysis*, Physical Review E **84**, 066306 (2011).