

Bibliography

- [1] W.W. Wood. Early history of computer simulation in statistical mechanics. In G. Ciccotti and W.G. Hoover, editors, *Molecular Dynamics Simulations of Statistical Mechanics Systems*, pages 2–14. Proceedings of the 97th Int. "Enrico Fermi" School of Physics, North Holland, Amsterdam, 1986.
- [2] G. Ciccotti, D. Frenkel, and I.R. McDonald. *Simulation of Liquids and Solids: Molecular Dynamics and Monte Carlo Methods in Statistical Mechanics*. North-Holland, Amsterdam, 1987.
- [3] J.A. Prins. Onze voorstelling omtrent de bouw van de stof. *Physica*, 8:257–268, 1928.
- [4] O.K. Rice. On the statistical mechanics of liquids, and the gas of hard elastic spheres. *J. Chem. Phys.*, 12:1–18, 1944.
- [5] J.D. Bernal. The Bakerian lecture, 1962: The structure of liquids. *Proc. R. Soc.*, 280:299–322, 1964.
- [6] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.N. Teller, and E. Teller. Equation of state calculations by fast computing machines. *J. Chem. Phys.*, 21:1087–1092, 1953.
- [7] N. Metropolis. The beginning of the Monte Carlo method. *Los Alamos Science*, 12:125–130, 1987.
- [8] E. Fermi, J.G. Pasta, and S.M. Ulam. Studies of non-linear problems. LASL Report LA-1940, 1955.
- [9] B.J. Alder and T.E. Wainwright. Molecular dynamics by electronic computers. In I. Prigogine, editor, *Proc. of the Int. Symp. on Statistical Mechanical Theory of Transport Processes (Brussels, 1956)*, pages 97–131. Interscience, Wiley, New York, 1958.
- [10] J.B. Gibson, A.N. Goland, M. Milgram, and G.-H. Vineyard. Dynamics of radiation damage. *Phys. Rev.*, 120:1229–1253, 1960.
- [11] G.-H. Vineyard. Autobiographical remarks of G.-H. Vineyard. In P.C. Gehlen, J.R. Beeler, and R.I. Jaffe, editors, *Interatomic Potentials and Simulation of Lattice Defects*, pages xiii–xvi. Plenum, New York, 1972.
- [12] A. Rahman. Correlations in the motion of atoms in liquid argon. *Phys. Rev.*, 136:A405–A411, 1964.
- [13] L. Verlet. Computer "experiments" on classical fluids. I. Thermodynamical properties of Lennard-Jones molecules. *Phys. Rev.*, 159:98–103, 1967.

- [14] J.A. Barker and R.O. Watts. Structure of water: A Monte Carlo calculation. *Chem. Phys. Lett.*, 3:144–145, 1969.
- [15] I.R. McDonald and K. Singer. Calculation of the thermodynamic properties of liquid argon from Lennard-Jones parameters by a Monte Carlo method. *Discuss. Faraday Soc.*, 43:40–49, 1967.
- [16] P.N. Vorontsov-Vel'yaminov, A.M. El'yashevich, and A.K. Kron. Theoretical investigation of the thermodynamics properties of solutions of strong electrolytes by the Monte Carlo method. *Elektrokhimiya*, 2:708–716, 1966.
- [17] B.J. Alder and T.E. Wainwright. Phase transition for a hard sphere system. *J. Chem. Phys.*, 27:1208–1209, 1957.
- [18] W.W. Wood and J.D. Jacobson. Preliminary results from a recalculation of the Monte Carlo equation of state of hard-spheres. *J. Chem. Phys.*, 27:1207–1208, 1957.
- [19] M.P. Allen and D.J. Tildesley. *Computer Simulation of Liquids*. Clarendon Press, Oxford, 1987.
- [20] J.M. Haile. *Molecular Dynamics Simulations: Elementary Methods*. Wiley, New York, 1992.
- [21] D.P. Landau and K. Binder. *A Guide to Monte Carlo Simulation in Statistical Physics*. Cambridge University Press, Cambridge, 2000.
- [22] D.C. Rapaport. *The Art of Molecular Dynamics Simulation*. Cambridge University Press, Cambridge, 1995.
- [23] M.E.J. Newman and G.T. Barkema. *Monte Carlo Methods in Statistical Physics*. Oxford University Press, Oxford, 1999.
- [24] R.W. Hockney and J.W. Eastwood. *Computer Simulations Using Particles*. McGraw-Hill, New York, 1981.
- [25] W.G. Hoover. *Molecular Dynamics*. Springer, Berlin, 1986.
- [26] W.G. Hoover. *Computational Physics Statistical Mechanics*. Elsevier Sci. Publ., Amsterdam, 1991.
- [27] F.J. Vesely. *Computational Physics. An Introduction*. Plenum, New York, 1994.
- [28] D.W. Heermann. *Computer Simulation Methods in Theoretical Physics*. Springer, Berlin, 1990.
- [29] D.J. Evans and G.P. Morriss. *Statistical Mechanics of Non-Equilibrium Liquids*. Academic Press, London, 1990.
- [30] S.E. Koonin. *Computational Physics*. Benjamin/Cummings, Menlo Park, Calif., 1986.
- [31] H. Gould and J. Tobochnik. *Computer Simulation Methods, Vols. I and II*. Addison-Wesley, Reading, Mass., 1988.
- [32] M.H. Kalos and P.A. Whitlock. *Monte Carlo Methods*. Wiley, New York, 1986.
- [33] W.H. Press, B.P. Flannery, S.A. Teukolsky, and W.T. Vetterling. *Numerical Recipes: The Art of Scientific Computing*. Cambridge University Press, Cambridge, 1986.
- [34] J.P. Valleau and S.G. Whittington. A guide to Monte Carlo simulations for statistical mechanics: 1. Highways. In B.J. Berne, editor, *Statistical Mechanics, Part A*, pages 137–168. Plenum, New York, 1977.

- [35] J.P. Valleau and S.G. Whittington. A guide to Monte Carlo simulations for statistical mechanics: 2. Byways. In B.J. Berne, editor, *Statistical Mechanics, Part A*, pages 169–194. Plenum, New York, 1977.
- [36] K. Binder. *Applications of the Monte Carlo Method in Statistical Physics*. Springer, Berlin, 1984.
- [37] K. Binder. *The Monte Carlo Method in Condensed Matter Physics*. Springer, Berlin, 1992.
- [38] O.G. Mouritsen. *Computer Studies of Phase Transitions and Critical Phenomena*. Springer, Berlin, 1984.
- [39] G. Ciccotti and W.G. Hoover. *Molecular-Dynamics Simulations of Statistical-Mechanical Systems. Proceedings of the 97th International "Enrico Fermi" School of Physics*. North-Holland, Amsterdam, 1986.
- [40] M. Meyer and V. Pontikis. *Proceedings of the NATO ASI on Computer Simulation in Materials Science*. Kluwer, Dordrecht, 1991.
- [41] M.P. Allen and D.J. Tildesley. *Proceedings of the NATO ASI on Computer Simulation in Chemical Physics*. Kluwer, Dordrecht, 1993.
- [42] M. Baus, L.F. Rull, and J.P. Ryckaert. *Observation, Prediction and Simulation of Phase Transitions*. Kluwer, Dordrecht, 1995.
- [43] R. Balian. *From Microphysics to Macrophysics*. Springer, Berlin, 1991.
- [44] L.E. Reichl. *A Modern Course in Statistical Physics*. University of Texas Press, Austin, 1980.
- [45] H. Goldstein. *Classical Mechanics*. Addison-Wesley, Reading, 2nd edition, 1980.
- [46] H.L. Anderson. Scientific uses of the MANIAC. *J. Stat. Phys.*, 43:731–748, 1986.
- [47] N.G. van Kampen. *Stochastic Processes in Physics and Chemistry*. North-Holland, Amsterdam, 1981.
- [48] K.A. Fichtorn and W.H. Weinberg. Theoretical foundations of dynamical Monte Carlo simulations. *J. Chem. Phys.*, 95:1090–1096, 1991.
- [49] W.W. Wood and F.R. Parker. Monte Carlo equation of state of molecular interactions with Lennard-Jones potential. I. A supercritical isotherm at about twice the critical temperature. *J. Chem. Phys.*, 27:720–733, 1957.
- [50] M.J. Mandel. On the properties of a periodic fluid. *J. Stat. Phys.*, 15:299–305, 1976.
- [51] J.G. Powles. The liquid-vapour coexistence line for Lennard-Jones-type fluids. *Physica*, 126A:289–299, 1984.
- [52] B. Smit and D. Frenkel. Vapour-liquid equilibria of the two dimensional Lennard-Jones fluid(s). *J. Chem. Phys.*, 94:5663–5668, 1991.
- [53] B. Smit. Phase diagrams of Lennard-Jones fluids. *J. Chem. Phys.*, 96:8639–8640, 1992.
- [54] V.I. Manousiouthakis and M.W. Deem. Strickt detiled balance is unnecessary in Monte Carlo simulation. *J. Chem. Phys.*, 110:2753–2756, 1999.
- [55] W.G.T. Kranendonk and D. Frenkel. Simulation of the adhesive-hard-sphere model. *Mol. Phys.*, 64:403–424, 1988.
- [56] R.D. Mountain and D. Thirumalai. Quantative measure of efficiency of Monte Carlo simulations. *Physica A*, 210:453–460, 1994.

- [57] F.J. Vesely. Angular Monte Carlo integration using quaternion parameters: A spherical reference potential for CCl_4 . *J. Comp. Phys.*, 47:291–296, 1982.
- [58] M. Fixman. Classical statistical mechanics of constraints: A theorem and application to polymers. *Proc. Natl. Acad. Sci. USA*, 71:3050–3053, 1974.
- [59] G. Ciccotti and J.P. Ryckaert. Molecular dynamics simulation of rigid molecules. *Comp. Phys. Rep.*, 4:345–392, 1986.
- [60] L.R. Dodd, T.D. Boone, and D.N. Theodorou. A concerted rotation algorithm for atomistic Monte Carlo simulation of polymer melts and glasses. *Mol. Phys.*, 78:961–996, 1993.
- [61] J.J. Nicolas, K.E. Gubbins, W.B. Streett, and D.J. Tildesley. Equation of state for the Lennard-Jones fluid. *Mol. Phys.*, 37:1429–1454, 1979.
- [62] J.K. Johnson, J.A. Zollweg, and K.E. Gubbins. The Lennard-Jones equation of state revisited. *Mol. Phys.*, 78:591–618, 1993.
- [63] Z.W. Salsburg and W.W. Wood. Equation of state of classical hard spheres at high density. *J. Chem. Phys.*, 37:798–804, 1962.
- [64] P. Diaconis, S. Holmes, and R.M. Neal. Analysis of a non-reversible Markov chain sampler. Technical Report BU-1385-M, Biometrics Unit, Cornell University, 1997.
- [65] M.A. Miller, L.M. Amon, and W.P. Reinhardt. Should one adjust the maximum step size in a Metropolis Monte Carlo simulation? *Chem. Phys. Lett.*, 331:278–284, 2000.
- [66] G.D. Quinlan and S. Tremaine. On the reliability of gravitational n-body integrations. *Mon. Not. R. Astron. Soc.*, 259:505–518, 1992.
- [67] R.E. Gillilan and K.R. Wilson. Shadowing, rare events, and rubber bands - A variational Verlet algorithm for molecular-dynamics. *J. Chem. Phys.*, 97:1757–1772, 1992.
- [68] S. Toxvaerd. Hamiltonians for discrete dynamics. *Phys. Rev. E*, 50:2271–2274, 1994.
- [69] W.C. Swope, H.C. Andersen, P.H. Berens, and K.R. Wilson. A computer simulation method for the calculation of equilibrium constants for the formation of physical clusters of molecules: Application to small water clusters. *J. Chem. Phys.*, 76:637–649, 1982.
- [70] H.J.C. Berendsen and W.F. van Gunsteren. Practical algorithms for dynamics simulations. In G. Ciccotti and W. G. Hoover, editors, *Molecular Dynamics Simulations of Statistical Mechanics Systems*, pages 43–65. Proceedings of the 97th Int. "Enrico Fermi" School of Physics, North Holland, Amsterdam, 1986.
- [71] M.E. Tuckerman, B.J. Berne, and G.J. Martyna. Reversible multiple time scale molecular dynamics. *J. Chem. Phys.*, 97:1990–2001, 1992.
- [72] J.C. Sexton and D.H. Weingarten. Hamiltonian evolution for the hybrid Monte Carlo algorithm. *Nucl. Phys. B*, 380:665–677, 1992.
- [73] H. Yoshida. Symplectic integrators for hamiltonian systems: Basic theory. In S. Ferraz-Mello, editor, *Chaos, Resonance and Collective Dynamical Phenomena in the Solar System*, pages 407–411. Kluwer, Dordrecht, 1992.
- [74] H. Yoshida. Recent progress in the theory and application of symplectic integrators. *Celest. Mech. Dyn. Astron.*, 56:27–43, 1993.

- [75] P. Saha and S. Tremaine. Symplectic integrators for solar system dynamics. *Astron. J.*, 104:1633–1640, 1992.
- [76] R. Olender and R. Elber. Calculation of classical trajectories with a very large time step: Formalism and numerical examples. *J. Chem. Phys.*, 105:9299–9315, 1996.
- [77] R. Elber, J. Meller, and R. Olender. Stochastic path approach to compute atomically detailed trajectories: Application to the folding of c peptide. *J. Phys. Chem. B*, 103:899–911, 1999.
- [78] L. Onsager and S. Machlup. Fluctuations and irreversible processes. *Phys. Rev.*, 91:1505–1512, 1953.
- [79] J.-P. Hansen and I.R. McDonald. *Theory of Simple Liquids*. Academic Press, London, 2nd edition, 1986.
- [80] J.L. Lebowitz, J.K. Percus, and L. Verlet. Ensemble dependence of fluctuations with application to machine computations. *Phys. Rev.*, 153:250–254, 1967.
- [81] J.-P. Hansen and L. Verlet. Phase transitions of the Lennard-Jones system. *Phys. Rev.*, 184:151–161, 1969.
- [82] A.J.C. Ladd and L.V. Woodcock. Triple-point coexistence properties of the Lennard-Jones system. *Chem. Phys. Lett.*, 51:155–159, 1977.
- [83] A.J.C. Ladd and L.V. Woodcock. Interfacial and co-existence properties of the Lennard-Jones system at the triple point. *Mol. Phys.*, 36:611–619, 1978.
- [84] H. Flyvbjerg and H.G. Petersen. Error estimates on averages of correlated data. *J. Chem. Phys.*, 91:461–466, 1989.
- [85] G.J. Martyna, M.E. Tuckerman, D.J. Tobias, and M.L. Klein. Explicit reversible integrators for extended systems dynamics. *Mol. Phys.*, 87:1117–1157, 1996.
- [86] J. Naghizadeh and S.A. Rice. Kinetic theory of dense fluids. X. measurement and interpretation of self-diffusion in liquid ar, kr, xe and ch₄. *J. Chem. Phys.*, 36:2710–2720, 1962.
- [87] J.J. Erpenbeck and W.W. Wood. Molecular dynamics techniques for hard-core systems. In B.J. Berne, editor, *Statistical Mechanics, Part B*, pages 1–40. Plenum, New York, 1976.
- [88] W.W. Wood. Monte Carlo calculations for hard disks in the isothermal-isobaric ensemble. *J. Chem. Phys.*, 48:415–434, 1968.
- [89] I.R. McDonald. NpT-ensemble Monte Carlo calculations for binary liquid mixtures. *Mol. Phys.*, 23:41–58, 1972.
- [90] R. Najafabadi and S. Yip. Observation of finite-temperature strain transformation (f.c.c. \leftrightarrow b.c.c.) in Monte Carlo simulation of iron. *Scripta Metall.*, 17:1199–1204, 1983.
- [91] G.E. Norman and V.S. Filinov. Investigation of phase transitions by a Monte-Carlo method. *High Temp. (USSR)*, 7:216–222, 1969.
- [92] D.J. Adams. Chemical potential of hard-sphere fluids by Monte Carlo methods. *Mol. Phys.*, 28:1241–1252, 1974.
- [93] M. Creutz. Microcanonical Monte Carlo simulation. *Phys. Rev. Lett.*, 50:1411–1414, 1983.

- [94] A.Z. Panagiotopoulos. Direct determination of phase coexistence properties of fluids by Monte Carlo simulation in a new ensemble. *Mol. Phys.*, 61:813–826, 1987.
- [95] P. Attard. On the density of volume states in the isobaric ensemble. *J. Chem. Phys.*, 103:9884–9885, 1995.
- [96] G.J.M. Koper and H. Reiss. Length scale for the constant pressure ensemble: Application to small systems and relation to einstein fluctuation theory. *J. Chem. Phys.*, 100:422–432, 1996.
- [97] R. Eppinga and D. Frenkel. Monte Carlo study of the isotropic and nematic phases of infinitely thin hard platelets. *Mol. Phys.*, 52:1303–1334, 1984.
- [98] K. Binder. Finite size scaling analysis of Ising model block distribution functions. *Z. Phys. B*, 43:119–140, 1981.
- [99] M. Rovere, D.W. Hermann, and K. Binder. Block density distribution function analyses of two-dimensional Lennard-Jones fluids. *Europhys. Lett.*, 6:585–590, 1988.
- [100] N.B. Wilding and A.D. Bruce. Density fluctuations and field mixing in the critical fluid. *J. Phys.: Condens. Matter*, 4:3087–3108, 1992.
- [101] M. Rovere, P. Nielaba, and K. Binder. Simulation studies of gas-liquid transitions in two dimensions via subsystem-block-density distribution analysis. *Z. Phys.*, 90:215–228, 1993.
- [102] M. Parrinello and A. Rahman. Crystal structure and pair potentials: A molecular-dynamics study. *Phys. Rev. Lett.*, 45:1196–1199, 1980.
- [103] M. Parrinello and A. Rahman. Polymorphic transitions in single crystals: A new molecular dynamics method. *J. Appl. Phys.*, 52:7182–7190, 1981.
- [104] H.C. Andersen. Molecular dynamics at constant pressure and/or temperature. *J. Chem. Phys.*, 72:2384–2393, 1980.
- [105] D.C. Wallace. Thermodynamic theory of stressed crystals and higher-order elastic constants. In H. Ehrenreich, F. Seitz, and D. Turnbull, editors, *Solid State Physics: Advances in Research and Applications*, pages 301–404. Academic Press, New York, 1970.
- [106] D.J. Adams. Grand canonical ensemble Monte Carlo for a Lennard-Jones fluid. *Mol. Phys.*, 29:307–311, 1975.
- [107] D.J. Adams. Calculating the low temperature vapour line by Monte Carlo. *Mol. Phys.*, 32:647–657, 1976.
- [108] D.J. Adams. Calculating the high-temperature vapour line by Monte Carlo. *Mol. Phys.*, 37:211–221, 1979.
- [109] L.A. Rowley, D. Nicholson, and N.G. Parsonage. Monte Carlo grand canonical ensemble calculation in a gas-liquid transition region for 12-6 argon. *J. Comp. Phys.*, 17:401–414, 1975.
- [110] J. Yao, R.A. Greenkorn, and K.C. Chao. Monte Carlo simulation of the grand canonical ensemble. *Mol. Phys.*, 46:587–594, 1982.
- [111] M. Mezei. A cavity-biased (T, V, μ) Monte Carlo method for the computer simulation of fluids. *Mol. Phys.*, 40:901–906, 1980.
- [112] J.P. Valleau and L.K. Cohen. Primitive model electrolytes. I. Grand canonical Monte Carlo computations. *J. Chem. Phys.*, 72:5935–5941, 1980.

- [113] W. van Meegen and I.K. Snook. The grand canonical ensemble Monte Carlo method applied to the electrical double layer. *J. Chem. Phys.*, 73:4656–4662, 1980.
- [114] H.J.F. Stroud, E. Richards, P. Limcharoen, and N.G. Parsonage. Thermodynamic study of the Linde 5A + methane system. *J. Chem. Soc., Faraday Trans. I*, 72:942–954, 1976.
- [115] C.R.A. Catlow. *Modelling of Structure and Reactivity in Zeolites*. Academic Press, London, 1992.
- [116] L.D. Gelb, K.E. Gubbins, R. Radhakrishnan, and M. Sliwinska-Bartkowiak. Phase separation in confined systems. *Rep. Prog. Phys.*, 62:1573–1659, 1999.
- [117] J.L. Soto and A.L. Myers. Monte Carlo studies of adsorption in molecular sieves. *Mol. Phys.*, 42:971–983, 1981.
- [118] G.B. Wood and J.S. Rowlinson. Computer simulations of fluids in zeolite X and Y. *J. Chem. Soc., Faraday Trans. 2*, 85:765–781, 1989.
- [119] S.J. Goodbody, K. Watanabe, D. MacGowan, J.P.R.B. Walton, and N. Quirke. Molecular simulations of methane and butane in silicalite. *J. Chem. Soc., Faraday Trans.*, 87:1951–1958, 1991.
- [120] R.Q. Snurr, R.L. June, A.T. Bell, and D.N. Theodorou. Molecular simulations of methane adsorption in silicalite. *Mol. Sim.*, 8:73–92, 1991.
- [121] F. Karavias and A.L. Myers. Isothermic heat of multicomponent adsorption: Thermodynamics and computer simulations. *Langmuir*, 7:3118–3126, 1991.
- [122] P.R. van Tassel, H.T. Davis, and A.V. McCormick. Open-system Monte Carlo simulations of Xe in NaA. *J. Chem. Phys.*, 98:8919–8929, 1993.
- [123] M.W. Maddox and J.S. Rowlinson. Computer simulation of the adsorption of a fluid mixture in zeolite Y. *J. Chem. Soc. Faraday Trans.*, 89:3619–3621, 1993.
- [124] B. Smit. Simulating the adsorption isotherms of methane, ethane, and propane in the zeolite silicalite. *J. Phys. Chem.*, 99:5597–5603, 1995.
- [125] L.F. Rull, G. Jackson, and B. Smit. The condition of microscopic reversibility in the Gibbs-ensemble Monte Carlo simulations of phase equilibria. *Mol. Phys.*, 85:435–447, 1995.
- [126] S. Nosé. A unified formulation of the constant temperature molecular dynamics method. *J. Chem. Phys.*, 81:511–519, 1984.
- [127] W. Feller. *An Introduction to Probability Theory and Its Applications, Vol I*. Wiley, New York, 1957.
- [128] W. Feller. *An Introduction to Probability Theory and Its Applications, Vol II*. Wiley, New York, 1966.
- [129] H. Tanaka, K. Nakanishi, and N. Watanabe. Constant temperature molecular dynamics calculation on Lennard-Jones fluid and its application to water. *J. Chem. Phys.*, 78:2626–2634, 1983.
- [130] S. Nosé. A molecular dynamics method for simulation in the canonical ensemble. *Mol. Phys.*, 52:255–268, 1984.
- [131] W.G. Hoover. Canonical dynamics: Equilibrium phase-space distributions. *Phys. Rev. A*, 31:1695–1697, 1985.
- [132] W.G. Hoover. Constant pressure equations of motion. *Phys. Rev. A*, 34:2499–2500, 1986.

- [133] S. Nosé. An extension of the canonical ensemble molecular dynamics method. *Mol. Phys.*, 57:187–191, 1986.
- [134] S. Toxvaerd and O.H. Olsen. Canonical molecular dynamics of molecules with internal degrees of freedom. *Ber. Bunsenges. Phys. Chem.*, 94:274–278, 1990.
- [135] M.E. Tuckerman, Yi Liu, G. Ciccotti, and G.J. Martyna. Non-Hamiltonian molecular dynamics: Generalizing Hamilton phase space principles to non-Hamiltonian systems. *J. Chem. Phys.*, 116:1678, 2001.
- [136] G.J. Martyna, M.L. Klein, and M.E. Tuckerman. Nosé-Hoover chains: The canonical ensemble via continuous dynamics. *J. Chem. Phys.*, 97:2635–2645, 1992.
- [137] M.E. Tuckerman and G.J. Martyna. Understanding modern molecular dynamics: Techniques and applications. *J. Phys. Chem. B*, 104:159–178, 2000.
- [138] G.J. Martyna, D.J. Tobias, and M.L. Klein. Constant-pressure molecular-dynamics algorithms. *J. Chem. Phys.*, 101:4177–4189, 1994.
- [139] H.J.C. Berendsen, J.P.M. Postma, W.F. van Gunsteren, A. DiNola, and J.R. Haak. Molecular dynamics with coupling to an external bath. *J. Chem. Phys.*, 81:3684–3690, 1984.
- [140] K. Binder. *Monte Carlo Methods in Statistical Physics*. Springer, Berlin, 1979.
- [141] B.J. Alder and T.E. Wainwright. Phase transition in elastic disks. *Phys. Rev.*, 127:359–361, 1962.
- [142] S. Toxvaerd and E. Praestgaard. Molecular dynamics calculation of the liquid structure up to a solid surface. *J. Chem. Phys.*, 67:5291–5295, 1977.
- [143] J.N. Cape and L.V. Woodcock. Molecular dynamics calculation of phase coexistence properties: The soft-sphere melting transition. *Chem. Phys. Lett.*, 59:271–274, 1978.
- [144] Y. Hiwatari, E. Stoll, and T. Schneider. Molecular-dynamics investigation of solid-liquid coexistence. *J. Chem. Phys.*, 68:3401–3404, 1978.
- [145] A. Ueda, J. Takada, and Y. Hiwatari. Molecular dynamics studies of solid-liquid interface of soft-core model. *J. Phys. Soc. Jpn.*, 50:307–314, 1981.
- [146] A.Z. Panagiotopoulos. Adsorption and capillary condensation of fluids in cylindrical pores by Monte Carlo simulation in the Gibbs ensemble. *Mol. Phys.*, 62:701, 1987.
- [147] A.Z. Panagiotopoulos, N. Quirke, M.R. Stapleton, and D.J. Tildesley. Phase equilibria by simulations in the Gibbs ensemble: Alternative derivation, generalization and application to mixtures and membrane equilibria. *Mol. Phys.*, 63:527–545, 1988.
- [148] B. Smit, Ph. de Smedt, and D. Frenkel. Computer simulations in the Gibbs ensemble. *Mol. Phys.*, 68:931–950, 1989.
- [149] D.A. Kofke. Gibbs-Duhem integration: A new method for direct evaluation of phase coexistence by molecular simulations. *Mol. Phys.*, 78:1331–1336, 1993.
- [150] D.A. Kofke. Direct evaluation of phase coexistence by molecular simulation via integration along the coexistence line. *J. Chem. Phys.*, 98:4149–4162, 1993.
- [151] R. Agrawal and D.A. Kofke. Solid-fluid coexistence for inverse-power potentials. *Phys. Rev. Lett.*, 74:122–125, 1995.

- [152] D.A. Kofke and P.T. Cummings. Quantitative comparison and optimization of methods for evaluating the chemical potential by molecular simulation. *Mol. Phys.*, 92:973–996, 1997.
- [153] S.W. de Leeuw, B. Smit, and C.P. Williams. Molecular dynamics studies of polar/nonpolar fluid mixtures: I. mixtures of Lennard-Jones and Stockmayer fluids. *J. Chem. Phys.*, 93:2704–2719, 1990.
- [154] J.G. Kirkwood. Statistical mechanics of fluid mixtures. *J. Chem. Phys.*, 3:300–313, 1935.
- [155] E.J. Meijer, D. Frenkel, R.A. LeSar, and A.J.C. Ladd. Location of melting point at 300 K of nitrogen by Monte Carlo simulation. *J. Chem. Phys.*, 92:7570–7575, 1990.
- [156] D. Frenkel. Free energy computations and first order phase transitions. In G. Ciccotti and W.G. Hoover, editors, *Molecular Dynamics Simulations of Statistical Mechanics Systems*, pages 151–188. Proceedings of the 97th Int. "Enrico Fermi" School of Physics, North Holland, Amsterdam, 1986.
- [157] E.J. Meijer and D. Frenkel. Melting line of Yukawa system by computer simulation. *J. Chem. Phys.*, 94:2269–2271, 1991.
- [158] D. Frenkel and B.M. Mulder. The hard ellipsoid-of-revolution fluid I. Monte Carlo simulations. *Mol. Phys.*, 55:1171–1192, 1985.
- [159] A. Stroobants, H.N.W. Lekkerkerker, and D. Frenkel. Evidence for one-, two-, and three-dimensional order in a system of hard parallel spherocylinders. *Phys. Rev. A*, 36:2929–2945, 1987.
- [160] D. Frenkel, H.N.W. Lekkerkerker, and A. Stroobants. Thermodynamic stability of a smectic phase in a system of hard rods. *Nature*, 332:822–823, 1988.
- [161] J.A.C. Veerman and D. Frenkel. Phase diagram of a system of hard spherocylinders by computer simulation. *Phys. Rev. A*, 41:3237–3244, 1990.
- [162] J.A.C. Veerman and D. Frenkel. Relative stability of columnar crystalline phases in a system of parallel hard spherocylinders. *Phys. Rev. A*, 43:4334–4343, 1991.
- [163] J.A.C. Veerman and D. Frenkel. Phase behaviour of disklike hard-core mesogens. *Phys. Rev. A*, 45:5632–5648, 1992.
- [164] W.G.T. Kranendonk and D. Frenkel. Computer simulation of solid-liquid coexistence in binary hard-sphere mixtures. *Mol. Phys.*, 72:679–697, 1991.
- [165] W.G.T. Kranendonk and D. Frenkel. Free energy calculations for solid solutions by computer simulations. *Mol. Phys.*, 72:715–733, 1991.
- [166] M.D. Eldridge, P.A. Madden, and D. Frenkel. Entropy-driven formation of a superlattice in a hard-sphere binary mixture. *Nature*, 365:35–37, 1993.
- [167] M.D. Eldridge, P.A. Madden, and D. Frenkel. The stability of the AB₁₃ crystal in a binary hard sphere system. *Mol. Phys.*, 79:105–120, 1993.
- [168] M.D. Eldridge, P.A. Madden, and D. Frenkel. A computer investigation into the stability of the AB₂ superlattice in a binary hard sphere system. *Mol. Phys.*, 80:987–995, 1993.
- [169] W.F. van Gunsteren, P.K. Weiner, and A. J. Wilkinson. *Computer Simulation of Biomolecular Systems: Theoretical and Experimental Applications*. Escom, Leiden, 1993.

- [170] M. Watanabe and W.P. Reinhardt. Direct dynamical calculation of entropy and free energy by adiabatic switching. *Phys. Rev. Lett.*, 65:3301–3304, 1990.
- [171] T.P. Straatsma, H.J.C. Berendsen, and J.P.M. Postma. Free energy of hydrophobic hydration: A molecular dynamics study of noble gases in water. *J. Chem. Phys.*, 85:6720–6727, 1986.
- [172] B. Widom. Some topics in the theory of fluids. *J. Chem. Phys.*, 39:2802–2812, 1963.
- [173] B. Widom. Structure of interfaces from uniformity of the chemical potential. *J. Stat. Phys.*, 19:563–574, 1978.
- [174] K.S. Shing. Infinite-dilution activity coefficients from computer simulation. *Chem. Phys. Lett.*, 119:149–151, 1985.
- [175] P. Sindzingre, G. Ciccotti, C. Massobrio, and D. Frenkel. Partial enthalpies and related quantities in mixtures from computer simulation. *Chem. Phys. Lett.*, 136:35–41, 1987.
- [176] R. Lustig. Statistical mechanics in the classical molecular dynamics ensemble. I. Fundamentals. *J. Chem. Phys.*, 101:3048–3059, 1994.
- [177] R. Lustig. Statistical thermodynamics in the classical molecular dynamics ensemble. II. Application to computer simulation. *J. Chem. Phys.*, 101:3060–3067, 1994.
- [178] U. Heinbruch and J. Fischer. On the application of Widom's test particle method to homogeneous and inhomogeneous fluids. *Mol. Sim.*, 1:109–120, 1987.
- [179] J.I. Siepmann, I.R. McDonald, and D. Frenkel. Finite-size corrections to the chemical potential. *J. Phys.: Condens. Matter*, 4:679–691, 1992.
- [180] K. Shing and S.T. Chung. Computer simulation methods for the calculation of the solubility in supercritical extraction systems. *J. Phys. Chem.*, 91:1674–1681, 1987.
- [181] P. Sindzingre, C. Massobrio, G. Ciccotti, and D. Frenkel. Calculation of partial enthalpies of an argon-krypton mixture by NPT molecular dynamics. *Chem. Phys.*, 129:213–224, 1989.
- [182] K.S. Shing and K.E. Gubbins. Free energy and vapour-liquid equilibria for a quadrupolar Lennard-Jones fluid. *Mol. Phys.*, 46:1109–1128, 1982.
- [183] K.S. Shing and K.E. Gubbins. The chemical potential in non-ideal liquid mixtures: Computer simulation and theory. *Mol. Phys.*, 49:1121–1138, 1983.
- [184] C.H. Bennett. Efficient estimation of free energy differences from Monte Carlo data. *J. Comp. Phys.*, 22:245–268, 1976.
- [185] A.M. Ferrenberg and R.H. Swendsen. Optimized Monte Carlo data analysis. *Phys. Rev. Lett.*, 63:1195–1198, 1989.
- [186] G.M. Torrie and J.P. Valleau. Nonphysical sampling distributions in Monte Carlo free-energy estimation: Umbrella sampling. *J. Comp. Phys.*, 23:187–199, 1977.
- [187] D. Chandler. *An Introduction to Modern Statistical Mechanics*. Oxford University Press, New York, 1987.
- [188] J.P. Valleau. Density-scaling: A new Monte Carlo technique in statistical mechanics. *J. Comp. Phys.*, 96:193–216, 1991.

- [189] J.P. Valleau. Monte Carlo: Choosing which game to play. In M. Meyer and V. Pontikis, editors, *Proceedings of the NATO ASI on Computer Simulation in Materials Science*, pages 67–84. Kluwer, Dordrecht, 1991.
- [190] J.P. Valleau. Density-scaling Monte Carlo study of subcritical Lennard-Jonesium. *J. Chem. Phys.*, 99:4718–4728, 1977.
- [191] I.R. McDonald and K. Singer. Machine calculation of thermodynamic properties of a simple fluid at supercritical temperatures. *J. Chem. Phys.*, 47:4766–4772, 1967.
- [192] I.R. McDonald and K. Singer. Examination of the adequacy of the 12-6 potential for liquid argon by means of Monte Carlo calculations. *J. Chem. Phys.*, 50:2308–2315, 1969.
- [193] C. Jarzynski. Non-equilibrium equality for free energy differences. *Phys. Rev. Lett.*, 78:2690–2693, 1997.
- [194] C. Jarzynski. Equilibrium free-energy differences from non-equilibrium measurements: A master-equation approach. *Phys. Rev. E*, 56:5018–5035, 1997.
- [195] G.E. Crooks. Non-equilibrium measurements of free energy differences for microscopically reversible markovian systems. *J. Stat. Phys.*, 90:1480–1487, 1997.
- [196] G.E. Crooks. Entropy production fluctuation theorem and the non-equilibrium work relation for free-energy differences. *Phys. Rev. E*, 60:2721–2726, 1999.
- [197] G.E. Crooks. Path-ensemble averages in systems driven far from equilibrium. *Phys. Rev. E*, 61:2361–2366, 2000.
- [198] D.A. Kofke and E.D. Glandt. Monte Carlo simulation of multicomponent equilibria in a semigrand canonical ensemble. *Mol. Phys.*, 64:1105–1131, 1988.
- [199] P. Tilwani and D. Wu. Direct simulation of phase coexistence in solids using the Gibbs ensemble: Configuration annealing Monte Carlo. Master's thesis, Department of Chemical Engineering, Colorado School of Mines, Golden, Colorado, USA, 1999.
- [200] P.G. Bolhuis and D. Frenkel. Prediction of an expanded-to-condensed transition in colloidal crystals. *Phys. Rev. Lett.*, 72:2211–2214, 1994.
- [201] A.Z. Panagiotopoulos. Direct determination of fluid phase equilibria by simulation in the Gibbs ensemble: A review. *Mol. Sim.*, 9:1–23, 1992.
- [202] D. Frenkel. Monte Carlo simulations. In C.R.A. Catlow, editor, *Computer Modelling of Fluids, Polymers and Solids*. NATO ASI, Kluwer, Dordrecht, 1990.
- [203] B. Smit and D. Frenkel. Calculation of the chemical potential in the Gibbs ensemble. *Mol. Phys.*, 68:951–958, 1989.
- [204] A. Lofti, J. Vrabec, and J. Fischer. Vapour liquid equilibria of the Lennard-Jones fluid from the NPT plus test particle method. *Mol. Phys.*, 76:1319–1333, 1992.
- [205] B. Smit. *Computer Simulation of Phase Coexistence: from Atoms to Surfactants*. Ph.D. thesis, Rijksuniversiteit Utrecht, The Netherlands, 1990.
- [206] J.S. Rowlinson and F.L. Swinton. *Liquids and Liquid Mixtures*. 3rd edn. Butterworth, London, 1982.
- [207] J.S. Rowlinson and B. Widom. *Molecular Theory of Capillarity*. Clarendon Press, Oxford, 1982.

- [208] A.Z. Panagiotopoulos. Molecular simulations of phase coexistence: Finite-size effects and the determination of critical parameters for two- and three dimensional Lennard-Jones fluids. *Int. J. Thermophys.*, 15:1057–1072, 1994.
- [209] M. Rovere, D.W. Hermann, and K. Binder. The gas-liquid transition of the two-dimensional Lennard-Jones fluid. *J. Phys.: Condens. Matter*, 2:7009–7032, 1990.
- [210] K.K. Mon and K. Binder. Finite size effects for the simulation of phase coexistence in the Gibbs ensemble near the critical point. *J. Chem. Phys.*, 96:6989–6995, 1992.
- [211] J.R. Recht and A.Z. Panagiotopoulos. Finite-size effects and approach to criticality in Gibbs ensemble simulations. *Mol. Phys.*, 80:843–852, 1993.
- [212] E. de Miguel, E. Martin del Rio, and M.M. Telo da Gama. Liquid-liquid phase equilibria of symmetrical mixtures by simulation in the semi-grand canonical ensemble. *J. Chem. Phys.*, 103:6188–6196, 1995.
- [213] A.Z. Panagiotopoulos. Molecular simulation of phase equilibria. In E. Kiran and J.M.H. Levelt Sengers, editors, *Supercritical Fluids: Fundamentals for Applications*, pages 411–437. NATO ASI, Kluwer, Dordrecht, 1994.
- [214] A.Z. Panagiotopoulos. Gibbs ensemble techniques. In M. Bauss *et al*, editor, *Observation, Prediction, and Simulation of Phase Transitions in Complex Fluids*, pages 463–501. NATO ASI, Kluwer, Dordrecht, 1995.
- [215] G.L. Deitrick, L.E. Scriven, and H.T. Davis. Efficient molecular simulation of chemical potentials. *J. Chem. Phys.*, 90:2370, 1989.
- [216] M.R. Stapleton and A.Z. Panagiotopoulos. Application of the excluded volume map sampling to phase equilibrium calculations in the Gibbs ensemble. *J. Chem. Phys.*, 92:1285–1293, 1990.
- [217] A.Z. Panagiotopoulos. Molecular simulation of phase equilibria: Simple, ionic and polymeric fluids. *Fluid Phase Equilibria*, 76:97–112, 1992.
- [218] J.P. Valleau. The Coulombic phase transition: Density-scaling Monte Carlo. *J. Chem. Phys.*, 95:584–589, 1991.
- [219] B. Smit, C.P. Williams, E.M. Hendriks, and S.W. de Leeuw. Vapour-liquid equilibria for Stockmayer fluids. *Mol. Phys.*, 68:765–769, 1989.
- [220] M.E. van Leeuwen, B. Smit, and E.M. Hendriks. Vapour-liquid equilibria of stockmayer fluids: computer simulations and perturbation theory. *Mol. Phys.*, 78:271–283, 1993.
- [221] P.G. de Gennes and P.G. Pincus. Pair correlations in a ferromagnetic colloid. *Phys. kondens. Materie*, 11:189–198, 1970.
- [222] V.I. Kalikmanov. Statistical thermodynamics of ferrofluids. *Physica A*, 183:25–50, 1992.
- [223] G.S. Rushbrooke, G. Stell, and J.S. Hoyer. Theory of polar liquids I. Dipolar hard spheres. *Mol. Phys.*, 26:1199–1215, 1973.
- [224] K.-C. Ng, J.P. Valleau, G.M. Torrie, and G.N. Patey. Liquid-vapour co-existence of dipolar hard spheres. *Mol. Phys.*, 38:781–788, 1979.
- [225] J.-M. Caillol. Search of the gas-liquid transition of dipolar hard spheres. *J. Chem. Phys.*, 98:9835–9849, 1993.

- [226] M.E. van Leeuwen and B. Smit. What makes a polar fluid a liquid? *Phys. Rev. Lett.*, 71:3991–3994, 1993.
- [227] J.J. Weis and D. Levesque. Chain formation in low density dipolar hard spheres: A Monte Carlo study. *Phys. Rev. Lett.*, 71:2729–2732, 1993.
- [228] P.J. Camp, J.C. Shelley, and G.N. Patey. Isotropic fluid phases of dipolar hard spheres. *Phys. Rev. Lett.*, 84:115–118, 2000.
- [229] T. Tlusty and S.A. Safran. Defect-induced phase separation in dipolar fluids. *Science*, 290:1328–1331, 2000.
- [230] M.E. van Leeuwen, C.J. Peter, J de Swaan Arons, and A.Z. Panagiotopoulos. Investigation of the transition to liquid-liquid immiscibility for Lennard-Jones (12,6) systems, using the Gibbs-ensemble molecular simulations. *Fluid Phase Equilibria*, 66:57–75, 1991.
- [231] V.I. Harismiadis, N.K. Koutras, D.P. Tassios, and A.Z. Panagiotopoulos. How good is conformal solution theory for phase equilibrium predictions. *Fluid Phase Equilibria*, 65:1–18, 1991.
- [232] A.Z. Panagiotopoulos. Exact calculations of fluid-phase equilibria by Monte Carlo simulations in a new ensemble. *Int. J. Thermophys.*, 10:447, 1989.
- [233] J.G. Amar. Application of the Gibbs ensemble to the study of fluid-fluid phase equilibria in a binary mixture of symmetric non-additive hard-spheres. *Mol. Phys.*, 4:739–745, 1989.
- [234] R.D. Mountain and A.H. Harvey. Computer simulation of fluid-fluid phase equilibria in mixtures of non-additive soft disks. *J. Chem. Phys.*, 94:2238–2243, 1991.
- [235] K.S. Shing. Infinite-dilution activity coefficients of quadrupolar Lennard-Jones mixtures from computer simulation. *J. Chem. Phys.*, 85:4633–4637, 1986.
- [236] W.G.T. Kranendonk and D. Frenkel. Thermodynamic properties of binary hard sphere mixtures. *Mol. Phys.*, 72:699–713, 1991.
- [237] J.K. Johnson, A.Z. Panagiotopoulos, and K.E. Gubbins. Reactive canonical Monte Carlo: A new simulation technique for reacting or associating fluids. *Mol. Phys.*, 81:717–733, 1994.
- [238] W.R. Smith and B. Triska. The reaction ensemble method for the computer simulation of chemical and phase equilibria. I. Theory and basic examples. *Macromol. Symp.*, 81:343–354, 1994.
- [239] M.R. Stapleton, D.J. Tildesley, and N. Quirke. Phase equilibria in polydisperse fluids. *J. Chem. Phys.*, 92:4456–4467, 1990.
- [240] R. Agrawal and D.A. Kofke. Thermodynamic and structural properties of model systems at solid-fluid coexistence: II. Melting and sublimation of the Lennard-Jones system. *Mol. Phys.*, 85:43–59, 1995.
- [241] M.H.J. Hagen, E.J. Meijer, G.C.A.M. Mooij, D. Frenkel, and H.N.W. Lekkerkerker. Does C_{60} have a liquid phase? *Nature*, 365:425–426, 1993.
- [242] E.J. Meijer and D. Frenkel. Colloids dispersed in polymer solution. A computer simulation study. *J. Chem. Phys.*, 100:6873–6887, 1994.
- [243] W.O. Haag. Catalysis by zeolites—science and technology. In J. Weitkamp, H.G. Karge, H. Pfeifer, and W. Hölderich, editors, *Zeolites and Related Microp-*

- orous Materials: State of the Art 1994, volume 84, pages 1375–1394. Studies in Surface Science and Catalysis, Elsevier, Amsterdam, 1994.
- [244] P.G. Bolhuis, M.H.J. Hagen, and D. Frenkel. Isostructural solid-solid transition in crystalline systems with short-ranged interactions. *Phys. Rev. E*, 50:4880–4890, 1994.
- [245] M. Dijkstra. *The Effect of Entropy on the Stability and Structure of Complex Fluids*. Ph.D. thesis, Rijksuniversiteit Utrecht, The Netherlands, 1994.
- [246] M. Dijkstra and D. Frenkel. Simulation study of a two-dimensional system of semiflexible polymers. *Phys. Rev. E*, 50:349–357, 1994.
- [247] P.G. Bolhuis and D.A. Kofke. Numerical study of freezing in polydisperse colloidal suspensions. *J. Phys.: Condens. Matt.*, 8:9627–9631, 1996.
- [248] P.G. Bolhuis and D. Frenkel. Tracing the phase boundaries of hard spherocylinders. *J. Chem. Phys.*, 106:666–687, 1997.
- [249] E.J. Meijer and F.E. Azhar. Novel procedure to determine coexistence lines by computer simulation. Application to hard-core Yukawa model for charge-stabilized colloids. *J. Chem. Phys.*, 106:4678–4683, 1997.
- [250] F.A. Escobedo and J.J. de Pablo. Pseudo-ensemble simulations and Gibbs-Duhem integrations for polymers. *J. Chem. Phys.*, 106:2911–2923, 1997.
- [251] F.A. Escobedo. Tracing coexistence lines in multicomponent fluid mixtures by molecular simulation. *J. Chem. Phys.*, 110:11999–12010, 1999.
- [252] W.G. Hoover and F.H. Ree. Melting transition and communal entropy for hard spheres. *J. Chem. Phys.*, 49:3609–3617, 1968.
- [253] G.S. Stringfellow, H.E. DeWitt, and W.L. Slattery. Equation of state of the one-component plasma derived from precision Monte Carlo calculations. *Phys. Rev. A*, 41:1105–1111, 1990.
- [254] W.G. Hoover, S.G. Gray, and K.W. Johnson. Thermodynamic properties of the fluid and solid phases for the inverse power potentials. *J. Chem. Phys.*, 55:1228–1136, 1971.
- [255] B.B. Laird and A.D.J. Haymet. Phase diagram for the inverse sixth power potential system from molecular dynamics simulations. *Mol. Phys.*, 75:71–80, 1992.
- [256] W.G. Hoover, M. Ross, K.W. Johnson, D. Henderson, J.A. Barker, and B.C. Brown. Soft-sphere equation of state. *J. Chem. Phys.*, 52:4931–4941, 1970.
- [257] J.-P. Hansen. Phase transition of the Lennard-Jones system. II. High-temperature limit. *Phys. Rev. A*, 2:221–230, 1970.
- [258] H. Ogura, H. Matsuda, T. Ogawa, N. Ogita, and A. Ueda. Computer simulations for the melting curve maximum phenomenon. *Prog. Theoret. Phys.*, 58:419–433, 1977.
- [259] D. Frenkel and A.J.C. Ladd. New Monte Carlo method to compute the free energy of arbitrary solids. Application to the fcc and hcp phases of hard spheres. *J. Chem. Phys.*, 81:3188–3194, 1984.
- [260] P.G. Bolhuis and D.A. Kofke. Monte Carlo study of freezing of polydisperse hard spheres. *Phys. Rev. E*, 54:634–643, 1996.
- [261] D.A. Kofke and P.G. Bolhuis. Freezing of polydisperse hard spheres. *Phys. Rev. E*, 59:618–622, 1999.

- [262] P.A. Monson and D.A. Kofke. Solid-fluid equilibrium: Insights from simple molecular models. In I. Prigogine and S.A. Rice, editors, *Advances in Chemical Physics*, volume 115, pages 113–179. Wiley, New York, 2000.
- [263] W.G. Hoover and F.H. Ree. Use of computer experiments to locate the melting transition and calculate the entropy in the solid phase. *J. Chem. Phys.*, 47:4873–4878, 1967.
- [264] E.J. Meijer. *Computer Simulations of Molecular Solids and Colloidal Dispersions*. Ph.D. thesis, Rijksuniversiteit Utrecht, The Netherlands, 1993.
- [265] D. Frenkel. Stability of the high-pressure body-centered-cubic phase of helium. *Phys. Rev. Lett.*, 56:858–860, 1986.
- [266] J.Q. Broughton and G.H. Gilmer. Molecular dynamics investigation of the crystal-fluid interface. I. Bulk properties. *J. Chem. Phys.*, 79:5095–5104, 1983.
- [267] J.A. Schouten. Phase equilibria in binary systems at very high pressures. *Phys. Rep.*, 172:33–92, 1989.
- [268] J.P. Ryckaert and G. Ciccotti. Introduction of Andersen's demon in the molecular dynamics of systems with constraints. *J. Chem. Phys.*, 78:7368–7374, 1983.
- [269] W.G. Hoover. Entropy for small classical crystals. *J. Chem. Phys.*, 49:1981–1982, 1968.
- [270] J.M. Polson, E. Trizac, S. Pronk, and D. Frenkel. Finite-size corrections to the free energies of crystalline solids. *J. Chem. Phys.*, 112:5339–5342, 2000.
- [271] R.J. Speedy. Pressure of the metastable hard-sphere fluid. *J. Phys.: Condensed Matter*, 9:8591–8599, 1997.
- [272] R.J. Speedy. Pressure and entropy of hard-sphere crystals. *J. Phys.: Condensed Matter*, 10:4387–4391, 1998.
- [273] B.J. Alder and T.E. Wainwright. Studies in molecular dynamics. II. Behavior of a small number of elastic spheres. *J. Chem. Phys.*, 33:1439–1451, 1960.
- [274] B. Smit and D. Frenkel. Explicit expression for finite size corrections to the chemical potential. *J. Phys.: Condens. Matt.*, 1:8659–8665, 1989.
- [275] M. Abramowitz and I. Stegun. *Handbook of Mathematical Functions*. Dover, New York, 1970.
- [276] L.V. Woodcock. Entropy difference between the face-centred cubic and hexagonal close-packed crystal structures. *Nature*, 385:141–143, 1997.
- [277] P.G. Bolhuis, D. Frenkel, S.-C. Mau, and D.A. Huse. Entropy differences between crystal phases. *Nature*, 388:235–237, 1997.
- [278] A.D. Bruce, N.B. Wilding, and G.J. Ackland. Free energy of crystalline solids: A lattice-switch Monte Carlo method. *Phys. Rev. Lett.*, 79:3002–3005, 1997.
- [279] B.A. Berg and T. Neuhaus. Multicanonical ensemble: A new approach to simulate first-order phase transitions. *Phys. Rev. Lett.*, 68:9–12, 1992.
- [280] S.-C. Mau and D.A. Huse. Stacking entropy of hard-sphere crystals. *Phys. Rev. E*, 59:4396–4401, 1999.
- [281] C.H. Bennett and B.J. Alder. Studies in molecular dynamics. IX. Vacancies in hard sphere crystals. *J. Chem. Phys.*, 54:4796–4808, 1970.
- [282] R.K. Bowles and R.J. Speedy. Cavities in the hard-sphere crystal and fluid. *Mol. Phys.*, 83:113–125, 1994.

- [283] W.C. Swope and H.C. Andersen. Thermodynamics, statistical mechanics and computer simulation of crystals with vacancies and interstitials. *Phys. Rev. A*, 46:4539–4548, 1992.
- [284] R.J. Speedy and H. Reiss. Cavities in the hard-sphere fluid and crystal and the equation of state. *Mol. Phys.*, 72:999–1014, 1991.
- [285] R.J. Speedy and H. Reiss. A computer simulation study of cavities in the hard-disc fluid and crystal. *Mol. Phys.*, 72:1015–1033, 1991.
- [286] M.A. Bates and D. Frenkel. Influence of vacancies on the melting transition of hard disks in two dimensions. *Phys. Rev. E*, 61:5223–5227, 2000.
- [287] S. Pronk and D. Frenkel. Vacancies and interstitials in hard sphere crystals. *J. Phys. Chem. B*, 105:6722–6727, 2001.
- [288] M. Müller and W. Paul. Measuring the chemical potential of polymer solutions and melts in computer simulations. *J. Chem. Phys.*, 100:719–724, 1994.
- [289] S.K. Kumar, I. Szleifer, and A.Z. Panagiotopoulos. Determination of the chemical potentials of polymeric systems from Monte Carlo simulations. *Phys. Rev. Lett.*, 66:2935–2938, 1991.
- [290] S.K. Kumar, I. Szleifer, and A.Z. Panagiotopoulos. Determination of the chemical potentials of polymeric systems from Monte Carlo simulations. *Phys. Rev. Lett.*, 68:3658, 1992.
- [291] K.K. Mon and R.B. Griffiths. Chemical potential by gradual insertion of a particle in Monte Carlo simulation. *Phys. Rev. A*, 31:956–959, 1985.
- [292] B. Smit, G.C.A.M. Mooij, and D. Frenkel. Comment on “determination of the chemical potential of polymeric systems from Monte Carlo simulations”. *Phys. Rev. Lett.*, 68:3657, 1992.
- [293] J. Harris and S.A. Rice. A lattice model of a supported monolayer of amphiphilic molecules: Monte Carlo simulations. *J. Chem. Phys.*, 88:1298–1306, 1988.
- [294] J.I. Siepmann. A method for the direct calculation of chemical potentials for dense chain systems. *Mol. Phys.*, 70:1145–1158, 1990.
- [295] M.N. Rosenbluth and A.W. Rosenbluth. Monte Carlo simulations of the average extension of molecular chains. *J. Chem. Phys.*, 23:356–359, 1955.
- [296] D. Frenkel and B. Smit. Unexpected length dependence of the solubility of chain molecules. *Mol. Phys.*, 75:983–988, 1992.
- [297] D. Frenkel, G.C.A.M. Mooij, and B. Smit. Novel scheme to study structural and thermal properties of continuously deformable molecules. *J. Phys.: Condens. Matter*, 4:3053–3076, 1992.
- [298] J.J. de Pablo, M. Laso, and U.W. Suter. Estimation of the chemical potential of chain molecules by simulation. *J. Chem. Phys.*, 96:6157–6162, 1992.
- [299] K. Kremer and K. Binder. Monte Carlo simulations of lattice models for macromolecules. *Comp. Phys. Rep.*, 7:259–310, 1988.
- [300] J. Batoulis and K. Kremer. Statistical properties of biased sampling methods for long polymer chains. *J. Phys. A: Math. Gen.*, 21:127–146, 1988.
- [301] E.J. Maginn, A.T. Bell, and D.N. Theodorou. Sorption thermodynamics, siting and conformation of long n-alkanes in silicalite as predicted by

- configurational-bias Monte Carlo integration. *J. Phys. Chem.*, 99:2057–2079, 1995.
- [302] B. Smit and J.I. Siepmann. Simulating the adsorption of alkanes in zeolites. *Science*, 264:1118–1120, 1994.
- [303] B. Smit and J.I. Siepmann. Computer simulations of the energetics and siting of n-alkanes in zeolites. *J. Phys. Chem.*, 98:8442–8452, 1994.
- [304] B. Smit. Grand-canonical Monte Carlo simulations of chain molecules: Adsorption isotherms of alkanes in zeolites. *Mol. Phys.*, 85:153–172, 1995.
- [305] G.C.A.M. Mooij and D. Frenkel. The overlapping distribution method to compute chemical potentials of chain molecules. *J. Phys.: Condens. Matter*, 6:3879–3888, 1994.
- [306] P. Grassberger. Monte Carlo simulations of 3d self-avoiding walks. *J. Phys. A: Math. Gen.*, 26:2769–2776, 1993.
- [307] P. Grassberger and R. Hegger. Monte Carlo simulations of off-lattice polymers. *J. Phys.: Condens. Matter*, 7:3089–3097, 1993.
- [308] P. Grassberger and R. Hegger. Monte Carlo simulations of off-lattice polymers (corrections and additions). *J. Phys.: Condens. Matter*, 7:3089–3097, 1995.
- [309] T. Garel and H. Orland. Guided replication of random chains: a new Monte Carlo method. *J. Phys. A: Math. Gen.*, 23:L621–L626, 1990.
- [310] D. Frenkel. Numerical techniques to study complex liquids. In M. Baus *et al.*, editor, *Observation, Prediction and Simulation of Phase Transitions in Complex Fluids*, pages 357–419. NATO ASI, Kluwer, Dordrecht, 1995.
- [311] P. Grassberger. Pruned-enriched rosenbluth method: Simulations of theta polymers of chain length up to 1,000,000. *Phys. Rev. E*, 56:3682–3693, 1997.
- [312] H. Frauenkron, U. Bastolla, E. Gerstner, P. Grassberger, and W. Nadler. New Monte Carlo algorithm for protein folding. *Phys. Rev. Lett.*, 80:3149–3152, 1998.
- [313] H. Meirovitch. Scanning method as an unbiased simulation technique and its application to the study of self-attracting random walks. *Phys. Rev. A*, 32:3699–3708, 1985.
- [314] P.J. Steinbach and B.R. Brooks. New spherical-cutoff methods for long-range forces in macromolecular simulation. *J. Comp. Chem.*, 15:667–683, 1994.
- [315] J.W. Eastwood and R.W. Hockney. Shaping the force law in two-dimensional particle mesh models. *J. Comp. Phys.*, 16:342–359, 1974.
- [316] L. Greengard and V. Rokhlin. A fast algorithm for particle simulations. *J. Comp. Phys.*, 73:325–348, 1987.
- [317] T.A. Darden, D. York, and L. Pedersen. Particle mesh Ewald: An $N \log(N)$ method for Ewald sums in large systems. *J. Chem. Phys.*, 98:10089–10092, 1993.
- [318] P.P. Ewald. Die Berechnung optischer und elektrostatischer Gitterpotentiale. *Ann. Phys.*, 64:253–287, 1921.
- [319] S.W. de Leeuw, J.W. Perram, and E.R. Smith. Simulation of electrostatic systems in periodic boundary conditions. I. Lattice sums and dielectric constants. *Proc. R. Soc. London A*, 373:27–56, 1980.
- [320] S.W. de Leeuw, J.W. Perram, and E.R. Smith. Simulation of electrostatic systems in periodic boundary conditions. II. Equivalence of boundary conditions. *Proc. R. Soc. London A*, 373:56–66, 1980.

- [321] S.W. de Leeuw, J.W. Perram, and E.R. Smith. Simulation of electrostatic systems in periodic boundary conditions. III. Further theory and applications. *Proc. R. Soc. London A*, 388:177–193, 1983.
- [322] J.-P. Hansen. Molecular-dynamics simulations of Coulomb systems in two and three dimensions. In G. Ciccotti and W.G. Hoover, editors, *Molecular Dynamics Simulations of Statistical Mechanics Systems*, pages 89–129. Proceedings of the 97th Int. “Enrico Fermi” School of Physics, North Holland, Amsterdam, 1986.
- [323] M.P. Tosi. Cohesion of ionic solids in the Born model. In F. Seitz and D. Turnbull, editors, *Solid State Physics: Advances in Research and Applications*, pages 1–120. Academic Press, New York, 1964.
- [324] J.-M. Caillol and D. Levesque. Numerical simulations of homogeneous and inhomogeneous ionic systems: An efficient alternative to the Ewald method. *J. Chem. Phys.*, 94:597–607, 1991.
- [325] M. Neumann. Dipole moment fluctuation formulas in computer simulations of polar systems. *Mol. Phys.*, 50:841–858, 1983.
- [326] J.A. Kolafa and J.W. Perram. Cutoff errors in the Ewald summation formulae for point charge systems. *Mol. Sim.*, 9:351–368, 1992.
- [327] H.G. Petersen. Accuracy and efficiency of the particle mesh Ewald method. *J. Chem. Phys.*, 103:3668–3679, 1995.
- [328] K. Esselink. A comparison of algorithms for long-range interactions. *Comp. Phys. Comm.*, 87:375–395, 1995.
- [329] A.W. Appel. An efficient program for many-body simulation. *SIAM J. Sci. Stat. Comput.*, 6:85–103, 1985.
- [330] K. Esselink. The order of Appel’s algorithm. *Inf. Proc. Lett.*, 41:141–147, 1992.
- [331] J. Barnes and P. Hut. A hierarchical $O(N \log N)$ force-calculation algorithm. *Nature*, 324:446–449, 1986.
- [332] K.E. Schmidt and M.A. Lee. Implementing the fast multipole method in three dimensions. *J. Stat. Phys.*, 63:1223–1235, 1991.
- [333] H.Q. Ding, N. Karasawa, and W.A. Goddard III. Atomic level simulations on a million particles: The cell multipole method for Coulombic and London nonbond interactions. *J. Chem. Phys.*, 97:4309–4315, 1992.
- [334] M. Deserno and C Holm. How to mesh up Ewald sums. I. A theoretical and numerical comparison of various particle mesh routines. *J. Chem. Phys.*, 109:7678–7693, 1998.
- [335] U. Essmann, L. Perera, M.L. Berkowitz, T.A. Darden, H. Lee, and L. Pedersen. A smooth particle mesh Ewald method. *J. Chem. Phys.*, 103:8577–8593, 1995.
- [336] E.L. Pollock and J. Glosli. Comments on P^3M , FMM, and the Ewald method for large periodic Coulombic systems. *Comp. Phys. Comm.*, 95:93–110, 1996.
- [337] C. Sagui and T.A. Darden. Molecular dynamics simulations of biomolecules: Long-range electrostatic effects. *Annu. Rev. Biophys. Biomol. Struct.*, 28:155–179, 1999.
- [338] J.V.L. Beckers, C.P. Lowe, and S.W. de Leeuw. An iterative PPPM method for simulating Coulombic systems on distributed memory parallel computers. *Mol. Sim.*, 20:369–383, 1998.

- [339] M. Deserno and C Holm. How to mesh up Ewald sums. II. An accurate error estimate for the particle-particle-particle-mesh algorithm. *J. Chem. Phys.*, 109:7694–7701, 1998.
- [340] H.Q. Ding, N. Karasawa, and W.A. Goddard III. The reduced cell multipole method for coulombic interactions in periodic systems with million-atom unit cells. *Chem. Phys. Lett.*, 196:6–10, 1992.
- [341] B.A. Luty, I.G. Tironi, and W.F. van Gunsteren. Lattice-sum methods for calculating electrostatic interactions. *J. Chem. Phys.*, 103:3014–3021, 1995.
- [342] F. Figueirido, R.M. Levy, R. Zhou, and B.J. Berne. Large scale simulation of macromolecules in solution: Combining the periodic fast multipole method with multiple time step integrators. *J. Chem. Phys.*, 106:9835–9849, 1997.
- [343] D.M. Heyes, M. Barber, and J.H.R. Clarke. Molecular dynamics computer simulation of surface properties of crystalline potassium chloride. *J. Chem. Soc. Faraday Trans. II*, 73:1485–1496, 1977.
- [344] A. Grzybowski, E. Gwozdz, and A. Brodka. Ewald summation of electrostatic interactions in molecular dynamics of a three-dimensional system with periodicity in two directions. *Phys. Rev. B*, 61:6706–6712, 2000.
- [345] A.H. Widmann and D.B. Adolf. A comparison of Ewald summation techniques for planar surfaces. *Comput. Phys. Commun.*, 107:167–186, 1997.
- [346] S.W. de Leeuw and J.W. Perram. Electrostatic lattice sums for semi-infinite lattices. *Mol. Phys.*, 37:1313–1322, 1979.
- [347] E.R. Smith. Electrostatic potentials for simulations of thin layers. *Mol. Phys.*, 65:1089–1104, 1988.
- [348] E. Spohr. Effect of boundary conditions and system size on the interfacial properties of water and aqueous solutions. *J. Chem. Phys.*, 107:6342–6348, 1994.
- [349] J. Hautman and M.L. Klein. An Ewald summation method for planar surfaces and interfaces. *Mol. Phys.*, 75:379–395, 1992.
- [350] I.C. Yeh and M.L. Berkowitz. Ewald summation for systems with slab geometry. *J. Chem. Phys.*, 111:3155–3162, 1999.
- [351] E.R. Smith. Electrostatic energy in ionic crystals. *Proc. R. Soc. London A*, 375:475–505, 1981.
- [352] P.S. Crozier, R.L. Rowley, E. Spohr, and D. Henderson. Comparison of charged sheets and corrected 3D Ewald calculations of long-range forces in slab geometry electrolyte systems with solvent molecules. *J. Chem. Phys.*, 112:9253–9257, 2000.
- [353] R.F. Cracknell, D. Nicholson, N.G. Parsonage, and H. Evans. Rotational insertion bias: A novel method for simulating dense phases of structured particles, with particular application to water. *Mol. Phys.*, 71:931–943, 1990.
- [354] J.I. Siepmann and D. Frenkel. Configurational-bias Monte Carlo: A new sampling scheme for flexible chains. *Mol. Phys.*, 75:59–70, 1992.
- [355] J.J. de Pablo, M. Laso, and U.W. Suter. Simulation of polyethylene above and below the melting point. *J. Chem. Phys.*, 96:2395–2403, 1992.
- [356] G.C.A.M. Mooij, D. Frenkel, and B. Smit. Direct simulation of phase equilibria of chain molecules. *J. Phys.: Condens. Matter*, 4:L255–L259, 1992.

- [357] G.C.A.M. Mooij and D. Frenkel. A systematic optimization scheme for configurational bias Monte Carlo. *Mol. Sim.*, 17:41–55, 1996.
- [358] B. Chen and J.I. Siepmann. Transferable potentials for phase equilibria. 3. Explicit-hydrogen description of normal alkanes. *J. Phys. Chem. B*, 103:5370–5379, 1999.
- [359] M.D. Macedonia and E.J. Maginn. A biased grand canonical Monte Carlo method for simulating adsorption using all-atom and branched united atom models. *Mol. Phys.*, 96:1375–1390, 1999.
- [360] T.J.H. Vlucht. *Adsorption and Diffusion in Zeolites: A Computational Study*. Ph.D. thesis, University of Amsterdam, 2000.
- [361] T.J.H. Vlucht, R. Krishna, and B. Smit. Molecular simulations of adsorption isotherms for linear and branched alkanes and their mixtures in silicalite. *J. Phys. Chem. B*, 103:1102–1118, 1999.
- [362] M. Dijkstra. Confined thin films of linear and branched alkanes. *J. Chem. Phys.*, 107:3277–3288, 1997.
- [363] M.G. Martin and J.I. Siepmann. Novel configurational-bias Monte Carlo method for branched molecules. Transferable potentials for phase equilibria. 2. United-atom description of branched alkanes. *J. Phys. Chem. B*, 103:4508–4517, 1999.
- [364] D. Chandler and P.G. Wolynes. Exploiting the isomorphism between quantum theory and classical statistical mechanics of polyatomic fluids. *J. Chem. Phys.*, 74:4078–4095, 1981.
- [365] V.G. Mavrantzas, T.D. Boone, E. Zervopoulou, and D.N. Theodorou. End-bridging Monte Carlo: A fast algorithm for atomistic simulation of condensed phases of long polymer chains. *Macromolecules*, 32:5072–5096, 1999.
- [366] M. Dijkstra and D. Frenkel. Evidence for entropy-driven demixing in hard-core fluids. *Phys. Rev. Lett.*, 72:298–300, 1994.
- [367] M. Dijkstra, D. Frenkel, and J.-P. Hansen. Phase separation in binary hard-core mixtures. *J. Chem. Phys.*, 101:3179–3189, 1994.
- [368] H. Yamakawa. *Modern Theory of Polymer Solutions*. Harper and Row, New York, 1971.
- [369] M. Vendruscolo. Modified configurational bias Monte Carlo method for simulation of polymer systems. *J. Chem. Phys.*, 106:2970–2976, 1996.
- [370] C.D. Wick and J.I. Siepmann. Self-adapting fixed-end-point configurational-bias Monte Carlo method for the regrowth of interior segments of chain molecules with strong intramolecular interactions. *Macromolecules*, 33:7207–7218, 2000.
- [371] Z. Chen and F.A. Escobedo. A configurational-bias approach for the simulation of inner sections of linear and cyclic molecules. *J. Chem. Phys.*, 113:11382–11392, 2000.
- [372] P.V.K. Pant and D.N. Theodorou. Variable connectivity method for the atomistic Monte Carlo simulation of polydisperse polymer melts. *Macromolecules*, 28:7224–7234, 1995.

- [373] M.G. Wu and M.W. Deem. Analytical rebridging Monte Carlo: Application to cis/trans isomerization in proline-containing, cyclic peptites methods for cyclic peptides. *J. Chem. Phys.*, 111:6625–6632, 1999.
- [374] M.G. Wu and M.W. Deem. Efficient Monte Carlo methods for cyclic peptides. *Mol. Phys.*, 97:559–580, 1999.
- [375] T. Biben. *Structure et stabilité des fluides à deux composants: des fluides atomiques aux suspensions colloïdales*. Ph.D. thesis, Université Claude Bernard, Lyon, 1993.
- [376] T. Biben, P. Bladon, and D. Frenkel. Depletion effects in binary hard-sphere fluids. *J. Phys.: Condens. Matt.*, 8:10799–10821, 1996.
- [377] P.G. Bolhuis and D. Frenkel. Numerical study of the phase diagram of a mixture of spherical and rodlike colloids. *J. Chem. Phys.*, 101:9869–9875, 1995.
- [378] J.C. Shelley and G.N. Patey. A configurational bias Monte Carlo method for ionic solutions. *J. Chem. Phys.*, 100:8265–8270, 1994.
- [379] K. Esselink, L.D.J.C. Loyens, and B. Smit. Parallel Monte Carlo simulations. *Phys. Rev. E*, 51:1560–1568, 1995.
- [380] L.D.J.C. Loyens, B. Smit, and K. Esselink. Parallel Gibbs-ensemble simulations. *Mol. Phys.*, 86:171–183, 1995.
- [381] K. Esselink, P.A.J. Hilbers, S. Karaborni, J.I. Siepmann, and B. Smit. Simulating complex fluids. *Mol. Sim.*, 14:259–274, 1995.
- [382] T.J.H. Vlugt, M.G. Martin, B. Smit, J.I. Siepmann, and R. Krishna. Improving the efficiency of the cbmc algorithm. *Mol. Phys.*, 94:727–733, 1998.
- [383] B. Smit and T.L.M. Maesen. Commensurate “freezing” of alkanes in the channels of a zeolite. *Nature*, 374:42–44, 1995.
- [384] R. Evans. Microscopic theories of simple fluids and their interfaces. In J. Charvolin, J.F. Joanny, and J. Zinn-Justin, editors, *Liquides aux Interfaces/Liquids at interfaces*, pages 1–98. Les Houches, Session XLVIII, 1988, North Holland, Amsterdam, 1990.
- [385] S.J. Gregg and K.S.W. Sing. *Adsorption, Surface Area and Porosity*. Academic Press, London, 1982.
- [386] J.I. Siepmann, S. Karaborni, and B. Smit. Simulating the critical properties of complex fluids. *Nature*, 365:330–332, 1993.
- [387] W.J.M. van Well, J.P. Wolthuisen, B. Smit, J.H.C. van Hooff, and R.A. van Santen. Commensurate freezing of n-alkanes in silicalite. *Angew. Chem. (Int. Ed.)*, 34:2543–2544, 1995.
- [388] R. Krishna, B. Smit, and T.J.H. Vlugt. Sorption-induced diffusion-selective separation of hydrocarbon isomers using silicalite. *J. Phys. Chem. A*, 102:7727–7730, 1998.
- [389] G.C.A.M. Mooij. *Novel Simulation Techniques for the Study of Polymer Phase Equilibria*. Ph.D. thesis, Rijksuniversiteit Utrecht, The Netherlands, 1993.
- [390] B. Smit, S. Karaborni, and J.I. Siepmann. Computer simulations of vapour-liquid phase equilibria of n-alkanes. *J. Chem. Phys.*, 102:2126–2140, 1995. Erratum: *J. Chem. Phys.* 109:352, 1998.
- [391] M. Laso, J.J. de Pablo, and U.W. Suter. Simulation of phase equilibria for chain molecules. *J. Chem. Phys.*, 97:2817–2819, 1992.

- [392] J.I. Siepmann, S. Karaborni, and B. Smit. Vapor-liquid equilibria of model alkanes. *J. Am. Chem. Soc.*, 115:6454–6455, 1993.
- [393] C. Tsonopoulos. Critical constant of normal alkanes from methane to polyethylene. *AIChE Journal*, 33:2080–2083, 1987.
- [394] W.L. Jorgensen, J.D. Madura, and C.J. Swenson. Optimized intermolecular potential function for liquid hydrocarbons. *J. Am. Chem. Soc.*, 106:6638–6646, 1984.
- [395] S. Toxvaerd. Molecular dynamics calculation of the equation of state of alkanes. *J. Chem. Phys.*, 93:4290–4295, 1990.
- [396] C. Tsonopoulos and Z. Tan. Critical constant of normal alkanes from methane to polyethylene II. Application of the Flory theory. *Fluid Phase Equilibria*, 83:127–138, 1993.
- [397] M.J. Anselme, M. Gude, and A.S. Teja. The critical temperatures and densities of the n-alkanes from pentane to octadecane. *Fluid Phase Equilibria*, 57:317–326, 1990.
- [398] Y.-J. Sheng, A.Z. Panagiotopoulos, S.K. Kumar, and I. Szleifer. Monte Carlo calculation of phase equilibria for a bead-spring polymeric model. *Macromolecules*, 27:400–406, 1994.
- [399] F.A. Escobedo and J.J. de Pablo. Simulation and prediction of vapour-liquid equilibria for chain molecules. *Mol. Phys.*, 87:347–366, 1996.
- [400] M. Mondello and G.S. Grest. Molecular dynamics of linear and branched alkanes. *J. Chem. Phys.*, 103:7156–7165, 1995.
- [401] M. Mondello, G.S. Grest, E.B. Webb III, and P. Peczak. Dynamics of n-alkanes: Comparison to Rouse model. *J. Chem. Phys.*, 109:798–805, 1998.
- [402] J.D. Moore, S.T. Cui, H.D. Cochran, and P.T. Cummings. Rheology of lubricant basestocks: A molecular dynamics study of c-30 isomers. *J. Chem. Phys.*, 113:8833–8840, 2000.
- [403] C. McCabe, S.T. Cui, P.T. Cummings, P.A. Gordon, and R.B. Saeger. Examining the rheology of 9-octylheptadecane to giga-pascal pressures. *J. Chem. Phys.*, 114:1887–1891, 2001.
- [404] M.G. Martin and J.I. Siepmann. Transferable potentials for phase equilibria (trappe): I. united-atom description of n-alkanes. *J. Phys. Chem. B*, 102:2569–2577, 1998.
- [405] S.K. Nath, F.A. Escobedo, and J.J. de Pablo. On the simulation of vapor-liquid equilibria for alkanes. *J. Chem. Phys.*, 108:9905–9911, 1998.
- [406] C.D. Wick, M.G. Martin, and J.I. Siepmann. Transferable potentials for phase equilibria. 4. United-atom description of linear and branched alkenes and alkylbenzenes. *J. Phys. Chem. B*, 104:8008–8016, 2000.
- [407] S.K. Nath, B.J. Banaszak, and J.J. de Pablo. A new ninted atom force field for α -olefins. *J. Chem. Phys.*, 1114:3612–3161, 2001.
- [408] M.E. van Leeuwen and B. Smit. Molecular simulations of the vapour-liquid coexistence curve of methanol. *J. Phys. Chem.*, 99:1831–1833, 1995.
- [409] B. Chen, J.J. Potoff, and J.I. Siepmann. Monte Carlo calculations for alcohols and their mixtures with alkanes. transferable potentials for phase equilibria. 5.

- United-atom description of primary, secondary, and tertiary alcohols. *J. Phys. Chem. B*, 105:3093–3104, 2001.
- [410] S. Consta, N.B. Wilding, D. Frenkel, and Z. Alexandrowicz. Recoil growth: An efficient simulation method for multi-polymer systems. *J. Chem. Phys.*, 110:3220–3228, 1999.
- [411] S. Consta, T.J.H. Vlught, J. Wichers Hoeth, B. Smit, and D. Frenkel. Recoil growth algorithm for chain molecules with continuous interactions. *Mol. Phys.*, 97:1243–1254, 1999.
- [412] H. Meirovitch. Statistical properties of the scanning simulation method for polymer-chains. *J. Chem. Phys.*, 89:2514–2522, 1988.
- [413] Z. Alexandrowicz and N.B. Wilding. Simulation of polymers with rebound selection. *J. Chem. Phys.*, 109:5622–5626, 1998.
- [414] M. Falcioni and M.W. Deem. A biased Monte Carlo scheme for zeolite structure solution. *J. Chem. Phys.*, 110:1754–1766, 1999.
- [415] A.P. Lyubartsev, A.A. Martsinovski, S.V. Shevkunov, and P.N. Vorontsov-Vel'yaminov. New approach to Monte Carlo calculation of the free energy: Method of expanded ensembles. *J. Chem. Phys.*, 96:1776–1783, 1992.
- [416] E. Marinari and G. Parisi. Simulated tempering: A new Monte Carlo scheme. *Europhys. Lett.*, 19:451–458, 1992.
- [417] C.J. Geyer and E.A. Thompson. Annealing markov chain Monte Carlo with applications to the ancestral inference. *J. Am. Stat. Soc.*, 90:909–920, 1995.
- [418] S. Kirkpatrick, C.D. Gelatt Jr., and M.P. Vecchi. Optimization by simulated annealing. *Science*, 220:671–680, 1983.
- [419] C.J. Geyer. Markov chain Monte Carlo maximum likelihood. In *Computing Science and Statistics*, pages 156–163. Proceedings of the 23rd Symposium on the Interface, 1991.
- [420] D.D. Frantz, D.L. Freeman, and J.D. Doll. Reducing quasi-ergodic behaviour in Monte Carlo simulations by J-walking: Application to atomic clusters. *J. Chem. Phys.*, 93:2769–2784, 1990.
- [421] I. Nezbeda and J.A. Kolafa. A new version of the insertion particle method for determining the chemical potential by Monte Carlo simulation. *Mol. Sim.*, 5:391–403, 1991.
- [422] K. Shing and A.Z. Azadipour. A new simulation method for the grand canonical ensemble. *Chem. Phys. Lett.*, 190:386–390, 1992.
- [423] L.F. Vega, K.S. Shing, and L.F. Rull. A new algorithm for molecular dynamics simulations in the grand canonical ensemble. *Mol. Phys.*, 82:439–453, 1994.
- [424] Q.L. Yan and J.J. de Pablo. Hyper-parallel tempering Monte Carlo: Application to the Lennard-Jones fluid and the restricted primitive model. *J. Chem. Phys.*, 111:9509–9516, 1999.
- [425] Q.L. Yan and J.J. de Pablo. Hyperparallel tempering Monte Carlo simulation of polymeric systems. *J. Chem. Phys.*, 113:1276–1282, 2000.
- [426] A. Bunker and B. Dünweg. Parallel excluded volume tempering for polymer melts. *Phys. Rev. E*, 63:art. no. 010902, 2001.
- [427] S. Auer and D. Frenkel. Prediction of absolute crystal-nucleation rate in hard-sphere colloids. *Nature*, 409:1020–1023, 2001.

- [428] N.B. Wilding. Critical-point and coexistence-curve properties of the Lennard-Jones fluid: A finite-size scaling study. *J. Phys.: Condens. Matter*, 4:3087–3108, 1992.
- [429] A.M. Ferrenberg and R.H. Swendsen. New Monte Carlo technique for studying phase transitions. *Phys. Rev. Lett.*, 61:2635–2638, 1988.
- [430] S. Duane, A. Kennedy, B.J. Pendleton, and D. Roweth. Hybrid Monte Carlo. *Phys. Lett. B.*, 195:216–222, 1987.
- [431] B. Mehlig, D.W. Heermann, and B.M. Forrest. Exact Langevin algorithms. *Mol. Phys.*, 76:1347–1357, 1992.
- [432] B. Mehlig, D.W. Heermann, and B.M. Forrest. Hybrid Monte Carlo method for condensed matter systems. *Phys. Rev. B*, 45:679–685, 1992.
- [433] B.M. Forrest and U.W. Suter. Generalized coordinate Hybrid Monte Carlo. *Mol. Phys.*, 82:393–410, 1994.
- [434] G.M. Crippen. Conformational analysis by energy embedding. *J. Comp. Chem.*, 3:471–476, 1982.
- [435] R.H. Swendsen and J.-S. Wang. Nonuniversal critical dynamics in Monte Carlo simulations. *Phys. Rev. Lett.*, 58:86–88, 1987.
- [436] D. Wu, D. Chandler, and B. Smit. Electrostatic analogy for surfactant assemblies. *J. Phys. Chem.*, 96:4077–4083, 1992.
- [437] B. Smit, K. Esselink, P.A.J. Hilbers, N.M. van Os, and I. Szleifer. Computer simulations of surfactant self-assembly. *Langmuir*, 9:9–11, 1993.
- [438] F.H. Stillinger. Variational model for micelle structure. *J. Chem. Phys.*, 78:4654–4661, 1983.
- [439] G. Orkoulas and A.Z. Panagiotopoulos. Chemical potentials in ionic systems from Monte Carlo simulations with distance-biased test particle insertion. *Fluid Phase Equilibria*, 93:223–231, 1993.
- [440] G. Orkoulas and A.Z. Panagiotopoulos. Free energy and phase equilibria for the restricted primitive model of ionic fluids from Monte Carlo simulations. *J. Chem. Phys.*, 101:1452–1459, 1994.
- [441] D. Frenkel. Advanced Monte Carlo techniques. In M.P. Allen and D.J. Tildesley, editors, *Computer Simulation in Chemical Physics*, pages 93–152. NATO ASI, Kluwer, Dordrecht, 1993.
- [442] R. Car and M. Parrinello. Unified approach for molecular dynamics and density-functional theory. *Phys. Rev. Lett.*, 55:2471–2474, 1985.
- [443] J.P. Ryckaert, G. Ciccotti, and H.J.C. Berendsen. Numerical integration of the Cartesian equations of motion of a system with constraints: Molecular dynamics of n-alkanes. *J. Comp. Phys.*, 23:237–341, 1977.
- [444] S.W. de Leeuw, J.W. Perram, and H.G. Petersen. Hamilton's equations for constrained dynamical systems. *J. Stat. Phys.*, 61:1203–1222, 1990.
- [445] G. Ciccotti. Molecular dynamics simulations of nonequilibrium phenomena and rare dynamical events. In M. Meyer and V. Pontikis, editors, *Proceedings of the NATO ASI on Computer Simulation in Materials Science*, pages 119–137. Kluwer, Dordrecht, 1991.

- [446] G. Galli and A. Pasquarello. First-principle molecular dynamics. In M.P. Allen and D.J. Tildesley, editors, *Computer Simulation in Chemical Physics*, pages 261–313. NATO ASI, Kluwer, Dordrecht, 1993.
- [447] D.K. Remler and P.A. Madden. Molecular dynamics without effective potentials via the Carr-Parrinello approach. *Mol. Phys.*, 70:921–966, 1990.
- [448] H. Löwen, P.A. Madden, and J.-P. Hansen. Ab initio description of counterion screening in colloidal suspensions. *Phys. Rev. Lett.*, 68:1081–1084, 1992.
- [449] H. Löwen, P.A. Madden, and J.-P. Hansen. Nonlinear counterion screening in colloidal suspensions. *J. Chem. Phys.*, 98:3275–3289, 1993.
- [450] C.G. Gray and K.E. Gubbins. *Theory of Molecular Fluids. 1. Fundamentals*. Clarendon, Oxford, 1984.
- [451] M-L. Saboungi, A. Rahman, J.W. Halley, and M. Blander. Molecular dynamics studies of complexing in binary molten salts with polarizable anions: MAX₄. *J. Chem. Phys.*, 88:5818–5823, 1988.
- [452] M. Sprik and M.L. Klein. A polarizable model for water using distributed charge sites. *J. Chem. Phys.*, 89:7556–7560, 1988.
- [453] M. Wilson and P.A. Madden. Polarization effects in ionic systems from first principles. *J. Phys.: Condens. Matter*, 5:2687–2706, 1993.
- [454] M. Sprik. Computer simulation of the dynamics of induced polarization fluctuations in water. *J. Chem. Phys.*, 95:2283–2291, 1991.
- [455] P. Procacci and M. Marchi. Taming the Ewald sum in molecular dynamics simulations of solvated proteins via a multiple time step algorithm. *J. Chem. Phys.*, 104:3003–3012, 1996.
- [456] P. Procacci, M. Marchi, and G.J. Martyna. Electrostatic calculations and multiple time scales in molecular dynamics simulation of flexible molecular systems. *J. Chem. Phys.*, 108:8799–8803, 1998.
- [457] C.H. Bennett. Exact defect calculations in model substances. In A.S. Nowick and J.J. Burton, editors, *Diffusion in Solids: Recent Developments*, pages 73–113. Academic Press, New York, 1975.
- [458] D. Chandler. Statistical mechanics of isomerization dynamics in liquids and the transition state approximation. *J. Chem. Phys.*, 68:2959–2970, 1978.
- [459] B.J. Berne, G. Ciccotti, and D.F. Coker. *Classical and Quantum Dynamics in Condensed Phase Simulations*. World Scientific, Singapore, 1998.
- [460] M.J. Ruiz-Montero, D. Frenkel, and J.J. Brey. Efficient schemes to compute diffusive barrier crossing rates. *Mol. Phys.*, 90:925–941, 1997.
- [461] W.H. Miller. Importance of nonseparability in quantum mechanical transition-state theory. *Acc. Chem. Res.*, 9:306–312, 1976.
- [462] M.A. Wilson and D. Chandler. Molecular dynamics study of the cyclohexane interconversion. *Chem. Phys.*, 149:11–20, 1990.
- [463] M.H. Müser and G. Ciccotti. Two-dimensional orientational motion as a multichannel reaction. *J. Chem. Phys.*, 103:4273–4278, 1995.
- [464] H.A. Kramer. Brownian motion in a field of force and the diffusion model of chemical reactions. *Physica*, 7:284–304, 1940.
- [465] P.G. Bolhuis, C. Dellago, and D. Chandler. Sampling ensembles of deterministic transition pathways. *Faraday Discuss.*, 110:421–436, 1998.

- [466] D. Chandler. Finding transition pathways: Throwing ropes of rough mountain passes, in the dark. In B.J. Berne, G. Ciccotti, and D.F. Coker, editors, *Classical and Quantum Dynamics in Condensed Phase Simulations*, International School Enrico Fermi, pages 51–66. Italian Physical Society, World Scientific, Singapore, 1998.
- [467] C. Dellago, P.G. Bolhuis, F.S. Csajka, and D. Chandler. Transition path sampling and the calculation of rate constants. *J. Chem. Phys.*, 108:1964–1977, 1998.
- [468] C. Dellago, P.G. Bolhuis, and D. Chandler. On the calculation of reaction rate constants in the transition path ensemble. *J. Chem. Phys.*, 110:6617–6625, 1999.
- [469] L.R. Pratt. A statistical method for identifying transition states in high dimensional problems. *J. Chem. Phys.*, 9:5045–5048, 1986.
- [470] T.J.H. Vlugt and B. Smit. On the efficient sampling of pathways in the transition path ensemble. *Phys. Chem. Comm.*, 2:3–7, 2001.
- [471] P.L. Geissler, C. Dellago, and D. Chandler. Kinetic pathways of ion pair dissociation in water. *J. Phys. Chem. B*, 103:3706–3710, 1999.
- [472] G. Mills, H. Jonsson, and G.K. Schenter. Reversible work transition-state theory—Application to dissociative adsorption of hydrogen. *Surface Science*, 324:305–337, 1995.
- [473] G. Henkelman and H. Jonsson. A dimer method for finding saddle points on high dimensional potential surfaces using only first derivatives. *J. Chem. Phys.*, 111:7010–7022, 1999.
- [474] G. Henkelman, B.P. Uberuaga, and H. Jonsson. A climbing image nudged elastic band method for finding saddle points and minimum energy paths. *J. Chem. Phys.*, 113:9901–9904, 2000.
- [475] G. Henkelman and H. Jonsson. Improved tangent estimate in the nudged elastic band method for finding minimum energy paths and saddle points. *J. Chem. Phys.*, 113:9978–9985, 2000.
- [476] G.T. Barkema and N. Mousseau. Event-based relaxation of continuous disordered systems. *Phys. Rev. Lett.*, 77:4358–4361, 1996.
- [477] A.F. Voter. Hyperdynamics: Accelerated molecular dynamics of infrequent events. *Phys. Rev. Lett.*, 78:3908–3911, 1997.
- [478] M.R. Sorensen and A.F. Voter. Temperature-accelerated dynamics for simulation of infrequent events. *J. Chem. Phys.*, 112:9599–9606, 2000.
- [479] A.F. Voter. Parallel replica method for dynamics of infrequent events. *Phys. Rev. B*, 57:R13985–R13988, 1998.
- [480] P.J. Hoogerbrugge and J.M.V.A. Koelman. Simulating microscopic hydrodynamics phenomena with dissipative particle dynamics. *Europhys. Lett.*, 19:155–160, 1992.
- [481] J.M.V.A. Koelman and P.J. Hoogerbrugge. Dynamic simulation of hard-sphere suspensions under steady shear. *Europhys. Lett.*, 21:363–368, 1993.
- [482] A.J.C. Ladd. Short-time motion of colloidal particles - numerical-simulation via a fluctuating lattice-boltzmann equation. *Phys. Rev. Lett.*, 70:1339–1342, 1993.
- [483] A. Malevanets and R. Kapral. Solute molecular dynamics in a mesoscale solvent. *J. Chem. Phys.*, 112:7260–7269, 2000.

- [484] I. Pagonabarraga and D. Frenkel. Dissipative particle dynamics for interacting systems. *J. Chem. Phys.*, 115:5015–5026, 2001.
- [485] R.D. Groot and P.B. Warren. Dissipative particle dynamics: bridging the gap between atomistic and mesoscopic simulation. *J. Chem. Phys.*, 107:4423–4435, 1997.
- [486] C.P. Lowe. An alternative approach to dissipative particle dynamics. *Europhys. Lett.*, 47:145–151, 1999.
- [487] P. Español and P.B. Warren. Statistical mechanics of dissipative particle dynamics. *Europhys. Lett.*, 30:191–196, 1995.
- [488] P. Español. Hydrodynamics from dissipative particle dynamics. *Phys. Rev. E*, 52:1734–1742, 1995.
- [489] C.A. Marsh, G. Backx, and M.H. Ernst. Fokker-Planck-Boltzmann equation for dissipative particle dynamics. *Europhys. Lett.*, 38:411–415, 1997.
- [490] C.A. Marsh, G. Backx, and M.H. Ernst. Static and dynamic properties of dissipative particle dynamics. *Phys. Rev. E*, 56:1676–1691, 1997.
- [491] A.J. Masters and P.B. Warren. Kinetic theory for dissipative particle dynamics: The importance of collisions. *Europhys. Lett.*, 48:1–7, 1999.
- [492] C.A. Marsh and J.M. Yeomans. Dissipative particle dynamics: The equilibrium for finite time steps. *Europhys. Lett.*, 37:511–516, 1997.
- [493] I. Pagonabarraga, M.H.J. Hagen, and D. Frenkel. Self-consistent dissipative particle dynamics. *Europhys. Lett.*, 42:377–382, 1998.
- [494] S.M. Willemsen, T.J.H. Vlugt, H.C.J. Hoefsloot, and B. Smit. Combining dissipative particle dynamics and Monte Carlo techniques. *J. Comp. Phys.*, 147:507–517, 1998.
- [495] J.G. Kirkwood and F.P. Buff. *J. Chem. Phys.*, 17:338, 1949.
- [496] J.H. Irving and J.G. Kirkwood. *J. Chem. Phys.*, 18:817, 1950.
- [497] J.P.R.B. Walton, D.J. Tildesley, and J.S. Rowlinson. The pressure tensor at the planar surface of a liquid. *Mol. Phys.*, 48:1357–1368, 1983.
- [498] M.J.P. Nijmeijer, A.F. Bakker, C. Bruin, and J.H. Sikkenk. A molecular dynamics simulation of the Lennard-Jones liquid-vapour interface. *J. Chem. Phys.*, 89:3789–3792, 1988.
- [499] J. Bonet Avalos and A.D. Mackie. Dissipative particle dynamics with energy conservation. *Europhys. Lett.*, 40:141–146, 1997.
- [500] P. Español. Dissipative particle dynamics with energy conservation. *Europhys. Lett.*, 40:631–636, 1997.
- [501] J. Bonet Avalos and A.D. Mackie. Dynamic and transport properties of dissipative particle dynamics with energy conservation. *J. Chem. Phys.*, 111:5267–5276, 1997.
- [502] A.D. Mackie, J. Bonet Avalos, and V. Navas. Dissipative particle dynamics with energy conservation: Modelling of heat flow. *Phys. Chem. Chem. Phys.*, 1:2039–2049, 1999.
- [503] S.M. Willemsen, H.C.J. Hoefsloot, D.C. Visser, P.J. Hamersma, and P.D. Iedema. Modelling phase change with dissipative particle dynamics using a consistent boundary condition. *J. Comp. Phys.*, 162:385–394, 2000.

- [504] M. Ripoll, P. Español, and M.H. Ernst. Dissipative particle dynamics with energy conservation: Heat conduction. *Int. J. Mod. Phys. C*, 9:1329–1338, 1998.
- [505] R.D. Groot, T.J. Madden, and D.J. Tildesley. On the role of hydrodynamic interactions in block copolymer microphase separation. *J. Chem. Phys.*, 110:9739–9749, 1999.
- [506] G.R. McNamara and G. Zanetti. Use of the Boltzmann-equation to simulate lattice-gas automata. *Phys. Rev. Lett.*, 61:2332–2335, 1988.
- [507] R. Benzi, S. Succi, and M. Vergassola. The lattice Boltzmann-equation—Theory and applications. *Phys. Rep.*, 222:145–197, 1992.
- [508] S. Chen and G.D. Doolen. Lattice Boltzmann method for fluid flows. *Ann. Rev. Fluid Mech.*, 30:329–364, 1998.
- [509] U. Frisch, B. Hasslacher, and Y. Pomeau. Lattice-gas automata for the Navier-Stokes equation. *Phys. Rev. Lett.*, 56:1505–1508, 1986.
- [510] A.J.C. Ladd. Numerical simulations of particulate suspensions via a discretized Boltzmann-equation. 1. Theoretical foundation. *J. Fluid Mech.*, 271:285–309, 1994.
- [511] M.H.J. Hagen, C.P. Lowe, and D. Frenkel. Non-Boltzmann behavior from the Boltzmann equation. *Phys. Rev. E*, 51:4287–4291, 1995.
- [512] M.R. Swift, W.M. Osborn, and J.M. Yeomans. Lattice Boltzmann simulation of nonideal fluids. *Phys. Rev. Lett.*, 75:830–833, 1995.
- [513] G.A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Clarendon, Oxford, 1994.
- [514] F.J. Alexander, A.L. Garcia, and B.J. Alder. A consistent Boltzmann algorithm. *Phys. Rev. Lett.*, 74:5212–5215, 1995.
- [515] G.A. Bird. Recent advances and current challenges for DSMC. *Comput. Math. Appl.*, 35:1–14, 1998.
- [516] F.J. Alexander and A.L. Garcia. The direct simulation Monte Carlo method. *Comp. Phys.*, 11:588–593, 1997.
- [517] R.P. Feynman, R.B. Leighton, and M. Sands. *The Feynmann Lectures on Physics*. Addison-Wesley, Reading, Mass., 1965.
- [518] J.D. Meiss. Symplectic maps, variational principles, and transport. *Rev. Mod. Phys.*, 64:795–848, 1992.
- [519] S.K. Gray, D.W. Noid, and B.Q. Sumpter. Symplectic integrators for large-scale molecular-dynamics simulations - A comparison of several explicit methods. *J. Chem. Phys.*, 101:4062–4072, 1994.
- [520] M.E. Tuckerman, C.J. Mundy, and G.J. Martyna. On the classical statistical mechanics of non-Hamiltonian systems. *Europhys. Lett.*, 45:149–155, 2000.
- [521] K. Cho, J.D. Joannopoulos, and L. Kleinman. Constant temperature molecular dynamics with momentum conservation. *Phys. Rev. E*, 47:3145–3151, 1993.
- [522] D. Frenkel and A.J.C. Ladd. Elastic constants of hard-sphere crystals. *Phys. Rev. Lett.*, 59:1169, 1987.
- [523] D.R. Squire, A.C. Holt, and W.G. Hoover. Isothermal elastic constants for argon. Theory and Monte Carlo simulations. *Physica A*, 42:388–397, 1969.

- [524] M. Sprik, R.W. Impey, and M.L. Klein. Second-order elastic constants for the Lennard-Jones solid. *Phys. Rev. B*, 29:4368–4374, 1984.
- [525] O. Farago and Y. Kantor. Fluctuation formalism for elastic constants in hard-spheres-and-tethers systems. *Phys. Rev. E*, 61:2478–2489, 2000.
- [526] S. Sengupta, P. Nielaba, and K. Binder. Elastic moduli, dislocation core energy, and melting of hard disks in two dimensions. *Phys. Rev. E*, 61:6294–6301, 2000.
- [527] R. Zwanzig and N.K. Ailawadi. Statistical error due to finite averaging in computer experiments. *Phys. Rev.*, 182:280–283, 1969.
- [528] D. Frenkel. Intermolecular spectroscopy and computer simulations. In J. van Kranendonk, editor, *Intermolecular Spectroscopy and Dynamical Properties of Dense Systems*, International School of Physics “Enrico Fermi”, pages 156–201. Italian Physical Society, North Holland, Amsterdam, 1980.
- [529] G. Jacucci and A. Rahman. Comparing the efficiency of Metropolis Monte Carlo and molecular-dynamics methods for configuration space sampling. *Nuovo Cimento*, D4:341–356, 1984.
- [530] H. Bekker, E.J. Dijkstra, M.K.R. Renardus, and H.J.C. Berendsen. An efficient, box shape independent non-bonded force and virial algorithm for molecular dynamics. *Mol. Sim.*, 14:137–151, 1995.
- [531] D.J. Auerbach, W. Paul, C. Lutz, A.F. Bakker, W.E. Rudge, and F.F. Abraham. A special purpose parallel computer for molecular dynamics: motivation, design, implementation, and application. *J. Phys. Chem.*, 91:4881–4890, 1987.
- [532] D. Ruelle. *Statistical Mechanics: Rigorous Results*. Benjamin, Reading, Mass., 1969.
- [533] R.B. Dingle. *Asymptotic Expansions, Their Derivation and Interpretation*. Academic Press, New York, 1973.
- [534] I.M.J.J. van de Ven-Lucassen, T.J.H. Vlugt, A.J.J. van der Zanden, and P.J.A.M. Kerkhof. Using molecular dynamics to obtain Maxwell-Stefan diffusion coefficients in liquid systems. *Mol. Phys.*, 94:495–503, 1998.
- [535] <http://www.dl.ac.uk/CCP/CCP5/main.html>.
- [536] G. Ilario, I.G. Tironi, and W.F. van Gunsteren. A molecular dynamics study of chloroform. *Mol. Phys.*, 83:381–403, 1994.
- [537] <http://www.dsm.fordham.edu/ftnchek/>.
- [538] P. Hellekalek. Good random number generators are (not so) easy to find. *Math. Comput. Sim.*, 46:485–505, 1998.