

## References

- Aharoni, S. M. and N. S. Murthy (1983) "*Spherical Non-Draining Boc-Poly( $\alpha$ , $\epsilon$ -L-Lysine) Macromolecules: SAXS and Viscosity Studies*", Polym. Commun. **24**, 132-136.
- Allen, M. P. (1984) "*Atomic and molecular representations of molecular hydrodynamics variables*", Mol. Phys. **52**, 705-716.
- Allen, M. P. and D. J. Tildesley (1987) "*Computer Simulation of Liquids*", Oxford, Clarendon Press.
- Anderson, H. C. (1980) "*Molecular dynamics simulations at constant pressure and temperature*", J. Chem. Phys. **72**, 2384-2393.
- Aust, C., M. Kröger and S. Hess (1999) "*Structure and Dynamics of dilute Polymer Solutions under Shear Flow via Nonequilibrium Molecular Dynamics*", Macromolecules **32**, 5660-5672.
- Bair, S., C. McCabe and P. T. Cummings (2002) "*Comparison of Nonequilibrium Molecular Dynamics with Experimental Measurements in the Nonlinear Shear-Thinning Regime*", Phys. Rev. Lett. **88**, 058302.
- Bar, G., S. Rubin, R. Cutts, T. N. Taylor and T. A. Zawodzinski, Jr. (1996) "*Dendrimer-Modified Silicon Oxide Surfaces as Platforms for the Deposition of Gold and Silver Colloid Monolayers: Preparation Method, Characterization, and Correlation between Microstructure and Optical Properties*", Langmuir **12**, 1172-1179.
- Baranyai, A. and D. J. Evans (1990) "*New algorithm for constrained molecular dynamics simulation of liquid benzene and naphthalene*", Mol. Phys. **70**, 53-63.
- Berker, A., S. Chynoweth, U. C. Klomp and Y. Michopoulos (1992) "*Non-equilibrium Molecular Dynamics (NEMD) Simulations and the Rheological Properties of Liquid n-Hexadecane*", J. Chem. Soc. Faraday Trans. **88**, 1719-1725.
- Bird, R. B., C. F. Curtiss, R. C. Armstrong and O. Hassager (1987) "*Dynamics of Polymeric Liquids*", New York, John Wiley & Sons.
- Biswas, P. and B. J. Cherayil (1994) "*Radial dimensions of starburst polymers*", J. Chem. Phys. **100**, 3201-3209.
- Bodnár, I., A. S. Silva, Y. H. Kim and N. J. Wagner (2000) "*Structure and Rheology of Hyperbranched and Dendritic Polymers. II. Effects of Blending Acetylated and Hydroxy-Terminated Poly(propyleneimine) Dendrimers with Aqueous Poly(ethylene oxide) Solutions*", J. Polym. Sci.: Part B: Polym. Phys. **38**, 874-882.
- Bolhuis, P. G., A. A. Louis, J. P. Hansen and E. J. Meijer (2001) "*Accurate effective pair potentials for polymer solutions*", J. Chem. Phys. **114**, 4296-4311.

- Boris, D. and M. Rubinstein (1996) "*A Self-Consistent Mean Field Model of a Starburst Dendrimer: Dense Core vs Dense Shell*", *Macromolecules* **29**, 7251-7260.
- Bosman, A. W., H. M. Janssen and E. W. Meijer (1999) "*About Dendrimers: Structure, Physical Properties, and Applications*", *Chem. Rev.* **99**, 1665-1688.
- Buhleier, E., W. Wehner and F. Vögtle (1978) "*""Cascade"- and "Nonskid-Chain-like" Syntheses of Molecular Cavity Topologies*", *Synthesis* **2**, 155-158.
- Cagin, T., P. J. Miklis, G. Wang, G. Zamanakos, R. Martin, H. Li, D. T. Mainz, V. Nagarajan and W. A. Goddard III (1999). "*Recent Advances in Simulation of Dendritic Polymers*". "*Dynamics in Small Confining Systems V, Materials Research Society Symposium Proceedings Vol. 543*". J. M. Drake, G. S. Grest, J. Klafter and R. Kopelman. Warrendale, Pennsylvania, Materials Research Society.
- Cagin, T., G. Wang, R. Martin, N. Breen and W. A. Goddard III (2000) "*Molecular modelling of dendrimers for nanoscale applications*", *Nanotechnology* **11**, 77-84.
- Cai, C. and Z. Y. Chen (1997) "*Rouse Dynamics of a Dendrimer Model in the  $\theta$  Condition*", *Macromolecules* **30**, 5104-5117.
- Chai, M., Y. Niu, W. J. Youngs and P. L. Rinaldi (2001) "*Structure and Conformation of DAB Dendrimers in Solution via Multidimensional NMR Techniques*", *J. Am. Chem. Soc.* **123**, 4670-4678.
- Chen, Z. Y. and C. Cai (1999) "*Dynamics of Starburst Dendrimers*", *Macromolecules* **32**, 5423-5434.
- Chen, Z. Y. and S.-M. Gui (1996) "*Monte Carlo Simulations of Star-Burst Dendrimers*", *Macromolecules* **29**, 7943-7952.
- Cox, W. P. and E. H. Merz (1958) "*Correlation of dynamic and steady flow viscosities*", *J. Polym. Sci.* **28**, 619.
- Daivis, P. J. and D. J. Evans (1994) "*Comparison of constant pressure and constant volume nonequilibrium simulations of sheared model decane*", *J. Chem. Phys.* **100**, 541-547.
- Daivis, P. J., D. J. Evans and G. P. Morriss (1992) "*Computer simulation study of the comparative rheology of branched and linear alkanes*", *J. Chem. Phys.* **97**, 616-627.
- Daivis, P. J., M. L. Matin and B. D. Todd (2003) "*Nonlinear shear and elongational rheology of model polymer melts by non-equilibrium molecular dynamics*", *J. Non-Newtonian Fluid Mech.* **111**, 1-18.
- Daniels, D. R., T. C. B. McLeish, B. J. Crosby, R. N. Young and C. M. Fernyhough (2001) "*Molecular Rheology of Comp Polymer Melts. 1. Linear Viscoelastic Response*", *Macromolecules* **34**, 7025-7033.

- de Brabander-van den Berg, E. M. M., J. F. G. A. Jansen and E. W. Meijer (1995) "*The Dendritic Box: Shape-Selective Liberation of Encapsulated Guests*", *J. Am. Chem. Soc.* **117**, 4417-4418.
- de Gennes, P. G. (1979) "*Scaling Concepts in Polymer Physics*", Ithaca, Cornell University.
- de Gennes, P. G. and H. Hervet (1983) "*Statistics of 'starburst' polymers*", *J. Phys. Lett. Fr.* **44**, L351.
- de Groot, S. R. and P. Mazur (1962) "*Non-equilibrium thermodynamics*", Amsterdam, North-Holland Pub. Co.
- Delhommelle, J. and D. J. Evans (2001a) "*Comparison of thermostatting mechanisms in NVT and NPT simulations of decane under shear*", *J. Chem. Phys.* **115**, 43-49.
- Delhommelle, J. and D. J. Evans (2001b) "*Configurational temperature thermostat for fluids undergoing shear flow: application to liquid chlorine*", *Molecular Physics* **99**, 1825-1829.
- Doi, M. and S. F. Edwards (1986) "*The Theory of Polymer Dynamics*", Oxford, Clarendon Press.
- Edberg, R., D. J. Evans and G. P. Morriss (1986) "*Constrained molecular dynamics: Simulation of liquid alkanes with a new algorithm*", *J. Chem. Phys.* **84**, 6933-6939.
- Edberg, R., G. P. Morriss and D. J. Evans (1987) "*Rheology of n-alkanes by nonequilibrium molecular dynamics*", *J. Chem. Phys.* **86**, 4555-4570.
- Evans, D. J., H. J. M. Hanley and S. Hess (1984) "*Non-Newtonian phenomena in simple fluids*", *Physics Today* **37**, 26-33.
- Evans, D. J. and G. P. Morriss (1983a) "*Isothermal isobaric molecular dynamics*", *Chem. Phys.* **77**, 63-66.
- Evans, D. J. and G. P. Morriss (1983b) "*The isothermal isobaric molecular dynamics ensemble*", *Phys. Lett. A* **98**, 433-436.
- Evans, D. J. and G. P. Morriss (1984a) "*Nonlinear-response theory for steady planar Couette flow*", *Phys. Rev. A* **30**, 1528-1530.
- Evans, D. J. and G. P. Morriss (1984b) "*Non-Newtonian molecular dynamics*", *Comput. Phys. Rep.* **1**, 297-344.
- Evans, D. J. and G. P. Morriss (1990) "*Statistical Mechanics of Nonequilibrium Liquids*", London, Academic Press.
- Evans, D. J. and S. Sarman (1993) "*Equivalence of thermostatted nonlinear responses*", *Phys. Rev. E* **48**, 48-48.

- Farrington, P. J., C. J. Hawker, J. M. J. Fréchet and M. E. Mackay (1998) "*The Melt Viscosity of Dendritic Poly(benzyl ether) Macromolecules*", *Macromolecules* **31**, 5043-5050.
- Fischer, M. and F. Vögtle (1999) "*Dendrimers: From Design to Application - A Progress Report*", *Angew. Chem. Int. Ed.* **38**, 884-905.
- Flory, P. J. and W. R. Krigbaum (1950) "*Statistical Mechanics of dilute Polymer Solutions.II*", *J. Chem. Phys.* **18**, 1086-1094.
- Fréchet, J. M. J. (1994) "*Functional Polymers and Dendrimers: Reactivity, Molecular Architecture, and Interfacial Energy*", *Science* **263**, 1710-1715.
- Ganazzoli, F., R. La Ferla and G. Raffaini (2001) "*Intramolecular Dynamics of Dendrimers under Excluded-Volume Conditions*", *Macromolecules* **34**, 4222-4228.
- Ganazzoli, F., R. La Ferla and G. Terragni (2000) "*Conformational Properties and Intrinsic Viscosity of Dendrimers under Excluded-Volume Conditions*", *Macromolecules* **33**, 6611-6620.
- Ge, J., B. D. Todd, G.-W. Wu and R. J. Sadus (2003) "*Scaling behavior for the pressure and energy of shearing fluids*", *Phys. Rev. E* **67**, 061201.
- Gear, C. W. (1966) "*The numerical integration of ordinary differential equations of various orders*", Argonne National Laboratory.
- Gear, C. W. (1971) "*Numerical Initial Value Problems in Ordinary Differential Equations*", New York, Prentice-Hall, Englewood Cliffs.
- Grest, G. S. and K. Kremer (1986) "*Molecular dynamics simulation for polymers in the presence of a heat bath*", *Phys. Rev. A* **33**, 3628-3631.
- Grest, G. S., K. Kremer and T. A. Witten (1987) "*Structure of many arm star polymers: a molecular dynamics simulation*", *Macromolecules* **20**, 1376-1383.
- Harreis, H. M., C. N. Likos and M. Ballauff (2003) "*Can dendrimers be viewed as compact colloids? A simulation study of the fluctuation in a dendrimer of fourth generation*", *J. Chem. Phys.* **118**, 1979-1988.
- Hawker, C. J., P. J. Farrington, M. E. Mackay, K. L. Wooley and J. M. J. Fréchet (1995) "*Molecular Ball Bearings: The Unusual melt Viscosity Behavior of Dendritic macromolecules*", *J. Am. Chem. Soc.* **117**, 4409-4410.
- Hawker, C. J. and J. M. J. Fréchet (1990) "*Preparation of Polymers with Controlled Molecular Architecture. A New Convergent Approach to Dendritic Macromolecules*", *J. Am. Chem. Soc.* **112**, 7638-7647.
- Hawker, C. J., E. E. Malmström, C. W. Frank and J. P. Kampf (1997) "*Exact linear Analogs of Dendritic Polyether Macromolecules: Design, synthesis, and Unique Properties*", *J. Am. Chem. Soc.* **119**, 9903-9904.

- Hoover, W. G. (1985) "*Canonical dynamics: equilibrium phase-space distributions*", Phys. Rev. A **31**, 1695-1697.
- Hoover, W. G., D. J. Evans, R. B. Hickman, A. J. C. Ladd, W. T. Ashurst and B. Moran (1980) "*Lennard-Jones triple point bulk and shear viscosities. Green-Kubo theory, Hamiltonian mechanics and nonequilibrium molecular dynamics*", Phys. Rev. A **22**, 1690-1697.
- Hoover, W. G., A. J. C. Ladd and B. Moran (1982) "*High strain rate plastic flow studied via nonequilibrium molecular dynamics*", Phys. Rev. Lett. **48**, 1818-1820.
- Hunt, T. A. and B. D. Todd (2003) "*On the Arnold cat map and periodic boundary conditions for planar elongational flow*", Molecular Physics **101**, 3445-3454.
- Jabbarzadeh, A., J. D. Atkinson and R. I. Tanner (2003) "*Effect of Molecular Shape on Rheological Properties in Molecular Dynamics Simulation of Star, H, Comb, and linear Polymer Melts*", Macromolecules **36**, 5020-5031.
- Jackson, C. L., H. D. Chanzy, F. P. Booy, B. J. Drake, D. A. Tomalia, B. J. Bauer and E. J. Amis (1998) "*Visualization of Dendrimer Molecules by Transmission Electron Microscopy (TEM): Staining Methods and Cryo-TEM of Virtified Solutions*", Macromolecules **31**, 6259-6265.
- Karatasos, K., D. B. Adolf and G. R. Davies (2001) "*Statics and dynamics of model dendrimers as studied by molecular dynamics simulations*", J. Chem. Phys. **115**, 5310-5318.
- Khare, R., J. J. de Pablo and A. Yethiraj (1997) "*Rheological, thermodynamic, and structural studies of linear and branched alkanes under shear*", J. Chem. Phys. **107**, 6956-6964.
- Kim, Y. H. and O. W. Webster (1992) "*Hyperbranched polyphenylenes*", Macromolecules **25**, 5561-5572.
- Kioupis, L. I. and E. J. Maginn (1999) "*Molecular Simulation of Poly- $\alpha$ -olefin Synthetic Lubricants: Impact of Molecular Architecture on Performance Properties*", J. Phys. Chem. B **103**, 10781-10790.
- Kioupis, L. I. and E. J. Maginn (2000) "*Impact of Molecular Architecture on the High-Pressure Rheology of Hydrocarbon Fluids*", J. Phys. Chem. B **104**, 7774-7783.
- Kittel, C. (1976) "*Introduction to Solid State Physics*", New York, Wiley.
- Kremer, K. and G. S. Grest (1990) "*Dynamics of entangled linear polymer melts: A molecular-dynamics simulation*", J. Chem. Phys. **92**, 5057-5086.
- Kröger, M. and S. Hess (2000) "*Rheological Evidence for a Dynamical Crossover in Polymer Melts via Nonequilibrium Molecular Dynamics*", Phys. Rev. Lett. **85**, 1128-1131.

- Kröger, M., W. Loose and S. Hess (1993) "*Rheology and structural changes of polymer melts via nonequilibrium molecular dynamics*", J. Rheol. **37**, 1057-1079.
- La Ferla, R. (1997) "*Conformations and dynamics of dendrimers and cascade macromolecules*", J. Chem. Phys. **106**, 688-700.
- Ladd, A. J. C. (1984) "*Non-equilibrium molecular dynamics simulation of molecular fluids*", Mol. Phys. **53**, 459.
- Lees, A. W. and S. F. Edwards (1972) "*The computer study of transport processes under extreme conditions*", J. Phys. C **5**, 1921-1929.
- Lescanec, R. L. and M. Muthukumar (1990) "*Configurational Characteristics and Scaling Behavior of Starburst Molecules: A Computational Study*", Macromolecules **23**, 2280-2288.
- Likos, C. N., S. Rosenfeldt, N. Dingenouts, M. Ballauff, P. Lindner, W. N and F. Vögtle (2002) "*Gaussian effective interaction between flexible dendrimers of fourth generation: A theoretical and experimental study*", J. Chem. Phys. **117**, 1869-1877.
- Likos, C. N., M. Schmidt, H. Lowen, M. Ballauff, D. Potschke and P. Lindner (2001) "*Soft Interaction between Dissolved Flexible Dendrimers: Theory and Experiment*", Macromolecules **34**, 2914-2920.
- Louis, A. A., P. G. Bolhuis, J. P. Hansen and E. J. Meijer (2000) "*Can Polymer Coils Be Modeled as "soft Colloids"?*" Phys. Rev. Lett. **85**, 2522-2525.
- Lue, L. (2000a) "*Equation of state for polymer chains in good solvents*", J. Chem. Phys. **112**, 3442-3449.
- Lue, L. (2000b) "*Volumetric Behavior of Athermal Dendritic Polymers: Monte Carlo Simulation*", Macromolecules **33**, 2266-2272.
- Lue, L. and J. M. Prausnitz (1997) "*Structure and Thermodynamics of Homogenous-Dendritic-Polymer Solutions: Computer Simulation, Integral-Equation, and Lattice-Cluster Theory*", Macromolecules **30**, 6650-6657.
- Lyulin, A. V., D. B. Adolf and G. R. Davies (2001) "*Computer Simulations of Hyperbranched Polymers in Shear Flows*", Macromolecules **34**, 3783-3789.
- Lyulin, A. V., G. R. Davies and D. B. Adolf (2000) "*Brownian Dynamics Simulations of Dendrimers under Shear Flow*", Macromolecules **33**, 3294-3304.
- Mallamace, F., E. Canetta, D. Lombardo, A. Mazzaglia, A. Romeo, L. M. Scolaro and G. Maino (2002) "*Scaling properties in the internal structure of dendrimer systems*", Physica A **304**, 235-243.
- Mansfield, M. L. (2000) "*Monte Carlo Studies of Dendrimers. Additional Results for the Diamond Lattice Model*", Macromolecules **33**, 8043-8049.

- Mansfield, M. L. and M. Jeong (2002) "*Simulation of Lattice Dendrimers by a Monte Carlo Technique with Detailed Balance*", *Macromolecules* **35**, 9794-9798.
- Mansfield, M. L. and L. I. Klushin (1993) "*Monte Carlo Studies of Dendrimer Macromolecules*", *Macromolecules* **26**, 4262-4268.
- Mark, J. E., A. Eisenberg, W. W. Graessley, L. Mandelkern, E. T. Samulski, J. L. Koenig and G. D. Wignall (1993) "*Physical Properties of Polymers*", Washington DC, American Chemical Society.
- Matthews, O. A., A. N. Shipway and J. F. Stoddart (1998) "*Dendrimers - branching out from curiosities into new technologies*", *Prog. Polym. Sci.* **23**, 1-56.
- McCabe, C., S. Cui, P. T. Cummings, P. A. Gordon and R. B. Saeger (2001) "*Examining the rheology of 9-octylheptadecane to giga-pascal pressures*", *J. Chem. Phys.* **114**, 1887-1891.
- McCabe, C., C. W. Manke and P. T. Cummings (2002) "*Predicting the Newtonian viscosity of complex fluids from high strain rate molecular simulations*", *J. Chem. Phys.* **116**, 3339-3342.
- McLeish, T. C. B., J. Allgaier, D. K. Bick, G. Bishko, P. Biswas, R. Blackwell, B. Blottiere, N. Clarke, B. Gibbs, D. J. Groves, A. Hakiki, R. K. Heenan, J. M. Johnson, R. Kant, D. J. Read and R. N. Young (1999) "*Dynamics of Entangled H-Polymers: Theory, Rheology, and Neutron-Scattering*", *Macromolecules* **32**, 6734-6758.
- Morriss, G. P., P. J. Daivis and D. J. Evans (1991) "*The rheology of n alkanes: Decane and eicosane*", *J. Chem. Phys.* **94**, 7420-7433.
- Morriss, G. P. and D. J. Evans (1991) "*A constraint algorithm for the computer simulation of complex molecular liquids*", *Comput. Phys. Commun.* **62**, 267-278.
- Mourey, T. H., S. R. Turner, M. Rubinstein, J. M. J. Fréchet, C. J. Hawker and K. L. Wooley (1992) "*Unique Behavior of Dendritic Macromolecules: Intrinsic Viscosity of Polyether Dendrimers*", *Macromolecules* **25**, 2401-2406.
- Mundy, C. J., J. I. Siepmann and M. L. Klein (1995) "*Decane under shear: A molecular dynamics study using reversible NVT-SLLOD and NPT-SLLOD algorithms*", *J. Chem. Phys.* **103**, 10192-10200.
- Murat, M. and G. S. Grest (1996) "*Molecular Dynamics Study of Dendrimer Molecules in Solvents of Varying Quality*", *Macromolecules* **29**, 1278-1285.
- Naylor, A. M., W. A. Goddard, III, G. E. Kiefer and D. A. Tomalia (1989) "*Starburst Dendrimers. 5. Molecular Shape Control*", *J. Am. Chem. Soc.* **111**, 2239-2341.
- Newkome, G. R., C. N. Moorefield, G. R. Baker, M. J. Saunders and S. H. Grossman (1991) "*Unimolecular Micelles*", *Angew. Chem. Int. Ed.* **30**, 1178-1180.

- Newkome, G. R., C. N. Moorefield and F. Vögtle (2001) *"Dendrimers and Dendrons. Concepts, Syntheses, Applications"*, Weinheim, Wiley-Vch.
- Nosé, S. (1984) *"A molecular dynamics method for simulations in the canonical ensemble"*, Mol. Phys. **52**, 255-268.
- Nunez, C. M., B.-S. Chiou, A. L. Andrady and S. A. Khan (2000) *"Solution Rheology of Hyperbranched Polyesters and Their Blends with Linear Polymers"*, Macromolecules **33**, 1720-1726.
- Patrickios, C. S. and L. Lue (2000) *"Equation of state for star polymers in good solvents"*, J. Chem. Phys. **113**, 5485-5492.
- Pierleoni, C. and J.-P. Ryckaert (1991) *"Non-Newtonian viscosity of atomic fluids in shear and shear-free flows"*, Phys. Rev. A. **44**, 5314-5317.
- Prosa, T. J., B. J. Bauer and E. J. Amis (2001) *"From Start to Spheres: A SAXS Analysis of Dilute Dendrimer Solutions"*, Macromolecules **34**, 4897-4906.
- Prosa, T. J., B. J. Bauer, E. J. Amis, D. A. Tomalia and R. Scherrenberg (1997) *"A SAXS Study of the Internal Structure of Dendritic Polymer Systems"*, Journal of Polymer Science: Part B: Polymer Physics **35**, 2913-2924.
- Roovers, J. and B. Comanita (1999) *"Dendrimers and Dendrimer-Polymer Hybrids"*, Advances in Polymer Science **142**, 179-228.
- Rosenfeldt, S., N. Dingenouts, M. Ballauff, N. Werner, F. Vogtle and P. Lindner (2002) *"Distribution of End Groups within a Dendritic Structure: A SANS Study Including Contrast Variation"*, Macromolecules **35**, 8098-8105.
- Ryckaert, J.-P., A. Belleman, G. Ciccotti and G. V. Paolini (1988) *"Shear-Rate Dependence of the Viscosity of Simple Fluids by nonequilibrium Molecular Dynamics"*, Phys. Rev. Lett. **60**, 128-131.
- Sadus, R. J. (1999) *"Molecular Simulation of Fluids: Theory, Algorithms and Object-Oriented"*, Amsterdam, Elsevier.
- Scherrenberg, R., B. Coussens, P. van Vliet, G. Edouard, J. Brackman and E. de Brabander (1998) *"The Molecular Characteristics of Poly(propyleneimine) Dendrimers As Studied with Small-Angle Neutron Scattering, Viscosimetry, and Molecular Dynamics"*, Macromolecules **31**, 456-461.
- Sendjarevic, I. and a. J. McHugh (2000) *"Effects of Molecular Variables and Architecture on the Rheological Behavior of Dendritic Polymers"*, Macromolecules **33**, 590-596.
- Sheridan, P. F., D. B. Adolf, A. V. Lyulin, I. Neelov and G. R. Davies (2002) *"Computer simulations of hyperbranched polymers: The influence of the Wiener index on the intrinsic viscosity and radius of gyration"*, J. Chem. Phys. **117**, 7802-7812.

- Solc, K. (1971) *"Shape of a Random-Flight Chain"*, J. Chem. Phys. **55**, 335-344.
- Solc, K. and W. H. Stockmayer (1971) *"Shape of a Random-Flight Chains"*, J. Chem. Phys. **54**, 2756-2757.
- Stechemesser, S. and W. Eimer (1997) *"Solvent-Dependent Swelling of Poly(amido amine) Starburst Dendrimers"*, Macromolecules **30**, 2204-2206.
- Stevelmans, S., J. C. M. van Hest, J. F. G. A. Jansen, D. A. F. J. van Boxtl, E. M. M. de Brabander-van den Berg and E. W. Meijer (1996) *"Synthesis, Characterisation, and Guest-Host Properties of Inverted Unimolecular Dendritic Micelles"*, J. Am. Chem. Soc. **118**, 7398-7399.
- Suneel, G. R. S., D. M. A. Buzza, D. J. Groves and T. C. B. McLeish (2002) *"Rheology and Molecular Weight Distribution of Hyperbranched Polymers"*, Macromolecules **35**, 9605-9612.
- Tande, B. M., N. J. Wagner and Y. H. Kim (2003) *"Influence of End Groups on Dendrimer Rheology and Conformation"*, Macromolecules **36**, 4619-4623.
- Theodorou, D. N. and U. W. Suter (1985) *"Shape of Unperturbed Linear Polymers: Polypropylene"*, Macromolecules **18**, 1206-1214.
- Timoshenko, E. G., Y. A. Kuznetsov and R. Connolly (2002) *"Conformation of dendrimers in dilute solution"*, J. Chem. Phys. **117**, 9050-9062.
- Todd, B. D. and P. J. Daivis (1997) *"Elongational viscosities from nonequilibrium molecular dynamics simulations of oscillatory elongational flow"*, J. Chem. Phys. **107**, 1617-1624.
- Todd, B. D. and P. J. Daivis (1998) *"Nonequilibrium Molecular Dynamics Simulations of Planar Elongational Flow with Spatially and Temporally Periodic Boundary Conditions"*, Phys. Rev. Lett. **81**, 1118-1121.
- Todd, B. D. and P. J. Daivis (1999) *"A new algorithm for unrestricted duration nonequilibrium molecular dynamics simulations of planar elongational flow"*, Comput. Phys. Commun. **117**, 191-199.
- Todd, B. D. and P. J. Daivis (2000) *"The stability of nonequilibrium molecular dynamics simulations of elongational flows"*, J. Chem. Phys. **112**, 40-46.
- Tomalia, D. A., H. Baker, J. Dewald, M. Hall, G. Kallos, S. Martin, J. Roeck, J. Ryder and P. Smith (1986) *"Dendritic Macromolecules: Synthesis of Starburst Dendrimers"*, Macromolecules **19**, 2466-2468.
- Tomalia, D. A., H. Baker, J. R. Dewald, M. Hall, G. Kallos, S. Martin, J. Roeck, J. Ryder and P. Smith (1985) *"A new class of polymers: Starburst-dendritic macromolecules"*, Polym. J. **17**, 117-132.

- Tomalia, D. A., A. M. Naylor and W. A. Goddard III (1990) *"Starburst Dendrimers: Molecular-Level Control of Size, Shape, surface Chemistry, Topology, and Flexibility from Atoms to Macroscopic Matter"*, *Angew. Chem. Int. Ed. Engl.* **29**, 138-175.
- Topp, A., B. J. Bauer, J. W. Klimash, R. Splinder, D. A. Tomalia and E. J. Amis (1999) *"Probing the Location of the Terminal Groups of Dendrimers in Dilute Solution"*, *Macromolecules* **32**, 7226-7231.
- Travis, K. P., P. J. Daivis and D. J. Evans (1995a) *"Computer simulation algorithms for molecules undergoing planar Couette flow: A nonequilibrium molecular dynamics study"*, *J. Chem. Phys.* **103**, 1109-1118.
- Travis, K. P., P. J. Daivis and D. J. Evans (1995b) *"Thermostats for molecular fluids undergoing shear flow: Application to liquid chlorine"*, *J. Chem. Phys.* **103**, 10638-10651.
- Twyman, L. J., A. S. H. King and I. K. Martin (2002) *"Catalysis inside dendrimers"*, *Chem. Soc. Rev.* **31**, 69-82.
- Uppuluri, S., S. E. Keinath, D. A. Tomalia and P. R. Dvornic (1998) *"Rheology of Dendrimers. 1. Newtonian Flow Behaviour of Medium and Highly Concentrated Solutions of Polyamidoamine (PAMAM) Dendrimers in Ethylenediamine (EDA) Solvent"*, *Macromolecules* **31**, 4498-4510.
- Uppuluri, S., F. A. Morrison and P. R. Dvornic (2000) *"Rheology of Dendrimers. 2. Bulk Polyamidoamine Dendrimers under Steady Shear, Creep, and Dynamic Oscillatory Shear"*, *Macromolecules* **33**, 2551-2560.
- Vinogradov, C. V. and A. Y. Malkin (1980) *"Rheology of Polymers"*, Berlin, Springer.
- von Ferber, C. and A. Blumen (2002) *"Dynamics of dendrimers and of random built branched polymers"*, *J. Chem. Phys.* **116**, 8616-8624.
- Warner, H. R., Jr. (1972) *"Kinetic theory and rheology of dilute suspensions of finitely extensible dumbbells"*, *Ind. Eng. Chem. Fundam.* **11**, 379-387.
- Watanabe, S. and S. L. Regen (1994) *"Dendrimers as Building Blocks for Multilayer Construction"*, *J. Am. Chem. Soc.* **116**, 8855-8856.
- Weeks, J. D., D. Chandler and H. C. Anderson (1971) *"Role of repulsive forces in determining the equilibrium structure of simple liquids"*, *J. Chem. Phys.* **54**, 5237-5247.
- Wooley, K. L., C. A. Klug, K. Tasaki and J. Schaefer (1997) *"Shapes of Dendrimers from Rotational-Echo Double-Resonance NMR"*, *J. Am. Chem. Soc.* **119**, 53-58.
- Wu, G.-W. and R. J. Sadus (2005) *"Hard Sphere Compressibility Factors for Equation of State Development"*, *AIChE Journal* **51**, 309-313.
- Xu, Z., J. J. de Pablo and S. Kim (1995) *"Transport properties of polymer melts from nonequilibrium molecular dynamics"*, *J. Chem. Phys.* **102**, 5836-5844.

Xu, Z., R. Khare, J. J. de Pablo and S. Kim (1997) "*On the calculation of transport properties of polymer melts from nonequilibrium molecular dynamics*", J. Chem. Phys. **106**, 8285-8286.

Zacharopoulos, N. and I. G. Economou (2002) "*Morphology and Organization of Poly(propylene imine) Dendrimers in the Melt from Molecular Dynamics Simulation*", Macromolecules **35**, 1814-1821.

Zimmerman, S. C., F. Zeng, D. E. C. Reichert and S. V. Kolotuchin (1996) "*Self-Assembling Dendrimers*", Science **271**, 1095-1098.

Zook, T. C. and G. T. Pickett (2003) "*Hollow-Core Dendrimers Revisited*", Phys. Rev. Lett. **90**, 015502.