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Polymer 43 (2002) 357–368

polymer

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A dedication in honor of Professor Wayne Lee Mattice

'Gentle Scholar' was a nickname given to Wayne L. Mattice by a former graduate student. Those of us fortunate enough to work with Wayne know how well this phrase describes both his nature and professional abilities. With over 300 manuscripts published, Wayne is truly an inspiration to other scientists working in the field of polymer simulations.

Wayne's interest in conformational analysis was evident as early as the 1960s with his PhD work in biochemistry, under the guidance of Ronald C. Greene at Duke University. His 1968 dissertation was titled "Synthesis and Conformational Studies of a Block Copolymer of L-Alanine and Ethylene Glycol". After receiving his PhD, Wayne spent 2 years working with Leo Mandelkern as a USPHS Postdoctoral Fellow at Florida State University. During this time he performed a thorough investigation of the conformational properties of poly-L-proline. In 1970, Wayne became a member of the faculty at Louisiana State University in the Department of Biochemistry, where he continued to study polypeptides, and began research on synthetic-polymers. By the middle of the 1970s, Wayne had published his initial manuscripts on the use of the rotational isomeric state model to study macromolecules, an area to which he would continue to make contributions for many years, clearly establishing himself as the field's intellectual leader. From 1977 to 1986, Wayne was a faculty member in the Department of Chemistry at Louisiana State University, where he held the Boyd professorship. During this time, Wayne began investigations on polymeric proanthocyanidins, also known as condensed tannins. Over the next 10 years, Wayne would contribute some of the fundamental conformational studies on the condensed tannins. Since 1986, Wayne has been the Alex Schulman Professor in the Department of Polymer Science at the University of Akron. In this position he has completed computer simulations on a variety of polymers. Over the course of his career, Wayne has held positions as a Guggenheim Fellow with Paul J. Flory at Stanford University, a Visiting Professor with Harold. A. Scheraga at Cornell University, a Gastprofessor with Ulrich W. Suter at ETH, and a Sabbatical Faculty Member with John G. Curro at Sandia National Laboratory.

Through Wayne's research efforts including Monte Carlo methods, molecular dynamics, and most importantly, Rotational Isomeric State Theory, he continues to help develop the field of polymer simulations. He and Ulrich W. Suter coauthored the book "Conformation Theory of Large Molecules: The Rotational Isomeric State Model in Macromolecular Systems". As a result of his expertise, Wayne was invited by the American Chemical Society to create a short course entitled "Molecular Modeling of Polymers", which has been a mainstay of ACS's continuing education series for the past 10 years. Furthermore, Wayne currently is an Associate Editor for Macromolecules, a member of the editorial boards for both Computational and Theoretical Polymer Science and Macromolecular Theory and Simulations, and a member of the advisory board for Biopolymers. In addition to computational methods, Wayne has expertise in experimental methods such as circular dichroism, fluorescence spectroscopy, and nuclear magnetic resonance spectroscopy and their use to study conformational transitions.

As a faculty member and mentor, Wayne has directed 29 graduate students to the completion of their PhD Dissertations. His quiet manner allows his students ample freedom to explore their research projects, but he is always willing to spend time providing ideas and guidance, when necessary. In addition, he has the rare ability to make even complex topics like polymer simulations readily accessible to students and colleagues alike. His own hard work and dedication to his research provide motivation to his research group. Along with his scientific expertise, Wayne's caring and personal side is also evident to his research group from his one–on–one lunches after Friday group meetings to his group picnics, complete with nature hikes. Those who know and have worked with Wayne consider themselves very fortunate indeed to have the opportunity to learn from such an excellent teacher and scientist.

Carin A. Helfer
Guest Editor

As editor of this journal, I would like to add my thanks to Wayne Mattice for his many contributions in the area of polymer computations and theory. In the most general sense, all of us interested in this type of research can express our appreciation to Wayne for his numerous studies on polymeric systems, for the students he has produced who now make their own independent research contributions, and for the scholarly example he has set for many of us.

PII: S0032-3861(01)00434-7

In a more specific sense, it is important to acknowledge Wayne's contributions to our journal, Computational and Theoretical Polymer Science. Over this first 10-year period, he contributed twenty-two articles, and helped tremendously with the usual refereeing chores. In addition, he continues to be indispensable as a member of our Editorial Board, being one of our most effective advisors. The journal has benefited greatly from his participation, and Elsevier and I are greatly indebted to him.

J.E. Mark
Editor

List of publications

Wayne L. Mattice
Alex Schulman Professor
The University of Akron

Document update September 10, 2000

Books

[1] Williams VR, Mattice WL, Williams HB. Basic physical chemistry for the life sciences. 3rd ed. New York: Freeman, 1978. 442 p.
[2] Mattice WL, Suter UW. Conformational theory of large molecules. The rotational isomeric state model in macromolecular systems. New York: Wiley, 1994. ISBN 0-471-84338-5, 449 p.

Refereed publications
Summary by Location and Publisher

Location	Publisher	Number
Macromolecules	American Chemical Society	119
Biopolymers	John Wiley and Sons	30
J Chem Phys	American Institute of Physics	28
Comput Theor Polym Sci	Elsevier Science Ltd	22
J Am Chem Soc	American Chemical Society	17
Polymer	Elsevier Science Ltd	13
J Polym Sci, Polym Phys Ed	John Wiley and Sons	11
Macromol Theory Simul	Wiley–VCH	9
Langmuir	American Chemical Society	9
J Chem Soc, Perkin Trans II	Royal Society of Chemistry	5
J Phys Chem	American Chemical Society	5
Biochemistry	American Chemical Society	4
Int J Biol Macromol	Butterworth Scientific	4
Biochim Biophys Acta	Elsevier Biomedical Press	3
J Comput Chem	John Wiley and Sons	3
Polym Commun	Butterworth Scientific	3
Colloid Polym Sci	Steinkopff	2
J Comput-Aided Mater Des	Kluwer	2
J Fluorescence	Plenum Publishing Co.	2
J Membr Sci.	Elsevier Science Publishers	2
Miscellaneous		16
Refereed manuscripts published and in press		314

Complete citations for refereed publications

[1] Mattice WL, Mandelkern L. Conformational properties of poly-L-proline in concentrated salt solutions. Biochemistry 1970;9:1049–58.
[2] Mattice WL, Mandelkern L. The conformational transition induced in poly(4-hydroxy-L-proline) by calcium chloride. Macromolecules 1970;3:199–201.
[3] Mattice WL, Mandelkern L. Ordered structures in sequential copolypeptides containing L-proline or 4-hydroxy-L-proline. J Am Chem Soc 1970;92:5285–7.
[4] Mattice WL, Mandelkern L. Conformational properties of poly-L-proline Form II in dilute solution. J Am Chem Soc 1971;93:1769–77.
[5] Mattice WL, Mandelkern L. Development of ordered structures in sequential copolypeptides containing L-proline and γ-hydroxy-L-proline. Biochemistry 1971;10:1926–33.
[6] Mattice WL, Mandelkern L. Unperturbed dimensions of sequential copolypeptides containing glycine, L-alanine, L-proline, and γ-hydroxy-L-proline. Biochemistry 1971;10:1934–42.
[7] Mattice WL, Mandelkern L. On the heat precipitation of poly(L-proline). Macromolecules 1971;4:271–4.
[8] Mattice WL, Lo JT, Mandelkern L. A comparison of the effects of salt and temperature on charged and uncharged polypeptides in water. Macromolecules 1972;5:729–34.
[9] Mattice WL, Lo JT. Unperturbed dimensions of poly(N^5-ω-hydroxyethyl-L-glutamine) in water. Macromolecules 1972;5:734–9.
[10] Mattice WL, Nishikawa K, Ooi T. Conformational properties of poly(L-proline) containing a flexible pyrrolidine ring. Macromolecules 1973;6:443–6.
[11] Mattice WL. Minimum chain length required for the observation of a temperature-sensitive, salt-sensitive positive circular dichroism band in derivatives of L-alanine. J Am Chem Soc 1973;95:5800–2.
[12] Mattice WL. Comparison of the conformational map for poly(L-proline) with conformational maps for polysarcosine and poly(*N*-methyl-L-alanine). Macromolecules 1973;6:855–8.
[13] Rabenold DA, Mattice WL, Mandelkern L. Influence of conformational isomers on the circular dichroism of poly(L-prolylglycine). Macromolecules 1974;7:43–7.
[14] Mattice WL. The effect of temperature and salt concentration on the circular dichroism exhibited by unionized derivatives of L-alanine in aqueous solution. Biopolymers 1974;13:169–83.
[15] Ooi T, Clark DS, Mattice WL. Conformational properties of poly(γ-hydroxy-L-proline) based on rigid and flexible pyrrolidine rings. Macromolecules 1974;7:337–43.
[16] Arnett AF, Newkome G, Mattice WL, McGlynn SP. Excited electronic states of the α-dicarbonyls. J Am Chem Soc 1974;96:4385–92.
[17] Mattice WL, Harrison III WH. Estimation of the circular dichroism exhibited by statistical coils of poly(L-alanine) and unionized poly(L-lysine) in water. Biopolymers 1975;14:2025–33.
[18] Mattice WL. The configuration partition function, a priori probabilities, and conditional probabilities for branched macromolecules subject to the rotational isomeric state approximation. Macromolecules 1975;8:644–51.
[19] Lo JT, Mattice WL. Evidence from circular dichroism for the binding of hydrogen ions and calcium ions by poly(L-proline). Biopolymers 1976;15:15–19.
[20] Mattice WL. Conformational properties of a molecule consisting of three branches emanating from a common atom, evaluated using rotational isomeric state theory. Macromolecules 1976;9:48–52.
[21] Mattice WL, Carpenter DK. Mean-square unperturbed radii of gyration for molecules containing a single trifunctional or tetrafunctional branch point and having short-range interactions represented by a symmetric threefold rotation potential. Macromolecules 1976;9:53–8.

[22] Mattice WL, Harrison III WH. The importance of coulombic interactions for the induction of β structure in lysine oligomers by sodium dodecyl sulfate. Biopolymers 1976;15:559–67.
[23] Mattice WL, Carpenter DK. Behavior of the intramolecular scattering function in its representation by Nagai's series. J Chem Phys 1976;64:3261–5.
[24] Mattice WL. Mean-squared optical anisotropies for alkanes containing a single trifunctional or tetrafunctional branch point. J Am Chem Soc 1976;98:3466–70.
[25] Mattice WL, Riser JM, Clark DS. Conformational properties of the complexes formed by proteins and sodium dodecyl sulfate. Biochemistry 1976;15:4264–72.
[26] Carpenter DK, Mattice WL. Influence of fluctuations in electron density on the excess small-angle X-ray scattering from dilute solutions of macromolecules. Biopolymers 1977;16:67–80.
[27] Mattice WL, Carpenter DK. Effect of the fluctuations in electron density within a globular protein on the excess small-angle X-ray scattering. Biopolymers 1977;16:81–94.
[28] Mattice WL. Rotational isomeric state treatment of the cystine residue. Configuration partition function and its relationship to the optical activity exhibited by the disulfide bond. J Am Chem Soc 1977;99:2324–30.
[29] Clark DS, Mattice WL. Hydrodynamic properties and unperturbed dimensions of poly(γ-hydroxy-L-proline) in aqueous solution. Macromolecules 1977;10:369–74.
[30] McCord RW, Blakeney Jr EW, Mattice WL. Conformational changes induced in ionized poly(L-arginine) and poly(L-histidine) by sodium dodecyl sulfate. Biopolymers 1977;16:1319–29.
[31] Mattice WL. Unperturbed dimensions for homopolypeptides and sequential copolypeptides cross-linked via a disulfide bond. Macromolecules 1977;10:511–6.
[32] Mattice WL. Unperturbed dimensions of disordered proteins containing an interchain di-sulfide cross-link. Macromolecules 1977;10:516–20.
[33] Hawkins ER, Chang SH, Mattice WL. Kinetics of the renaturation of yeast $tRNA_3^{Leu}$. Biopolymers 1977;16:1557–66.
[34] Mattice WL. Configuration partition functions for vinyl polymers containing articulated side chains with threefold rotational potentials. Macromolecules 1977;10:1171–7.
[35] Mattice WL. Moment of inertia tensors and center of mass vectors for flexible molecules containing a trifunctional branch point. Macromolecules 1977;10:1177–81.
[36] Mattice WL. Persistence vectors, average center of mass vectors, and moment of inertia tensors for branched polymethylenes. Macromolecules 1977;10:1182–6.
[37] Mattice WL. Changes in unperturbed dimensions accompanying helix-coil transitions in cross-linked homopolypeptides, with special reference to poly(hydroxybutyl-L-glutamine). Macromolecules 1978;11:15–18.
[38] Mattice WL. Dependence of unperturbed dimensions and dipole moments of polydialkyl-siloxanes upon alkyl group length. Macromolecules 1978;11:517–21.
[39] Mattice WL, Saiz E. Dipole moment, optical anisotropy, and molar Kerr constant of triacetin. J Am Chem Soc 1978;100:6308–14.
[40] Mattice WL. Unperturbed dimensions of crosslinked histones evaluated using random-flight statistics and rotational isomeric state theory. Biopolymers 1979;18:225–37.
[41] Mattice WL. Size and asymmetry of spatial distributions for unperturbed triglycerides. J Am Chem Soc 1979;101:732–6.
[42] Mattice WL, McCord RW, Shippey PM. Disorder–order transitions induced in anionic homo-polypeptides by cationic detergents. Biopolymers 1979;18:723–30.
[43] Schwartz RW, Mattice WL, Spirtes MA. Melanostatin conformations in solution. Biopolymers 1979;18:1835–48.
[44] Newkome GR, Nayak A, Fronczek F, Kawato T, Taylor HCR, Meade L, Mattice W. Synthesis and temperature-dependent conformational preferences of macrocycles containing the 2,2′-bipyridyl moiety. J Am Chem Soc 1979;101:4472–7.
[45] Mattice WL, Newkome GR. Molecular origin of the temperature-dependent nmr spectrum of 1:1 crown ether macrocycles containing a 2,2′-bipyridyl subunit. J Am Chem Soc 1979;101:4478–80.
[46] Mattice WL. Dimensional changes accompanying the formation of poly(oxyethylene) macro-cycles. Macromolecules 1979;12:944–8.
[47] Mattice WL. Radius of gyration, asymmetry, and head-group orientation in unperturbed lecithins. J Am Chem Soc 1979;101:7651–4.
[48] Mattice WL. Macrocyclization of poly(thiaethylene). J Am Chem Soc 1980;102:2242–5.
[49] Mattice WL. Asymmetry of flexible chains, macrocycles, and stars. Macromolecules 1980;13:506–11.
[50] Mattice WL. Averaged principal moments of the inertia tensor for unperturbed poly(hydroxy-butyl-L-glutamine) as it passes through the helix–coil transition. Macromolecules 1980;13:904–9.
[51] Mattice WL, Srinivasan G, Santiago G. Helix end effects in block copolypeptides, proteins, and protein–detergent complexes. Macromolecules 1980;13:1254–60.
[52] McCord RW, Madison EL, Mattice WL. Experimental characterization of poly(hydroxyalkyl-L-glutamine) conformations in aqueous calcium chloride and sodium perchlorate solutions. Biopolymers 1980;19:1923–41.
[53] Mattice WL, Santiago G. Matrix treatment of configuration-dependent physical properties of simple chains perturbed by long-range interactions. Macromolecules 1980;13:1560–7.
[54] Mattice WL. Configurational statistics of unperturbed wormlike and rotational isomeric state stars of finite size. Macromolecules 1981;14:143–7.
[55] Skolnick J, Mattice WL. Rates of conformational transitions in branched chain molecules. Macromolecules 1981;14:292–9.
[56] Mattice WL, Skolnick J. Conformational properties of bolaform electrolytes. Macromolecules 1981;14:863–7.
[57] Mattice WL, Robinson RM. Conformational properties of central nervous system myelin basic protein, β-endorphin, and β-lipotropin in water and in the presence of anionic lipids. Biopolymers 1981;20:1421–34.
[58] Mattice WL, Napper DH. End effects and asymmetries of the distribution of chain atoms in polymethylene chains perturbed by attachment to an impenetrable interface. Macromolecules 1981;14:1066–71.
[59] Santiago G, Maroun RC, Hawkins ER, Mattice WL. Electrostatic interactions in ionic homo-polypeptides in solutions of moderate ionic strength. Biopolymers 1981;20:2181–94.
[60] Mattice WL, Skolnick J. Trans placements, expansion, and asymmetry of starlike poly-ethylenes bearing similarly charged ends. Macromolecules 1981;14:1463–8.
[61] Mattice WL, Stehling FC. Branch formation in low-density polyethylene. Macromolecules 1981;14:1479–84.
[62] Mattice WL. Generator matrix and Monte Carlo treatments of simple chains with excluded volume. Asymmetry and overall expansion of finite chains. Macromolecules 1981;14:1485–90.
[63] Mattice WL. Subchain expansion in generator matrix and Monte Carlo treatments of simple chains with excluded volume. Macromolecules 1981;14:1491–5.
[64] Mattice WL. Angular scattering functions for subchains defined by a generator matrix treatment of simple chains with excluded volume. Macromolecules 1981;15:579–82.
[65] Robinson RM, Blakeney Jr. EW, Mattice WL. Lipid-induced conformational changes in glucagon, secretin, and vasoactive intestinal peptide. Biopolymers 1982;21:1217–28.
[66] Mattice WL, Tobiason FL, Houglum K, Shanafelt A. Conformational analysis and dipole moments of tetra-*O*-methyl-(+)-epicatechin. J Am Chem Soc 1982;10:3359–62.
[67] Mattice WL, Skolnick J. Stability of the cross-linked tropomyosin dimer: cross-link effect on the cooperativity of the ordering process

and on the maximum in the helix probability profile. Macromolecules 1982;15:1088–93.
[68] Salinovich O, Mattice WL, Blakeney Jr. EW. Effects of temperature, pH, and detergents on the molecular conformations of the enterotoxin of *Clostridium perfringens*. Biochim Biophys Acta 1982;707:147–53.
[69] Mattice WL, Newkome GR. Monte Carlo study of macrocyclization to form benzo-crown ethers. J Am Chem Soc 1982;104:5942–4.
[70] Darsey JA, Mattice WL. Local configuration of poly (L-proline) in dilute solution. Macromolecules 1982;15:1626–31.
[71] Mattice WL. Unperturbed rotational isomeric state and wormlike polymethylene stars of high branch point functionality. Macromolecules 1982;15:1633–4.
[72] Hawkins ER, Robinson RM, Mattice WL. Helix initiation and propagation by (hydroxyethyl)-L-glutaminyl residues in water. Macromolecules 1983;16:158–61.
[73] Mattice WL. Complex branch formation in low-density polyethylene. Macromolecules 1983;16:487–90.
[74] Hamed MM, Robinson RM, Mattice WL. Behavior of amphipathic helices on analysis via matrix methods, with application to glucagon, secretin, and vasoactive intestinal peptide. Biopolymers 1983;22:1003–21.
[75] Hamed MM, Robinson RM, Mattice WL. Helix formation upon acidification of protein–dodecyl sulfate complexes. Biochim Biophys Acta 1983;743:260–7.
[76] Erie D, Darsey JA, Mattice WL. Representative configurations of unperturbed poly(L-alanine) chains. Macromolecules 1983;16:910–4.
[77] Mattice WL. Expansion of perturbed rotational isomeric state polymethylene stars. Macromolecules 1983;16:1623–7.
[78] Maroun RC, Mattice WL. Influence of L-cystinyl side-chain configurations on the melting of cross-linked α-tropomyosin dimers. Biochim Biophys Acta 1984;784:133–9.
[79] Hamed MM, Mattice WL. Mean-square hydrophobic moment for partially helical polypeptides. Biopolymers 1984;23:201–12.
[80] Mattice WL. Changes in unperturbed dimensions upon formation of regular β meanders. Macromolecules 1984;17:407–14.
[81] Mattice WL. Rotational isomeric state polymethylene stars in which atoms participating in long-range interactions behave as hard spheres. Macromolecules 1984;17:415–8.
[82] Mattice WL, Carpenter DK. Mean square dipole moments in rotational isomeric state chains containing atoms that behave as hard spheres. Macromolecules 1984;17:625–30.
[83] Hamed MM, Mattice WL. Mean-square helical hydrophobic moments in partially ordered proteins. Biopolymers 1984;23:1057–66.
[84] Baldwin DT, Mattice WL, Gandour RD. Molecular mechanics assessment of the configurational statistics of polyoxyethylene. J Comput Chem 1984;5:241–7.
[85] Mattice WL, Porter LJ. Molecular weight averages and ^{13}C NMR intensities provide evidence for branching in proanthocyanidin polymers. Phytochemistry 1984;23:1039–311.
[86] Overgaard T, Erie D, Darsey JA, Mattice WL. Helix formation by hydroxyamyl-L-glutaminyl residues in water and aqueous sodium dodecyl sulfate. Biopolymers 1984;23:1595–603.
[87] Mattice WL, Scheraga HA. Matrix formulation of the transition from a statistical coil to an intramolecular antiparallel β sheet. Biopolymers 1984;23:1701–24.
[88] Fronczek FR, Gannuch G, Mattice WL, Tobiason FL, Broeker JL, Hemingway RW. Dipole moment, solution, and solid state structure of (−)-epicatechin, a monomer unit of procyanidin polymers. J Chem Soc, Perkin Trans II 1984:1611–6.
[89] Mattice WL, Scheraga HA. Suppression of the statistical coil state during the $\alpha \rightarrow \beta$ transition in homopolypeptides. Biopolymers 1984;23:2879–90.
[90] Mattice WL, Scheraga HA. Practical estimates of the upper limit for the distribution function for strand lengths in large homopolymers containing intramolecular antiparallel sheets with tight bends. Macromolecules 1984;17:2690–6.
[91] Mattice WL. Expansion of the end-to-end distance and radius of gyration in perturbed poly-methylene chains. J Phys Chem 1984;88:6492–4.
[92] Hamed MM, Mattice WL. Helical hydrophobic moment profiles in α and β tropomyosin. Int J Biol Macromol 1985;7:15–18.
[93] Mattice WL, Lee E, Scheraga HA. Dominance of irregular structures in the formation of intra-molecular antiparallel β sheets by homopolyamino acids. Can J Chem 1985;63:140–6.
[94] Mattice WL, Scheraga HA. Role of interstrand loops in the formation of intramolecular cross-β-sheets by homopolyamino acids. Biopolymers 1985;24:565–79.
[95] Viswanadhan VN, Mattice WL. Poly(vinyl acetate) as a test of the Roedel mechanism for short branch formation. Makromol Chem 1985;186:633–40.
[96] Mattice WL. Similar matrix expressions describe configuration partition functions for intrachain formation of antiparallel β sheets and interacting α helices. Macromolecules 1985;18:1345–6.
[97] Fronczek FR, Gannuch G, Mattice WL, Hemingway RW, Chiari G, Tobiason FL, Houglum K, Shanafelt A. Preference for occupancy of axial positions by substituents bonded to the heterocyclic ring in penta-*O*-acetyl-(+)-catechin in the crystalline state. J Chem Soc Perkin Trans II 1985:1383–6.
[98] Viswanadhan VN, Mattice WL. Short-branch formation via the Roedel mechanism in copolymers of ethylene and vinyl acetate. J Polym Sci, Polym Phys Ed 1985;23:1957–65.
[99] Mattice WL, Carpenter DK, Barkley MD, Kestner NR. The multivariate gaussian distribution and the dipole moments of perturbed chains. Macromolecules 1985;18:2236–8.
[100] Mattice WL. Stabilization of short helices by intramolecular cluster formation. Biopolymers 1985;24:2231–42.
[101] Lin TH, Cherry WR, Mattice WL. Acridine fluoresence as a probe of micelle formation by sodium dodecyl sulfate in the presence of poly[*N*-(ω-hydroxyalkyl)-L-glutamines]. Polym Commun 1986;27:37–8.
[102] Mattice WL, Viswanadhan VN. Stereochemical selectivity during the formation of $CH_2R–CH_2–CHR–CH2–$ branches in the free radical initiated polymerization of monosubstituted vinyl monomers. Macromolecules 1986;19:568–71.
[103] Maroun RC, McCord RW, Mattice WL. Triangular matrix representation of dimensionless helical hydrophobic moment ratios. Int J Biol Macromol 1986;8:73–78.
[104] Porter LJ, Wong RY, Benson M, Chan BG, Viswanadhan VN, Gandour RD, Mattice WL. Conformational analysis of flavans: ^1H NMR and molecular mechanical (MM2) studies of the benzpyran ring of 3′,4′, 5,7-tetrahydroxyflavan-3-ols: the crystal and molecular structure of the procyanidin (2*R*,3*S*,4*R*)-3prime;,4′,5,7-tetramethoxy-4-(2,4,6-trimethoxyphenyl)-flavan-3-ol. J Chem Res (S) 1986: 86–87, J Chem Res (M) 1986: 0830–0880.
[105] Tilstra L, Strickland TC, Clark DS, Mattice WL. Helix formation by polybis(hydroxyethyl)-L-glutamine. Colloid Polym Sci 1986;264:469–72.
[106] Mattice WL. Helix breakers in block copolypeptides. Biopolymers 1986;25:1449–59.
[107] Mattice WL, Lloyd AC. Dipole moments of perturbed poly(vinyl chloride), poly(vinyl bromide), and poly(*p*-chlorostyrene). Macromolecules 1986;19:2250–3.
[108] Mattice WL. Reduction of the unperturbed dimensions of the main chain when ethyl groups are attached to a poly(methylene) backbone. Macromolecules 1986;19:2303–5.
[109] Mandelkern L, Alamo R, Mattice WL, Snyder RG. Observation of the Raman D-LAM band in ethylene copolymers: hydrogenated polybutadiene. Macromolecules 1986;19:2404–8.
[110] Mattice WL, Saiz E. Response of the mean-square optical anisotropy of chain molecules to the imposition of excluded volume. J Polym Sci, Polym Phys Ed 1986;24:2669–79.

[111] Viswanadhan VN, Mattice WL. Conformational analysis of the sixteen C(4)–C(6) and C(4)–C(8) dimers of (+)-catechin and (−)-epicatechin. J Comput Chem 1986;78:711–7.
[112] Mattice WL, Tilstra L. Basis for large differences in the cooperativity of the formation of antiparallel β-sheets and clusters of interacting α-helices in isolated chains. Biopolymers 1987;26:203–11.
[113] Viswanadhan VN, Mattice WL. Assessment of bond rotation interdependence in polymer chains: an information theory approach. Macromolecules 1987;20:685–8.
[114] Viswanadhan VN, Mattice WL. Assessment by molecular mechanics of the preferred conformations of the sixteen C(4)–C(6) and C(4)–C(8) linked dimers of (+)-catechin and (−)-epicatechin with axial or equatorial dihydroxyphenyl substituents at C(2). J Chem Soc Perkin Trans II 1987:739–43.
[115] Viswanadhan VN, Bergmann WR, Mattice WL. Configurational statistics of C(4)–C(8) linked homopolymers of (+)-catechin or (−)-epicatechin. Macromolecules 1987;20:1539–43.
[116] Mathur SC, Mattice WL. Ties, loops, and tight folds in ethylene-1-alkene copolymers with different 1-alkene components. Macromolecules 1987;20:2165–7.
[117] Bergmann WR, Barkley MD, Hemingway RW, Mattice WL. Heterogeneous fluorescence decay of (4β → 6)- and (4β → 8)-linked dimers of (+)-catechin and (−)-epicatechin as a result of rotational isomerism. J Am Chem Soc 1987;109:6614–9.
[118] Mattice WL. The role of $\langle r^2\,\mu^2\rangle_0$ in the response of the mean square dipole moment to the expansion of a family of model chains. J Chem Phys 1987;87:5512–7.
[119] Lin TH, Leed AR, Scheraga HA, Mattice WL. Helix initiation and propagation by isolated arginine residues in aqueous sodium dodecyl sulfate. Macromolecules 1988;21:131–6.
[120] Bergmann WR, Viswanadhan VN, Mattice WL. Conformations of polymeric proantho-cyanidins composed of (+)-catechin or (−)-epicatechin joined by 4β → 6 interflavan bonds. J Chem Soc Perkin Trans II 1988:45–47.
[121] Viswanadhan VN, Mattice WL. Configurational statistics of C(4)–C(8) linked polymers of (+)-catechin or (−)-epicatechin with mixed axial/equatorial substituents at C(2). Int J Biol Macromol 1988;10:9–14.
[122] Tilstra LF, Mattice WL. Collapse of a polypeptide chain as a result of the intramolecular formation of antiparallel β sheets. Biopolymers 1988;27:805–19.
[123] Mendicuti F, Viswanadhan VN, Mattice WL. Dependence of the occupancy of excimer-forming conformations on the size of the flexible spacer in polyesters from terephthalic acid and mono, di or triethylene glycol. Polymer 1988;29:875–9.
[124] Mathur SC, Mattice WL. Nonuniform distribution of short branches in two-dimensional simulations of the amorphous regions between two crystalline lamellae. Macromolecules 1988;21:1354–60.
[125] Bahar I, Mattice WL. The configurational contribution to the segmental orientation in network chains subject to perturbation by the excluded volume effect. J Chem Phys 1988;89:1153–8.
[126] Quirk RP, Perry S, Mendicuti F, Mattice WL. New method for quantitative functionalization of the terminus in poly(styrene). Naphthalene functionalization. Macromolecules 1988;21:2294–5.
[127] Viswanadhan VN, Mattice WL. Conformation of monomers and dimers of 2,3-*trans* and 2,3-*cis* flavan-3-ols with differing hydroxylation patterns in the B-ring. Int J Biol Macromol 1988;10:209–12.
[128] Lin TH, Leed AR, Scheraga HA, Mattice WL. Helix destabilization caused by the interaction of unaggregated sodium dodecyl sulfate with isolated lysine residues. Macromolecules 1988;21:2447–52.
[129] Mattice WL, Snyder RG. Configurational properties of finite cyclic alkanes. Macromolecules 1988;21:2452–6.
[130] Tilstra LF, Maeda H, Mattice WL. Interaction of (+)-catechin with the edge of the β sheet formed by poly(*S*-carboxymethyl-L-cysteine). J Chem Soc Perkin Trans II 1988:1613–6.
[131] Mendicuti F, Patel B, Viswanadhan VN, Mattice WL. Identification of conformations conducive to intramolecular excimer formation in polyesters with different numbers of methylene units between aromatic rings. Polymer 1988;29:1669–74.
[132] Mattice WL, Némethy G, Scheraga HA. Conformational entropy associated with the forma-tion of internal loops in collagen. Macromolecules 1988;21:2811–8.
[133] Mattice WL. Behavior of $\langle r^2\mu^2\rangle$ in several monosubstituted vinyl polymers. Macromolecules 1988;21:3320–4.
[134] Mathur SC, Mattice WL. On the additive nature of the first-order interactions at the tri-functional branch points in copolymers of ethylene and a larger 1-alkene. Makromol Chem 1988;189:2893–7.
[135] Mattice WL, Sienicki K. Extent of the correlation between the squared radius of gyration and squared end-to-end distance in random flight chains. J Chem Phys 1989;90:1956–8.
[136] Shannon VL, Strauss HL, Snyder RG, Elliger CA, Mattice WL. Conformation of the cyclo-alkanes $C_{14}H_{28}$, $C_{16}H_{32}$, and $C_{22}H_{44}$ in the liquid and high-temperature crystalline phases by vibrational spectroscopy. J Am Chem Soc 1989;111:1947–58.
[137] Sienicki K, Mattice WL. Forward and reverse energy transfer in the presence of energy migration and correlations. J Chem Phys 1989;90:6187–92.
[138] Bahar I, Mattice WL. Dynamics of conformational transitions to isomeric states favoring intramolecular excimer formation in polymeric chains. Application to dimer models of poly-styrene. J Chem Phys 1989;90:6775–82.
[139] Bahar I, Mattice WL. Dynamics of conformational transitions to isomeric states favoring intramolecular excimer formation in aromatic polyesters with methylene or oxyethylene spacers. J Chem Phys 1989;90:6783–90.
[140] Mathur SC, Rodrigues K, Mattice WL. Influence of a few short branches on the amorphous region of a semicrystalline polymer: simulation on a cubic lattice. Macromolecules 1989;22:2781–5.
[141] Sienicki K, Mattice WL. Self-consistent approximation to fluorescence decay in macromolecules with energy migration and dissociating traps. Macromolecules 1989;22:2854–7.
[142] Sienicki K, Mattice WL. Monomer–excimer–acceptor kinetics in the presence of diffusion and excimer dissociation. J Lumin 1989;43:233–41.
[143] Mendicuti F, Patel B, Waldeck DH, Mattice WL. Intramolecular excimer formation by phthaloyl, isophthaloyl, and terephthaloyl groups in polyesters with different numbers of methylene and oxyethylene spacers. Polymer 1989;30:1680–4.
[144] Neuburger NA, Mattice WL. Interpretation of the mean square dipole moment of poly(A-B) by use of the mean square end-to-end distance for its didymous partner. Macromolecules 1989;22:3694–7.
[145] Sienicki K, Itagaki H, Mattice WL. On theory of concentration depolarization of fluorescence in one and two-component systems for multipole interactions in one, two, and three dimensional medium. J Chem Phys 1989;91:4515–21.
[146] Bruno KR, Mattice WL. Enhancement at low concentration of the efficiency of inter-molecular nonradiative singlet energy transfer in labelled poly(L-lysine). Polym Commun 1989;30:310–2.
[147] Cho D, Mattice WL, Porter LJ, Hemingway RW. Use of the fluorescence quantum yield for the determination of the number-average molecular weight of polymers of epicatechin with 4β → 8 interflavan bonds. Polymer 1989;30:1955–8.
[148] Pannikottu A, Mattice WL. Adaptation of macrocyclization equilibrium theory to the formation of intramolecular excimers in end-labelled linear chains. Macromolecules 1990;23:867–70.
[149] Cho D, Mattice WL, Porter LJ. Anisotropy of the fluorescence from the monomer, five oligomers, and a polymer of epicatechin. Biopolymers 1990;29:57–60.
[150] Tanpipat N, Mattice WL. Range of the influence of the carbohydrate moiety on the conformation of the poly(amino acid) backbone in glycosylated mucins. Biopolymers 1990;29:377–83.

[151] Mendicuti F, Patel B, Mattice WL. Intramolecular excimer formation in model compounds for polyesters prepared from 2,6-naphthalene dicarboxylic acid and eight different glycols. Polymer 1990;31:453–7.
[152] Galiatsatos V, Mattice WL. Efficient formulation of the large generator matrices required for computation of the higher moments, and mixed moments, of conformation-dependent properties of chain molecules with independent bonds. J Comput Chem 1990;11:396–400.
[153] Rodrigues K, Mathur SC, Mattice WL. Influence of polyethylene-like short-range intra-molecular interactions on the segregation of short branches and growth of the interfacial region in simulations of lightly branched semicrystalline polymers. Macromolecules 1990;23:2482–8.
[154] Mendicuti F, Kulkarni R, Patel B, Mattice WL. Identification of the short-range intra-molecular excimers in polyacenaphthalene. Macromolecules 1990;23:2560–6.
[155] Cho D, Mattice WL. Quenching of the fluorescence of monomeric procyanidins by dimethyl sulfoxide. J Phys Chem 1990;94:3847–51.
[156] Bahar I, Mattice WL. Efficient calculation of the intramolecular contribution to orientational autocorrelation functions using dynamic rotational isomeric state theory. Macromolecules 1990;23:2719–23.
[157] Cho D, Tian R, Porter LJ, Hemingway RW, Mattice WL. Variations in the heterogeneity of the decay of the fluorescence in six procyanidin dimers. J Am Chem Soc 1990;112:4273–7.
[158] Zúñiga I, Rodrigues K, Mattice WL. Analytical and Monte Carlo studies of the interfacial region in semicrystalline polymers with first and second order intrachain interactions. Macromolecules 1990;23:4108–14.
[159] Darsey JA, Mattice WL. A harmonic oscillator model of the conformationally flexible helical polymeric molecules. J Math Chem 1990;4:383–94.
[160] Mendicuti F, Saiz E, Patel B, Dodge R, Mattice WL. Kerr constants of methyl benzoate and the dimethyl esters of phthalic, isophthalic, and terephthalic acids. J Phys Chem 1990;94:8374–8.
[161] Mendicuti F, Patel B, Mattice WL. Intramolecular formation of excimers in model com-pounds for polyesters containing naphthalene units. α,ω -diesters from 1-naphthoic acid and five glycols. Polymer 1990;31:1877–82.
[162] Chakraborty DK, Heitzhaus KD, Hamilton FJ, Harwood HJ, Mattice WL. Experimental characterization and molecular modeling of the intramolecular excimers in poly(*p-tert*-butyl-styrene). Macromolecules 1991;24:75–78.
[163] Rodrigues K, Mattice WL. Simulation of the steric stabilization of polymer colloids by diblock copolymers. J Chem Phys 1991;94:761–6.
[164] Bahar I, Mattice WL. Bimodal distribution of relaxational modes for the helix–coil transition in poly(oxymethylene). Macromolecules 1991;24:877–82.
[165] Mattice WL, Mandelkern L. Occurrence of irregular structures at the termination of the transition from a disordered chain to an intramolecular antiparallel sheet. Comput Polym Sci 1991;1:30–34.
[166] Mattice WL, Zúñiga I, Dodge R, Bahar I. Use of molecular dynamics trajectories for the formulation of the statistical weight matrices for chains of bonds with symmetric three-fold rotation potentials. Comput Polym Sci 1991;1:35–40.
[169] Yu WC, Mattice WL. A novel chromatographic method for determining the polydispersity index for polymers with a specified number of functional groups. J Polym Sci, Polym Phys Ed 1991;29:715–21.
[168] Dodge R, Mattice WL. Simulation by molecular dynamics of poly(1,4-*trans*-butadiene) as an inclusion complex in the channel in crystalline perhydrotriphenylene. Macromolecules 1991;24:2709–14.
[169] Bahar I, Zúñiga I, Dodge R, Mattice WL. Conformational statistics of poly(dimethyl sil-oxane). I. Probability distribution of rotational isomers from molecular dynamics simulations. Macromolecules 1991;24:2986–92.
[170] Bahar I, Zúñiga I, Dodge R, Mattice WL. Conformational statistics of poly(dimethyl sil-oxane). II. Rotational isomeric state approach with modified energy parameters. Macromolecules 1991;24:2993–8.
[171] Mattice WL, Tanpipat N. Reduction in the unperturbed dimensions of poly(vinyl chloride) upon the random incorporation of chloromethyl branches. Macromolecules 1991;24:3400–3.
[172] Cho D, Porter LJ, Mattice WL. Conformations and time-resolved fluorescence of oligomers of (−)-epicatechin with 4β → 8 interflavan bonds. Biopolymers 1991;30:537–45.
[173] Rodrigues K, Mattice WL. Segmental distribution functions for a micelle comprised of symmetric diblock copolymers (short chain amphiphiles). J Chem Phys 1991;95:5341–7.
[174] Zúñiga I, Bahar I, Dodge R, Mattice WL. Molecular dynamics analysis of transitions between rotational isomers in polymethylene with discrete hydrogen atoms. J Chem Phys 1991;95:5348–54.
[175] Zhan Y, Mattice WL. Molecular dynamics of dimeric models for polyesters with flexible spacers of different size. Comput Polym Sci 1991;1:166–72.
[176] Mattice WL. Implication of recent refinements in the intramolecular interactions in *n*-alkanes for the rotational isomeric state treatment of polymethylene. Comput Polym Sci 1991;1:173–8.
[177] Chakraborty DK, Kurian J, Kennedy JP, Mattice WL. An atom-based explanation for the absence of excimer emission in the fluorescence of dilute solutions of poly(pentafluoro-styrene). Colloid Polym Sci 1991;269:807–11.
[178] Lee KJ, Mattice WL. Population of rotational isomers and the unperturbed dimensions of poly(vinyl chloride) with and without chloromethyl branches, as deduced from molecular dynamics trajectories. Comput Polym Sci 1991;1:213–24.
[179] Cho D, Neuburger NA, Mattice WL. Correlations of nearest neighbor bonds at short times in the internal dynamics of polyisobutylene. Macromolecules 1992;25:322–6.
[180] Bruno KR, Mattice WL. Long-range intermolecular interactions in dilute aqueous solutions of ionized poly(L-lysine) at low ionic strength. Macromolecules 1992;25:327–30.
[181] Rodrigues K, Mattice WL. Intraparticle distribution functions for a micelle formed by a small symmetric triblock copolymer in a poor solvent for the terminal blocks. Langmuir 1992;8:456–9.
[182] Zhan Y, Mattice WL. The conformation and mobility of poly(1,4-*trans*-butadiene) in the crystalline state. Macromolecules 1992;25:1554–61.
[183] Zhan Y, Mattice WL. Creation, migration, and termination of conformational defects in poly-(1,4-*trans*-butadiene) in Form II and in the inclusion complex in perhydrotriphenylene. J Chem Phys 1992;96:3279–84.
[184] Patel B, Mendicuti F, Mattice WL. Dependence on spacer size of the intramolecular excimer emission from model compounds for polyesters derived from isophthalic or terephthalic acid. Polymer 1992;33:239–42.
[185] Neuburger N, Bahar I, Mattice WL. Molecular dynamics simulations of poly(dialkyl sil-oxanes). Conformational statistics and unperturbed chain dimensions. Macromolecules 1992;25:2447–54.
[186] Lee KJ, Mattice WL. Modeling of glassy poly(vinyl chloride) starting from a random model. Comput Polym Sci 1992;2:55–63.
[187] Lee KJ, Mattice WL, Snyder RG. Molecular dynamics of paraffins in the *n*-alkane/urea clathrate. J Chem Phys 1992;96:9138–43.
[188] Mendicuti F, Saiz E, Zúñiga I, Patel B, Mattice WL. Intramolecular excimer formation in model compounds for polyesters. Diesters from 2-naphthol and aliphatic dicarboxylic acids. Polymer 1992;33:2031–5.
[189] Zhan Y, Mattice WL. Simulation of the molecular dynamics of poly(1,4-*trans*-isoprene) and isoprene as inclusion complexes in crystalline perhydrotriphenylene. Macromolecules 1992;25:3439–42.

[190] Wang Y, Mattice WL, Napper DH. Simulation of the self-assembly of symmetric triblock copolymers in dilute solution. Macromolecules 1992;25:4073–7.
[191] Zhan Y, Mattice WL. Mobility of polyethylene in the inclusion complex with perhydrotriphenylene. Macromolecules 1992;25:4078–83.
[192] Bahar I, Neuburger N, Mattice WL. Mechanism of local conformational transitions in poly-(dialkyl siloxanes). Molecular dynamics simulations and dynamic rotational isomeric state approach. Macromolecules 1992;25:4619–25.
[193] Zhang R, Mattice WL. Evaluation of the persistence length of the rigid-rod polymers poly-(benzobisoxazole) and poly(benzobisthiazole) using molecular dynamics simulations. Macromolecules 1992;25:4937–41.
[194] Li Y, Mattice WL. Atom based modeling of amorphous 1,4-*cis*-polybutadiene. Macromolecules 1992;25:4942–7.
[195] Mendicuti F, Mattice WL. Intramolecular excimer formation in polyesters from terephthalic acid and cyclohexanediols with different stereochemical compositions. Polymer 1992;33:4180–3.
[196] Mendicuti F, Saiz E, Mattice WL. Intramolecular energy migration in polyesters from 2,6-naphthalene dicarboxylic acid. Polarization of fluorescence in the polymers and in bichromophoric model compounds. Polymer 1992;33:4908–12.
[197] Mendicuti F, Mattice WL. Intramolecular complexes in bichromophoric model compounds for polyesters with one, two, three or four oxyethylene spacers. Comput Polym Sci 1992;2:203–7.
[198] Wang Y, Mattice WL, Napper DH. Simulation of the formation of micelles by diblock copolymers under weak segregation. Langmuir 1993;9:66–70.
[199] Chakraborty DK, Kurian J, Trumbo D, Harwood HJ, Kennedy JP, Mattice WL. Electronic vs. steric effects of substituents on the intramolecular excimer fluorescence from dilute solutions of halogen-substituted polystyrenes. Makromol Chem 1993;194:329–38.
[200] Fronczek FR, Hemingway RW, McGraw GW, Steynberg JP, Helfer CA, Mattice WL. Crystal structure and conformational analysis of tetra-*O*-methyl-(+)-catechin. Biopolymers 1993;33:275–82.
[201] Dodge R, Mattice WL. The conformation of the intramolecular dimer in poly(ethylene terephthalate) . J Polym Sci, Polym Phys Ed 1993;31:207–12.
[202] Mendicuti F, Saiz E, Mattice WL. The ratio of excimer to monomer emission in diesters of 1-pyrenoic acid and five glycols. J Polym Sci, Polym Phys Ed 1993;31:213–20.
[203] Zhan Y, Mattice WL, Napper DH. Monte Carlo simulation of the adsorption of diblock copolymers from a nonselective solvent. I. Adsorption kinetics and adsorption isotherms. J Chem Phys 1993;98:7502–7.
[204] Zhan Y, Mattice WL, Napper DH. Monte Carlo simulation of the adsorption of diblock copolymers from a nonselective solvent. II. Structure of adsorbed layer. J Chem Phys 1993;98:7508–14.
[205] Makowski MP, Mattice WL. Characterization of rigid rod poly(pyridinium salts) by conformational analysis, molecular dynamics, and steady state and time resolved fluorescence. Polymer 1993;34:1606–12.
[206] Haliloglu T, Mattice WL. Analysis of orientation auto- and cross-correlation functions for polyethylene in the inclusion complex with perhydrotriphenylene. Macromolecules 1993;26:3137–42.
[207] Wang Y, Mattice WL. Simulation of the adsorption of symmetric diblock copolymers at the interface between the two homopolymers. J Chem Phys 1993;98:9861–87.
[208] Zhang R, Mattice WL. Molecular dynamics study of the conformational properties of cyclo-hexadecane. J Chem Phys 1993;98:9888–94.
[209] Kim EG, Misra S, Mattice WL. Atomistic models of amorphous polybutadienes II: poly(1,2-butadiene), poly(1,4-*trans*-butadiene) and a random copolymer of 1,4-*trans*-butadiene, 1,4-*cis*-butadiene and 1,2-butadiene. Macromolecules 1993;26:3424–31.
[210] Gallego J, Mendicuti F, Saiz E, Mattice WL. Intramolecular excimers and energy migration in polyesters with 2,6-naphthalene dicarboxylic acid units separated by spacers of 1–4 ethylene oxide units. Polymer 1993;34:2475–80.
[211] Balaji R, Wang Y, Foster MD, Mattice WL. A Monte Carlo study of the microphase separation transition in a diblock copolymer melt. Comput Polym Sci 1993;3:15–22.
[212] Zhang R, Mattice WL. Persistence length of the rodlike molecule trans-PBT revisited again. Macromolecules 1993;26:4384–5.
[213] Cho D, Mattice WL. Chiroptical properties and intrachromophoric interactions in oligomeric and polymeric molecules of procyanidins. Korea Polym J 1993;1:27–33.
[214] Wang Y, Li Y, Mattice WL. Simulation of the adsorption of unsymmetric diblock copolymers at the interface between the two monomeric homopolymers. J Chem Phys 1993;99:4068–75.
[215] Mendicuti F, Mattice WL. Intramolecular excimer formation in polyesters from terephthalic acid and six 2*R*,2*R*′-propanediols. Makromol Chem 1993;194:2851–60.
[216] Zhang R, Mattice WL. The flexibility of a new thermoplastic polyimide studied with molecular simulations. Macromolecules 1993;26:6100–5.
[217] Misra S, Mattice WL. Atomistic models of amorphous polybutadienes. 3. Static free volume. Macromolecules 1993;26:7274–81.
[218] Mendicuti F, Mattice WL. A rationalization of Hirayama's $n = 3$ rule for the intramolecular formation of excimers. Comput Polym Sci 1993;3:131–6.
[219] Zhan Y, Mattice WL. Self-assembly and adsorption of diblock copolymers from selective solvents. 1. Self-assembly. Macromolecules 1994;27:677–82.
[220] Zhan Y, Mattice WL. Self-assembly and adsorption of diblock copolymers from selective solvents. 2. Surface adsorption. Macromolecules 1994;27:683–8.
[221] Haliloglu T, Balaji R, Mattice WL. Mobility of the free ends and junction points in a lamellar block copolymer. Macromolecules 1994;27:1473–6.
[222] Misra S, Mattice WL. Telechelic polymers between two impenetrable adsorbing surfaces. Macromolecules 1994;27:2058–65.
[223] Adriani P, Wang Y, Mattice WL. Influence of chain stiffness on the micellization of block copolymers in a selective solvent as observed in Monte Carlo simulations. J Chem Phys 1994;100:7718–21.
[224] Bravo J, Mendicuti F, Mattice WL. Intramolecular formation of excimers in model compounds for polyesters obtained from 2,6-naphthalene dicarboxylic acid and cyclo-hexanediols. J Polym Sci, Part B: Polym Phys 1994;32:1511–9.
[225] Wang Y, Mattice WL. Adsorption of homopolymers on a solid surface. A comparison between Monte Carlo simulation and the Scheutjens–Fleer mean-field lattice theory. Langmuir 1994;10:2281–8.
[226] Misra S, Nguyen-Misra M, Mattice WL. Bridging by reversibly adsorbed telechelic polymers: a transient network. Macromolecules 1994;27:5037–42.
[227] Gallego J, Mendicuti F, Mattice WL. Molecular dynamics of dimeric model compounds for polyesters with 2,6-naphthalene dicarboxylate units separated by flexible oxyethylene spacers. Comput Polym Sci 1994;4:7–11.
[228] Haliloglu T, Mattice WL. Monte Carlo lattice simulation of the interchange of chains between micelles of diblock copolymers. Chem Engng Sci 1994;49:2851–7.
[229] Kim EG, Mattice WL. Local chain dynamics of bulk amorphous polybutadienes: a molecular dynamics study. J Chem Phys 1994;101:6242–54.
[230] Bravo J, Mendicuti F, Saiz E, Mattice WL. Intramolecular energy transfer in bichromophoric diesters containing anthracene and naphthalene groups separated by different numbers of methylene spacers. Macromol Chem Phys 1994;195:3411–24.
[231] Mattice WL, Napper DH. Distribution function for the radius of gyration for theta chains attached at one end to an impenetrable surface. Macromol Theory Simul 1994;3:931–7.

[232] Zhan Y, Mattice WL. Molecular dynamics simulation of the collapse of poly(1,4-*trans*-butadiene) to a globule and to a thin film. Macromolecules 1994;27:7056–62.
[233] Misra S, Mattice WL, Napper DH. Structure of polyelectrolyte stars and convex poly-electrolyte brushes. Macromolecules 1994;27:7090–8.
[234] Mattice WL, Misra S, Napper DH. Collapse of tethered chains due to *n*-clusters, when binary interactions are weakly repulsive, but ternary interactions are weakly attractive. Europhys Lett 1994;28:603–8.
[235] Mendicuti F, Saiz E, Bravo J, Mattice WL. Intramolecular energy transfer in polyesters and model compounds containing anthracene and naphthalene groups separated by methylene and oxyethylene spacers. Polym Int 1995;36:137–46.
[236] Wang Y, Kausch CM, Chun M, Quirk RP, Mattice WL. Exchange of chains between micelles of labeled polystyrene-block-polyoxyethylene, as monitored by non-radiative singlet energy transfer. Macromolecules 1995;28:904–11.
[237] Tanaka G, Mattice WL. Chain collapse by atomistic simulation. Macromolecules 1995;28:1049–59.
[238] Nguyen-Misra M, Mattice WL. Micellization and gelation of symmetric triblock copolymers with insoluble end blocks. Macromolecules 1995;218:1444–57.
[239] Martín O, Mendicuti F, Saiz E, Mattice WL. Rationalization of the ratio of excimer-to-monomer fluorescence emission intensity in bichromophoric diesters of 1-pyrenoic acid and mono-, di-, tri- and tetramethylene glycols. J Polym Sci, Part B: Polym Phys 1995;33:1107–16.
[240] Zhang NR, Mattice WL. Influence of channel diameter on the dynamics of polyethylene in its inclusion complex with perhydrotriphenylene. Acta Polym 1995;46:139–44.
[241] Wang Y, Rajagopalan R, Mattice WL. Kinetics of desorption of homopolymers from a solid surface. Phys Rev Lett 1995;74:2503–6.
[242] Zhan Y, Xing L, Mattice WL. Simulations of self-assembled monolayers with the same surface density, but different grafting patterns. Langmuir 1995;11:2103–8.
[243] Pozuelo J, Mendicuti F, Mattice WL. Intramolecular excimer formation in naphthalene-containing polyesters. Bichromophoric model compounds derived from phthalic, succinic or malonic acid and 2-hydroxynaphthalene or 2-hydroxymethylnaphthalene. Macromol Chem Phys 1995;196:1779–90.
[244] Haliloglu T, Mattice WL. The role of χ and N on the dynamics of the exchange of chains between micelles formed by diblock copolymers in selective solvents at concentrations slightly above the critical micelle concentration. Comput Polym Sci 1995;5:65–70.
[245] Steynberg JP, Brandt EV, Ferreira D, Helfer CA, Mattice WL, Gornik D, Hemingway RW. Conformational analysis of oligomeric flavanoids 2 * — methyl ether acetate derivatives of profisetinidins. Magn Reson Chem 1995;33:611–20.
[246] Rapold RF, Mattice WL. New high coordination lattice model for rotational isomeric state (RIS) polymer chains. J Chem Soc Faraday Trans 1995;91:2435–41.
[247] Ko MB, Mattice WL. Monte Carlo simulation of concentrated diblock copolymers in a selective solvent: anisotropy of the diffusion. Macromolecules 1995;28:6871–7.
[248] Nguyen-Misra MT, Mattice WL. Dynamics of end-associated triblock copolymer networks. Macromolecules 1995;28:6976–85.
[249] Wang Y, Rajagopalan R, Mattice WL. The exchange kinetics of macromolecules adsorbed on a solid surface: a theoretical investigation. Macromolecules 1995;28:7058–63.
[250] Zhang R, Mattice WL. Atomistic modeling of a new thermoplastic polyimide in the amorphous state: structure and energetics. Macromolecules 1995;28:7454–60.
[251] Misra S, Fleming III PD, Mattice WL. Structure and energy of thin films of poly(1,4-*cis*-butadiene): a new atomistic approach. J Comput-Aided Mater Des 1995;2:101–12.
[252] Zhang R, Mattice WL. Atomistic modeling of the diffusion of small penetrant molecules in the bulk amorphous polyimide of 3,3′,4,4′-benzophenonetetracarboxylic dianhydride and 2,2-dimethyl-1,3-(4-aminophenoxy)propane. J Membr Sci 1995;108:15–23.
[253] Pozuelo J, Mendicuti F, Mattice WL. Intramolecular face-to-face sandwich complexes of next-to-nearest neighbor rings in polyesters from terephthalic, isophthalic, or phthalic acid and $-(CH_2)_m-$ spacers. Comput Polym Sci 1995;5:179–85.
[254] Zhang R, Mattice WL. Molecular dynamics study of the persistence lengths of a new class of polyimide fibers. J Polym Sci, Part B: Polym Phys 1996;34:565–73.
[255] Nguyen-Misra M, Misra S, Mattice WL. Bridging by end-adsorbed triblock copolymers. Macromolecules 1996;29:1407–15.
[256] Rapold RF, Mattice WL. Introduction of short and long range energies to the simulation of real chains on the 2nd lattice. Macromolecules 1996;29:2457–66.
[257] Bravo J, Mendicuti F, Saiz E, Mattice WL. Intramolecular energy transfer in compounds with two 1-pyrenoate groups separated by methylene spacers. J Fluoresc 1996;6:41–50.
[258] Haliloglu T, Bahar I, Erman B, Kim EG, Mattice WL. A dynamic rotational isomeric state approach for extension of the time scale of the local dynamics observed in fully atomistic molecular dynamics simulations: application to polybutadiene. J Chem Phys 1996;104:4828–34.
[259] Bravo J, Mendicuti F, Saiz E, Mattice WL. The Förster radius for energy transfer from naphthalene to anthracene in polyesters with oxyethylene spacers. Macromol Chem Phys 1996;197:1349–60.
[260] Doruker P, Rapold RF, Mattice WL. Rotational isomeric state models for polyoxyethylene and polythiaethylene on a high coordination lattice. J Chem Phys 1996;104:8742–9.
[261] Tanaka G, Mattice WL. Chain collapse by lattice simulation. Macromol Theory Simul 1996;6:499–523.
[262] Wu H, Foster MD, Ross SA, Mattice WL, Matties MA. Temporal stability of a bilayer in a Langmuir–Blodgett multilayer and its dependence on multilayer structure. Langmuir 1996;12:3015–23.
[263] Xing L, Mattice WL. Atomistic simulations of self-assembled monolayers that contain azo-benzene. Langmuir 1996;12:3024–30.
[264] Haliloglu T, Bahar I, Erman B, Mattice WL. Mechanisms of the exchange of diblock copolymers between micelles at dynamic equilibrium. Macromolecules 1996;29:4764–71.
[265] Misra S, Tirrell M, Mattice WL. Interaction between polyelectrolyte brushes in poor solvents. Macromolecules 1996;29:6056–60.
[266] Martín O, Mendicuti F, Saiz E, Mattice WL. Intramolecular formation of excimers in model compounds for polymers of 2,6-naphthalene dicarboxylic acid and five glycols in media of different viscosity. J Polym Sci, Part B: Polym Phys 1996;34:2623–33.
[267] Haliloglu T, Bahar I, Erman B, Mattice WL. Relative contributions of coupled rotations and small amplitude torsions to conformational relaxation in polymers. Macromolecules 1996;29:8942–7.
[268] Pozuelo J, Madrid JM, Mendicuti F, Mattice WL. Inclusion complexes of chain molecules with cycloamyloses. 1. Conformational analysis of isolated cycloamyloses using molecular dynamics simulations. Comput Theor Polym Sci 1996;6:125–34.
[269] Cho J, Mattice WL. Estimation of long range interaction in coarse-grained rotational isomeric state polyethylene chains on a high coordination lattice. Macromolecules 1997;30:637–44.
[270] Haliloglu T, Stevenson DC, Mattice WL. Monte Carlo simulation of the adsorption from a nonselective solvent of symmetric triblock copolymers with sticky end blocks. J Chem Phys 1997;106:3365–9.
[271] Xing L, Mattice WL. Geometric properties of micelles formed by triblock copolymers and solubilizates in dilute solution. Macromol Theory Simul 1997;6:553–63.
[272] Xing L, Mattice WL. Solubilization of small molecules by triblock-copolymer micelles in selective solvents. Macromolecules 1997;30:1711–7.
[273] Martín O, Sánchez-Camacho A, Mendicuti F, Mattice WL. Effect of the directionality of the ester group on the formation of hairpins in

polyesters containing naphthalene and a flexible spacer. J Polym Sci, Part B: Polym Phys 1997;35:1127–33.
[274] Haliloglu T, Mattice WL. Conformational transitions of end-adsorbed triblock copolymers in a nonselective solvent. Macromol Theory Simul 1997;6:667–77.
[275] Pozuelo J, Mendicuti F, Mattice WL. Inclusion complexes of chain molecules with cyclo-amyloses. 2. Molecular dynamics simulations of polyrotaxanes formed by poly(ethylene glycol) and α-cyclodextrins. Macromolecules 1997;30:3685–90.
[276] He D, Reneker DH, Mattice WL. Fully atomistic models of the surface of amorphous polyethylene. Comput Theor Polym Sci 1997;7:19–24.
[277] Doruker P, Mattice WL. Reverse mapping of coarse grained polyethylene chains from the second nearest neighbor diamond lattice to an atomistic model in continuous space. Macromolecules 1997;30:5520–6.
[278] Natarajan U, Mattice WL. Atomistic simulations of phenoxy ring flips in the glassy region of a semi-crystalline polyimide. Macromol Theory Simul 1997;6:949–63.
[279] Madrid JM, Pozuelo J, Mendicuti F, Mattice WL. A molecular mechanics study of the inclusion complexes of 2-methyl naphthoate with α- and β-cyclodextrins. J Colloid Interface Sci 1997;193:112–20.
[280] Tanaka G, Mattice WL. Simulation of rodlike molecules represented by anisotropic Lennard–Jones potentials. Macromol Theory Simul 1997;6:1119–37.
[281] Sánchez-Camacho A, Pozuelo J, Mendicuti F, Mattice WL. Intramolecular energy transfer in naphthalene-containing polyesters: experiment and simulation for model compounds derived from five aliphatic dicarboxylic acids and 2-hydroxynaphthalene. J Fluoresc 1997;7:113–20.
[282] Natarajan U, Tanaka G, Mattice WL. Atomistic simulations of the surfaces of thin films of random copolymers. J Comput-Aided Mater Des 1997;4:193–205.
[283] Doruker P, Mattice WL. Simulation of polyethylene thin films on a high coordination lattice. Macromolecules 1998;31:1418–26.
[284] Hubbard PA, Brittain WJ, Mattice WL, Brunelle DJ. Ring-size distribution in the depolymerization of poly(butylene terephthalate). Macromolecules 1998;31:1518–22.
[285] von Meerwall E, Beckman S, Jang J, Mattice WL. Diffusion of liquid *n*-alkanes: free volume and density effects. J Chem Phys 1998;108:4299–304.
[286] Madrid JM, Mendicuti F, Mattice WL. Inclusion complexes of 2-methylnaphthoate and (-cyclodextrin. Experimental thermodynamics and molecular mechanics calculations. J Phys Chem B 1998;102:2037–44.
[287] Haliloglu T, Mattice WL. Mapping of rotational isomeric state chains with asymmetric torsional potential energy functions on a high coordination lattice: application to poly-propylene. J Chem Phys 1998;108:6989–95.
[288] Pozuelo J, Mendicuti F, Mattice WL. Inclusion complexes of chain molecules with cyclo-amyloses III. Molecular dynamics simulations of polyrotaxanes formed by poly(propylene glycol) and β cyclodextrins. Polym J 1998;30:479–84.
[289] Martín O, Mendicuti F, Saiz E, Mattice WL. Intramolecular energy transfer in naphthalene-containing polymers: molecular dynamics simulations for trichromophoric model compounds of polyesters derived from 2,6-naphthalene dicarboxylic acid and aliphatic glycols. Comput Theor Polym Sci 1998;7:149–57.
[290] Xing L, Mattice WL. Internal structures of micelles of triblock copolymers with small insoluble molecules in their cores. Langmuir 1998;14:4074–80.
[291] Natarajan U, Mattice WL. Interaction of toluene, hexadecane and water with the surfaces of random copolymers of styrene and butadiene. J Membr Sci 1998;146:135–42.
[292] Kim WK, Mattice WL. Molecular modeling of a thin film of polybenzoxazine. Langmuir 1998;14:6588–93.
[293] Jang JH, Mattice WL. Time scales for three processes in the interdiffusion across inter-faces. Polymer 1998;40:1911–4.
[294] Haliloglu T, Cho J, Mattice WL. Simulations of rotational isomeric state models for poly-propylene melts on a high coordination lattice. Macromol Theory Simul 1998;7:613–7.
[295] Natarajan U, Misra S, Mattice WL. Atomistic simulation of a polymer–polymer interface: interfacial energy and work of adhesion. Comput Theor Polym Sci 1998;8:323–9.
[296] Kim WK, Mattice WL. Conformational statistics of a polybenzoxazine. Comput Theor Polym Sci 1998;8:339–51.
[297] Kim WK, Mattice WL. A fully atomistic model of an amorphous polybenzoxazine at bulk density. Comput Theor Polym Sci 1998;8:353–61.
[298] Kim WK, Mattice WL. Static and dynamic behavior of H_2O and O_2 penetrants in a poly-benzoxazine. Macromolecules 1998;31:9337–44.
[299] Doruker P, Mattice WL. Segregation of chain ends is only a weak contributor to increased mobility at free polymer surfaces. J Phys Chem B 1999;103:178–83.
[300] Doruker P, Mattice WL. Mobility of the surface and interior of thin films composed of amorphous polyethylene. Macromolecules 1999;32:194–8.
[301] Martín O, Mendicuti F, Saiz E, Mattice WL. Intramolecular excited state complexes in tri-chromophoric model compounds for polyesters derived from 2,6-naphthalenedicarboxylic acid and aliphatic glycols. Experiment, rotational isomeric state model, and molecular dynamics. J Polym Sci, Polym Phys Ed 1999;37:253–66.
[302] Lee S, Mattice WL. A phantom bubble model for the distribution of free volume in polymers. Comput Theor Polym Sci 1999;9:57–61.
[303] Jang JH, Mattice WL. The effect of solid wall interaction on an amorphous polyethylene thin film, using a Monte Carlo simulation on a high coordination lattice. Polymer 1999;40:4685–94.
[304] von Meerwall E, Feick EJ, Ozisik R, Mattice WL. Diffusion in binary liquid *n*-alkane and alkane–polyethylene blends. J Chem Phys 1999;111:750–7.
[305] Mattice WL, Clancy TC. Unperturbed dimensions and local stiffness of poly(vinyl chloride) with stereochemical sequences composed of repeating units. Macromolecules 1999;32:5444–9.
[306] Clancy TC, Mattice WL. Computer simulation of polyolefin interfaces. Comput Theor Polym Sci 1999;9:261–70.
[307] Haliloglu T, Mattice WL. Detection of the onset of demixing in simulations of polypropylene melts in which the chains differ only in stereochemical composition. J Chem Phys 1999;111:4327–33.
[308] Doruker P, Mattice WL. A second generation of mapping/reverse mapping of coarse-grained and fully atomistic models of polymer melts. Macromol Theory Simul 1999;8:463–78.
[309] Vao-soongnern V, Doruker P, Mattice WL. Simulation of an amorphous polyethylene nano-fiber on a high coordination lattice. Macromol Theory Simul 2000;9:1–13.
[310] Jang JH, Mattice WL. A Monte Carlo simulation for the effect of compression on an amorphous polyethylene melt in very thin confined geometry. Macromolecules 2000;33:1467–72.
[311] Jang JH, Haliloglu T, von Meerwall ED, Mattice WL. Effect of vinyl content on self-diffusion in polybutadiene melts. Macromolecules 2000;33:4271–7.
[312] Clancy TC, Mattice WL. Rotational isomeric state chains on a high coordination lattice: dynamic Monte Carlo algorithm details. J Chem Phys 2000;112:10049–55.
[313] Ozisik R, Doruker P, Mattice WL, von Meerwall ED. Translational diffusion in Monte Carlo simulations of polymer melts: center of mass displacement vs. integrated velocity auto-correlation function. Comput Theor Polym Sci 2000;10:411–8.
[314] Vao-soongnern V, Mattice WL. Dynamic properties of an amorphous polyethylene nano-fiber. Langmuir 2000;16:6757–8.
[315] Doruker P, Wang Y, Mattice WL. Simulation of the random scission of C–C bonds in the initial stage of the thermal degradation of polyethylene. Comput Theor Polym Sci 2000; 10, Galley 22 September, 1999.

[316] Vao-soongnern V, Mattice WL. Topological effects on static and dynamic properties in an amorphous nanofiber composed of cyclic polymers. Macromol Theory Simul 2000;9:570–7.
[317] Jang JH, Ozisik R, Mattice WL. A Monte Carlo simulation on the effects of chain end modification on freely standing thin films of amorphous polyethylene melts. Macromolecules 2000;33:7663–71.
[318] Ozisik R, von Meerwall ED, Mattice WL. Comparison of the diffusion coefficients of unentangled linear and cyclic alkanes. Phys Rev E, revision in progress.
[319] Meng H, Saito T, Rinaldi PL, Wyzgoski F, Helfer CA, Mattice WL, Harwood HJ. 3D NMR characterization of chain ends formed in phosphinyl radical initiated polymerization of styrene. Macromolecules, submitted for publication.
[320] Gallego J, Pérez-Foullerat D, Mendicuti F, Mattice WL. Configurations conducive to the formation of intramolecular excimers in poly(*N*-vinyl carbazole) and its copolymers. J Polym Sci, Part B: Polym Phys, submitted for publication.
[321] Clancy TC, Pütz M, Weinhold JD, Curro JG, Mattice WL. Mixing of isotactic and syndio-tactic polypropylenes in the melt. Macromolecules, submitted for publication.
[322] Doruker P, Mattice WL. Effect of surface roughness on structure and dynamics in thin films. Macromol Theory Simul, submitted for publication.
[323] Pugh C, Small AC, Helfer CA, Mattice WL. Induction of smectic layering in nematic liquid crystals using immiscible components. IV. The effect of bulky lateral carboxyl substituents on the thermotropic behavior of 2,5-bis[(4′-(*n*-(perfluoroheptyl)octyloxy)benzoyl)oxy]-toluene. Liq Cryst, to be submitted.

Reviews, chapters in books

[1] Mandelkern L, Mattice WL. The conformational and optical properties of poly-L-proline and related polymers. Conformation of biological molecules and polymers, The Jerusalem Symposia on Quantum Chemistry and Biochemistry V. Jerusalem: The Israel Academy of Sciences and Humanities, 1973. p. 121–39.
[2] Mattice WL, Scheraga HA. Long-range aspects of the formation of intramolecular antiparallel β sheets. In: Eisenfield J, DeLisi C, editors. Mathematics and computers in biomedical applications. Amsterdam: Elsevier, 1985. p. 13–17.
[3] Mattice WL. Interaction of anionic detergents with cationic residues in polypeptides: conformational changes. In: Eisenberg A, Bailey FE, editors. Coulombic interactions in macromolecular systems, ACS Symp Ser, 302. 1986. p. 232–7.
[4] Scheraga HA, Mattice WL. In: Kroschwitz JI, editor. Encyclopedia of polymer science and engineering, 2nd ed. Helix–coil transitions, vol. 7. New York: Wiley-Interscience, 1987. p. 685–98.
[5] Bergmann WR, Mattice WL. Specific interactions of (+)-catechin and (−)-epicatechin with polymers that contain the L-prolyl residue. Photophysics of polymers. Hoyle CE, Torkelson JM, editors. ACS Symp Ser 1987;358:162–7.
[6] Mattice WL. The β sheet to coil transition. Annu Rev Biophys Biophys Chem 1989;18:93–111.
[7] Mattice WL. Configuration-dependent properties of polymers. In: Saegusa T, Higashimura T, Abe A, editors. Frontiers of macromolecular science. Oxford: Blackwell Scientific, 1989. p. 277–82.
[8] Mattice WL. Conformational analysis of oligomeric proanthocyanidins. In: Hemingway RW, Karchesy JJ, editors. The chemistry and significance of condensed tannins. New York: Plenum Press, 1989. p. 119–30.
[9] Tilstra LF, Cho D, Bergmann WR, Mattice WL. Complexes of condensed tannins with biopolymers. In: Hemingway RW, Karchesy JJ, editors. The chemistry and significance of condensed tannins. New York: Plenum Press, 1989. p. 335–41.
[10] Mattice WL. Determination of the unperturbed dimensions of polymers of (+)-catechin and (−)-epicatechin. (+)-catechin and (−)-epicatechin. Glass JE, editor. Adv Chem Ser 1989;223:285–93.
[11] Scheraga HA, Mattice WL. Helix–coil transitions. In: Kroschwitz JI, editor. Concise encyclopedia of polymer science and engineering. New York: Wiley, 1990. p. 447–9.
[12] Neuburger NA, Mattice WL. Behavior of the correlation coefficient for r^2 and s^2 in rotational isomeric state chains of finite n. In: Roe RJ, editor. Computer simulation of polymers. Englewood Cliffs, NJ: Prentice-Hall, 1990. p. 341–53.
[13] Mattice WL. Fluorescence of oligomers that contain catechin or epicatechin. In: Hemingway RW, Laks PE, editors. Plant polyphenols: biogenesis, chemical properties, and significance. New York: Plenum Press, 1992. p. 447–58.
[14] Helfer CA, Mattice WL. Conformational analysis of profisetinidin dimers. In: Hemingway RW, Laks PE, editors. Plant poly-phenols: biogenesis, chemical properties, and significance. New York: Plenum Press, 1992. p. 479–85.
[15] Mattice WL. Computer modeling of polymer structure and fundamental properties. In: Aggarwal SL, Russo S, editors. Comprehensive polymer science supplement 1. Oxford: Pergamon Press, 1992. p. 159–66.
[16] Wang Y, Mattice WL, Napper DH. Roles of A-B, A-solvent, and B-solvent interactions in the critical micelle concentration of A–B diblock copolymers. Colloid–polymer interactions: particulate, amphiphilic, and biological surfaces. Dubin PL, Tong P, editors. ACS Symp Ser 1993;532:45–52.
[17] Zhan Y, Mattice WL. Molecular modeling of polymers in inclusion complexes. Trends Polym Sci (Cambridge, UK) 1993;1:343–9.
[18] Misra S, Mattice WL, Varanasi S. A self consistent field theory for polyelectrolyte brushes. Trends Macromol Res 1994;1:269–89.
[19] Helfer CA, Mattice WL. Conformation and dynamics of condensed tannins. Trends Polym Sci (Cambridge, UK) 1995;3:117–22.
[20] Tilstra LF, Mattice WL. The β sheet ↔ coiltransition of polypeptides, as determined by circular dichroism. In: Fasman GD, editor. Circular dichroism: conformational analysis of biomolecules. New York: Plenum Press, 1996. p. 261–83.
[21] Mattice WL. Masses, sizes, and shapes of macromolecules from multifunctional monomers. In: Newkome GR, Vögtle F, editors. Dendritic macromolecules. Weinheim: VCH, 1996. p. 1–13.
[22] Haliloglu T, Mattice WL. Monte Carlo simulation of self-assembly in macromolecular systems. In: Webber SE, Munk P, Tuzar Z, editors. NATO ASI Series, Series E: Applied Sciences, vol. 327. Dordrecht, The Netherlands: Kluwer Academic Publishers, 1996. p. 167–96.
[23] Nguyen-Misra M, Misra S, Wang Y, Rodrigues K, Mattice WL. Simulation of self-assembly in solution by triblock copolymers with sticky blocks at their ends. Progr Colloid Polym Sci 1997;103:138–45.
[24] Bahar I, Cho J, Doruker P, Erman B, Haliloglu T, Kim EG, Mattice WL, Monnerie L, Rapold RF. Three approaches that may permit more efficient simulation of the dynamics of atomistic models of polymers . Trends Polym Sci (Cambridge, UK) 1997;5:155–60.
[25] Rehahn M, Mattice WL, Suter UW. Rotational isomeric state models in macromolecular systems. Adv Polym Sci 1997;131/132. 450 p.
[26] Haliloglu T, Mattice WL. Simulation of rotational isomeric state models for polypropylene melts on a high coordination lattice. Rev Chem Engng 1999;15:293–305.
[27] Baschnagel J, Binder K, Doruker P, Gusev AA, Hahn O, Kremer K, Mattice WL, Müller-Plathe F, Murat M, Paul W, Santos S, Suter UW, Tries V. Bridging the gap between atomistic and coarse-grained models of polymers: status and perspectives. Adv Polym Sci 2000;152:41–156.
[28] Mattice WL, Pugh C. Masses, sizes, and shapes of macromolecules from multifunctional monomers. In: Newkome GR, Vögtle F, editors. Dendritic macromolecules, 2nd ed. Weinheim: VCH, 2001, in press.
[29] Akten ED, Mattice WL, Suter UW. Rotational isomeric state (RIS) calculations, with an illustrative application to head-to-head, tail-to-tail polypropylene. In: Kotelyanskii M, Theodorou DN, editors.

Simulation methods for modeling polymers. New York: Marcel Dekker, 2001, in press.
[30] Vao-soongnern V, Doruker P, Mattice WL. Simulations of thin films and fibers of amorphous polymers. In: Dadmun M, Noid D, Sumpter B, editors. Computational studies, nanotechnology, and solution thermodynamics of polymer systems. New York: Plenum Press, 2000. p. 117–26.
[31] Helfer CA, Mendicuti F, Mattice WL. Steady-state fluorescence of polymers. In: Brady RF, editor. Comprehensive desk reference on polymer characterization and analysis. Oxford: Oxford University Press, 2001 in press.
[32] Mattice WL, Helfer CA. The rotational isomeric state model. Czecaj C, editor. Encyclopedia of polymer science and technology. 3rd ed. New York: Wiley, submitted for publication.

Unfereeed preprints, communications, biographies, etc.

[1] Mattice WL. Comparison of the conformational map for poly(L-proline) to the conformational map for polysarcosine near $\phi = 120°$. Polym Prepr (Am Chem Soc Div Polym Chem) 1973;14:1108–11.
[2] Igou DK, Lo JT, Clark DS, Mattice WL, Younathan ES. On the nature of interaction of dodecyl sulfate with proteins. Evidence from uncharged polypeptides. Biochem Biophys Res Commun 1974;60:140–5.
[3] Mattice WL. Interaction of peptides and proteins with small ions. Polym Prepr (Am Chem Soc Div Polym Chem) 1974;16:2–7.
[4] Clark DS, Mattice WL. Hydrodynamic properties of poly(γ-hydroxy-L-proline). Polym Prepr (Am Chem Soc Div Polym Chem) 1976;17:859–63.
[5] Spirtes MA, Schwartz RW, Mattice WL, Coy DH. Circular dichroism and absorption study of the structure of methionine–enkephalin in solution. Biochem Biophys Res Commun 1978;81:602–9.
[6] McCord RW, Mattice WL. Salt-induced helix–coil transitions in non-ionic homopolypeptides. Polym Prepr (Am Chem Soc Div Polym Chem) 1979;19:1021–4.
[7] Mattice WL. Branched molecules in biological membranes. Polym Prepr (Am Chem Soc Div Polym Chem) 1979;20:175–8.
[8] Mandelkern L, Mattice WL. Macromolecules in the first physical chemistry course. Org Coat Plast Prepr (Am Chem Soc Div Org Coat and Plast) 1979;41:113–5.
[9] Mattice WL. Polymer chemistry at Louisiana State University. Polym News 1980;6:234–6.
[10] Mattice WL, Robinson RM. Conformational changes expected in endogenous opioid peptides upon their interaction with acidic lipids. Biochem Biophys Res Commun 1981;101:1311–7.
[11] Maroun RC, Mattice WL. Solution conformations of the pituitary opioid peptide dynorphin(1–13). Biochem Biophys Res Commun 1981;103:442–6.
[12] Robinson RM, Hamed MH, Mattice WL. Sheet to α helix transition in the binding subunit of cholera toxin. Biochem Biophys Res Commun 1981;105:398–403.
[13] Mattice WL. Macromolecules in undergraduate physical chemistry. J Chem Ed 1981;58:911–3.
[14] Mattice WL. Unperturbed and perturbed rotational isomeric state polymethylene regular stars of high branch point functionality. Polym Prepr (Am Chem Soc Div Polym Chem) 1982;23:135–6.
[15] Mattice WL. Rotational isomeric state treatment of chain molecules. JEMMSE 1982;4:759–79.
[16] Mattice WL, Scheraga HA. Evaluation of intramolecular antiparallel sheet formation by matrix methods. Polym Prepr (Am Chem Soc Div Polym Chem) 1984;25:276–7.
[17] Blumenstein R, Carraher CE, Coker H, Fowkes F, Hellmuth E, Karl D, Mandelkern L, Mark JE, Mattice W, Rodriguez F, Rogers C, Sperling L, Stein R. Polymer principles in the undergraduate physical chemistry course. Part 1. J Chem Ed 1985;62:780–6.
[18] Blumenstein R, Carraher CE, Coker H, Fowkes F, Hellmuth E, Karl D, Mandelkern L, Mark JE, Mattice W, Rodriguez F, Rogers C, Sperling L, Stein R. Polymer principles in the undergraduate physical chemistry course. Part 2. J Chem Ed 1985;62:1030–6.
[19] Bergmann WR, Barkley MD, Mattice WL. Fluorescence of polymers of (+)-catechin and (−)-epicatechin. Polym Prepr (Am Chem Soc Div Polym Chem) 1986;27(2):320–1.
[20] Mandelkern L, Van Wart H, Mattice WL. Harold A. Scheraga. Macromolecules 1986;19:2469.
[21] Mark JE, Mattice WL. Leo Mandelkern, one of the pioneers of polymer science. Macromolecules 1987;20:235–6.
[22] Mendicuti F, Viswanadhan VN, Mattice WL. Excimers in polyesters from terephthalic acid and mono, di, or triethylene glycol. Polym Prepr (Am Chem Soc, Div Polym Chem) 1987;28(2):82–3.
[23] Mathur SC, Mattice WL. Chain conformations in the amorphous regions of copolymers of ethylene and various 1-alkenes. Polym Prepr (Am Chem Soc Div Polym Chem) 1987;28(2):335–6.
[24] Mattice WL, Tilstra L. Fluorescence: a tool for the study of conformational transition and intermolecular interactions in water soluble polymers . Polym Mater Sci Engng Prepr (Am Chem Soc Div Polym Mater Sci Engng) 1987;57:8–12.
[25] Bruno KR, Mattice WL. Conformational control of the onset of intermolecular interactions in poly(L-lysine). Polym Prepr (Am Chem Soc Div Polym Chem) 1988;29(1):184–5.
[26] Mathur SC, Mattice WL. Lattice simulations of amorphous regions between two crystalline lamellae: the influence of the presence of short branches . Polym Prepr (Am Chem Soc Div Polym Chem) 1988;29(1):240–1.
[27] Mendicuti F, Patel B, Viswanadhan VN, Mattice WL. An odd-even effect in excimer formation in polyesters with different numbers of methylene units between aromatic rings . Polym Prepr (Am Chem Soc Div Polym Chem) 1988;29(1):505–6.
[28] Ghosh K, Neuburger N, Mattice WL. Correlation coefficients for pairs of conformational properties. Polym Prepr (Am Chem Soc Div Polym Chem) 1989;30(2):7–8.
[29] Rodrigues K, Mathur SC, Mattice WL. Branch segregation and the interfacial region in ethylene — 1-alkene copolymers. Polym Prepr (Am Chem Soc Div Polym Chem) 1989;30(2):275–6.
[30] Mendicuti F, Mattice WL. Suppression of the influence of stray light on quantitative measurement of I_d/I_m for weakly emitting dilute solutions of polymers. Polym Bull (Berlin) 1989;22:557–63.
[31] Quirk RP, Kim J, Rodrigues K, Mattice WL. Anionic synthesis and characterization of poly(styrene-block-ethylene oxide) polymers with fluorescent probes at the block junctions. Polym Prepr (Am Chem Soc Div Polym Chem) 1990;31(1):87–8.
[32] Cho D, Mattice WL. Fluorescence and conformation of procyanidins. Polym Prepr (Am Chem Soc Div Polym Chem) 1990;31(1):203–4.
[33] Mattice WL. Simulation using rotational isomeric state theory of the formation of intramolecular excimers in polymers. Polym Prepr (Am Chem Soc Div Polym Chem) 1990;31(1):706–7.
[34] Mattice WL. Analysis of the conformations of poly(amino acids) using rotational isomeric state theory. Models of Biopolymers. Proceeding of U.S. — Polish Workshop, Warsaw-Lód'z 1990. p. 89–90.
[35] Galiatsatos V, Mattice WL. The correlation between r^2 and μ^2 for chains with symmetric rotation potentials. Polym Prepr (Am Chem Soc Div Polym Chem) 1990;31(2):588–9.
[36] Chakraborty DK, Heitzhaus KD, Hamilton FJ, Harwood HJ, Mattice WL. Intramolecular excimers in poly(*p-t*-butylstyrene). Polym Prepr (Am Chem Soc Div Polym Chem) 1990;31(2):590–1.
[37] Bruno KR, Mattice WL. Aggregate size in solutions of poly(L-lysine) at low ionic strength. Polym Prepr (Am Chem Soc Div Polym Chem) 1990;31(2):592–3.
[38] Rodrigues K, Mattice WL. Micelles and networks formed by symmetric triblock copolymers in dilute solutions that are poor solvents for the terminal blocks. Polym Bull (Berlin) 1991;25:239–43.
[39] Dodge R, Mattice WL. Molecular dynamics of a chain of poly(1,4-*trans*-butadiene) in the channel of crystalline perhydrotriphenylene. Polym Prepr (Am Chem Soc Div Polym Chem) 1991;32(1):267–8.

[40] Rodrigues K, Mattice WL. Simulation of diblock copolymers as steric stabilizers of polymer colloids. Polym Prepr (Am Chem Soc Div Polym Chem) 1991;32(1):269–70.
[41] Bahar I, Lee KJ, Mattice WL. Relaxation of runs of trans rotational isomers in single racemic poly(vinyl chloride) chains. Polym Prepr (Am Chem Soc Div Polym Chem) 1991;32(2):277–8.
[42] Neuburger NA, Mattice WL. The effect of the length of the side branches on the chain statistics of siloxanes. Polym Prepr (Am Chem Soc Div Polym Chem) 1991;32(2):279–80.
[43] Quirk RP, Kim J, Rodrigues K, Mattice WL. Anionic synthesis and characterization of poly(styrene-block-ethylene oxide) polymers with fluorescent probes at the block junctions. Makromol Chem Macromol Symp 1991;42/43:462–73.
[44] Rodrigues K, Kausch CM, Kim J, Quirk RP, Mattice WL. On the location of the free ends of the insoluble blocks in micelles formed by diblock copolymers. Polym Bull (Berlin) 1991;26:695–700.
[45] Lenz RW, Lovinger AJ, Mattice WL, Morawetz H. A quarter-century of macromolecules. Macromolecules 1992;25:1–2.
[46] Zhan Y, Dodge RW, Lee KJ, Mattice WL. Molecular dynamics of flexible chains confined by narrow channels. Polym Prepr (Am Chem Soc Div Polym Chem) 1992;33(1):564–5.
[47] Makowski MP, Mattice WL. Fluorescence and conformation of a rigid rod poly(pyridinium salt). Polym Prepr (Am Chem Soc Div Polym Chem) 1992;33(1):833–4.
[48] Dodge RW, Lee KJ, Zhan Y, Mattice WL. Molecular dynamics of common polymers in unusual environments. SPE/ANTEC 1992 Proc 1992. p. 1985–1987.
[49] Neuburger NA, Bahar I, Mattice WL. Computational statistics of poly(dialkyl siloxanes) from molecular dynamics simulations. SPE/ANTEC 1992 Proc 1992. p. 2282–6.
[50] Wang Y, Balaji R, Quirk RP, Mattice WL. Detection of the rate of exchange of chains between micelles formed by diblock copolymers in aqueous solution. Polym Bull (Berlin) 1992;28:333–8.
[51] Wang Y, Mattice WL. Intramolecular vs. intermolecular formation of bityrosine upon photoreaction of poly(L-tyrosine) in dilute aqueous solution. Polym Bull (Berlin) 1992;28:345–9.
[52] Reneker DH, Mattice WL, Quirk RP, Kim SJ. Macromolecular smart materials and structures. J Smart Mater Struct 1992;1:84–90.
[53] Helfer CA, Mattice WL. Comparison of the photophysical properties of profisetinidin dimers with procyanidin dimers. Polym Prepr (Am Chem Soc Div Polym Chem) 1992;33(2):256–7.
[54] Matties MA, Mattice WL. Intramolecular interactions between phenyl and terephthaloyl groups: implications for the interpretation of the red-shifted emission in poly(ethylene terephthalate). Polym Prepr (Am Chem Soc Div Polym Chem) 1992;33(2):258–9.
[55] Zhan Y, Mattice WL. Twiston vs. random fluctuation as the source of the source of the rapid motion of polyethylene in the inclusion complex with perhydrotriphenylene. Makromol Chem, Macromol Symp 1993;65:145–51.
[56] Zhang R, Mattice WL. Atomistic modeling of amorphous PI-2: cohesive energy, Hildebrand solubility parameter, and pair distribution functions. Polym Prepr (Am Chem Soc Div Polym Chem) 1993;34(2):450–1.
[57] Zhan Y, Mattice WL. Self-assembly and adsorption of a copolymer from a selective solvent. Polym Prepr (Am Chem Soc Div Polym Chem) 1993;34(2):452–3.
[58] Misra S, Mattice WL. Atomistic models of amorphous polybutadiene: static free volume. Polym Prepr (Am Chem Soc Div Polym Chem) 1993;34(2):454–5.
[59] Matties MA, Mattice WL. In vacuo molecular dynamics simulation of single chain poly-(ethylene terephthalate) and model compounds. Polym Prepr (Am Chem Soc Div Polym Chem) 1993;34(2):456–7.
[60] Kim EG, Mattice WL. Local motions in bulk polybutadienes: a molecular dynamics study. Polym Prepr (Am Chem Soc Div Polym Chem) 1993;34(2):458–9.
[61] Haliloglu T, Mattice WL. Monte Carlo lattice simulation of the exchange of chains between micelles of diblock copolymers. Polym Prepr (Am Chem Soc Div Polym Chem) 1993;34(2):460–1.
[62] Wang Y, Mattice WL. Simulation of the adsorption of diblock copolymers at the interface of the two monomeric homopolymers. Polym Prepr (Am Chem Soc Div Polym Chem) 1993;34(2):462–3.
[63] Balaji R, Mattice WL. Monte Carlo simulations of a diblock copolymer in solution. Polym Prepr (Am Chem Soc Div Polym Chem) 1993;34(2):464–5.
[64] Haliloglu T, Mattice WL. Exchange of chains between micelles formed by block copolymers. Polym Prepr (Am Chem Soc Div Polym Chem) 1994;35(1):572–3.
[65] Misra S, Napper DH, Mattice WL. Structure of polyelectrolyte brushes in poor solvents. Polym Mater Sci Engng Prepr (Am Chem Soc Div Polym Mater Sci Engng) 1994;71:603–4.
[66] Nguyen-Misra M, Mattice WL. Self-association of triblock copolymers with insoluble end blocks. Polym Mater Sci Engng Prepr (Am Chem Soc Div Polym Mater Sci Engng) 1994;71:605–6.
[67] Helfer CA, Sun JS, Matties MA, Mattice WL, Hemingway RW, Steynberg JP, Kelley LA. Implications of the fluorescence for the conformational analysis of polymeric profisetinidins and procyanidins. Polym Bull (Berlin) 1995;34:79–85.
[68] Matties MA, Mattice WL. Photophysical models of aromatic polyesters: excited state inter-actions in bis(phenalkyl)terephthalates. Polym Bull (Berlin) 1995;34:369–75.
[69] Xing L, Mattice WL. Atomistic simulations of self-assembled monolayers that contain azo-benzene. Polym Mater Sci Engng Prepr (Am Chem Soc Div Polym Mater Sci Engng) 1995;73:400–1.
[70] Rapold RF, Mattice WL. New high coordination lattice model for RIS polymer chains. Polym Mater Sci Engng Prepr (Am Chem Soc Div Polym Mater Sci Engng) 1995;73:402–3.
[71] Tanaka G, Mattice WL. Collapse of lattice chains. Polym Prepr (Am Chem Soc Div Polym Chem) 1995;36(2):53–4.
[72] Haliloglu T, Mattice WL. The molecular dynamics of poly(1,4-*trans*-butadiene) in the amorphous state and in an inclusion complex. Macromol Symp 1996;101:435–42.
[73] Sun JS, Mattice WL. Interaction of catechin with poly(L-proline). Polym Bull (Berlin) 1996;37:691–8.
[74] Kim WK, Mattice WL. Molecular modeling of polybenzoxazine: thin film and the diffusion of small penetrant molecules in the bulk. Polym Mater Sci Engng Prepr (Am Chem Soc Div Polym Mater Sci Engng) 1997;77:608–9.
[75] Jang JH, Mattice WL. Cohesion of two thin films of polyethylene melt by Monte Carlo simulation on a high coordination lattice. Polym Mater Sci Engng Prepr (Am Chem Soc Div Polym Mater Sci Engng) 1997;77:610–1.
[76] Doruker P, Mattice WL. Dynamics of polyethylene films on a high coordination lattice. Polym Mater Sci Engng Prepr (Am Chem Soc Div Polym Mater Sci Engng) 1998;78:257–8.
[77] Haliloglu T, Cho J, Mattice WL. Simulation of rotational isomeric state models for poly-propylene melts on a high coordination lattice. Polym Mater Sci Engng Prepr (Am Chem Soc Div Polym Mater Sci Engng) 1998;78:259–60.
[78] Doruker P, Mattice WL. Dynamics of bulk polyethylene on a high coordination lattice. Macromol Symp 1998;133:47–70.
[79] Ozisik R, Mattice WL. Diffusion coefficients of single component linear *n*-alkanes. SPE ANTEC 99 1999. p. 2412–6.
[80] Lee S, Mattice WL. Morphology in the box: atomic force calculation and phantom bubble analysis in the interface. Polym Mater Sci Engng Prepr (Am Chem Soc Div Polym Mater Sci Engng) 1999;81:451–2.
[81] Doruker P, Mattice WL. The effect of chain end segregation on the mobility of thin films. Polym Mater Sci Engng Prepr (Am Chem Soc Div Polym Mater Sci Engng) 1999;81:555–6.
[82] Doruker P, Mattice WL. Coarse-grained simulations on the stability of thin films. Polym Mater Sci Engng Prepr (Am Chem Soc Div Polym Mater Sci Engng) 2000;83:418–9.