ADVANCES IN POLYMER SCIENCE 195

Volume Editor A. R. Khokhlov

Conformation-Dependent Design of Sequences in Copolymers I

Springer

063
C748
V.1

Conformation-Dependent Design of Sequences in Copolymers I

Volume Editor: Alexei R. Khokhlov

With contributions by
P. G. Khalatur · A. R. Khokhlov · E. E. Makhaeva
I. M. Okhapkin · C. Wu · G. Zhang

Springer

The series *Advances in Polymer Science* presents critical reviews of the present and future trends in polymer and biopolymer science including chemistry, physical chemistry, physics and material science. It is adressed to all scientists at universities and in industry who wish to keep abreast of advances in the topics covered.
As a rule, contributions are specially commissioned. The editors and publishers will, however, always be pleased to receive suggestions and supplementary information. Papers are accepted for *Advances in Polymer Science* in English.
In references *Advances in Polymer Science* is abbreviated *Adv Polym Sci* and is cited as a journal.

Springer WWW home page: http://www.springer.com
Visit the APS content at http://www.springerlink.com/

Library of Congress Control Number: 2005934719

ISSN 0065-3195
ISBN-10 3-540-29513-5 Springer Berlin Heidelberg New York
ISBN-13 978-3-540-29513-6 Springer Berlin Heidelberg New York
DOI 10.1007/11569572

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilm or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer. Violations are liable for prosecution under the German Copyright Law.

Springer is a part of Springer Science+Business Media

springer.com

© Springer-Verlag Berlin Heidelberg 2006
Printed in Germany

The use of registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Cover design: *Design & Production* GmbH, Heidelberg
Typesetting and Production: LE-TEX Jelonek, Schmidt & Vöckler GbR, Leipzig

Printed on acid-free paper 02/3141 YL – 5 4 3 2 1 0

195
Advances in Polymer Science

Editorial Board:

A. Abe · A.-C. Albertsson · R. Duncan · K. Dušek · W. H. de Jeu
J.-F. Joanny · H.-H. Kausch · S. Kobayashi · K.-S. Lee · L. Leibler
T. E. Long · I. Manners · M. Möller · O. Nuyken · E. M. Terentjev
B. Voit · G. Wegner · U. Wiesner

Advances in Polymer Science

Recently Published and Forthcoming Volumes

Supramolecular Polymers/Oligomers/ Polymeric Betains
Vol. 201, 2006

Ordered Polymeric Nanostructures at Surfaces
Materials, Chemistry, Formation, Properties, and Applications
Volume Editor: Vansco, G. J.
Vol. 200, 2006

Emissive Materials/Nanomaterials
Vol. 199, 2006

Surface-Initiated Polymerization II
Volume Editor: Jordan, R.
Vol. 198, 2006

Surface-Initiated Polymerization I
Volume Editor: Jordan, R.
Vol. 197, 2006

Conformation-Dependent Design of Sequences in Copolymers II
Volume Editor: Khokhlov, A. R.
Vol. 196, 2006

Conformation-Dependent Design of Sequences in Copolymers I
Volume Editor: Khokhlov, A. R.
Vol. 195, 2006

Enzyme-Catalyzed Synthesis of Polymers
Volume Editors: Kobayashi, S., Ritter, H., Kaplan, D.
Vol. 194, 2006

Polymer Therapeutics II
Polymers as Drugs, Conjugates and Gene Delivery Systems
Volume Editors: Satchi-Fainaro, R., Duncan, R.
Vol. 193, 2006

Polymer Therapeutics I
Polymers as Drugs, Conjugates and Gene Delivery Systems
Volume Editors: Satchi-Fainaro, R., Duncan, R.
Vol. 192, 2006

Interphases and Mesophases in Polymer Crystallization III
Volume Editor: Allegra, G.
Vol. 191, 2005

Block Copolymers II
Volume Editor: Abetz, V.
Vol. 190, 2005

Block Copolymers I
Volume Editor: Abetz, V.
Vol. 189, 2005

Intrinsic Molecular Mobility and Toughness of Polymers II
Volume Editor: Kausch, H.-H.
Vol. 188, 2005

Intrinsic Molecular Mobility and Toughness of Polymers I
Volume Editor: Kausch, H.-H.
Vol. 187, 2005

Polysaccharides I
Structure, Characterization and Use
Volume Editor: Heinze, T.
Vol. 186, 2005

Advanced Computer Simulation Approaches for Soft Matter Sciences II
Volume Editors: Holm, C., Kremer, K.
Vol. 185, 2005

Crosslinking in Materials Science
Vol. 184, 2005

此为试读,需要完整PDF请访问: www.ertongbook.com

Volume Editor

Prof. Alexei R. Khokhlov
Physics Department
Moscow State University
119992 Moscow, Russia
khokhlov@polly.phys.msu.ru

Editorial Board

Prof. Akihiro Abe
Department of Industrial Chemistry
Tokyo Institute of Polytechnics
1583 Iiyama, Atsugi-shi 243-02, Japan
aabe@chem.t-kougei.ac.jp

Prof. A.-C. Albertsson
Department of Polymer Technology
The Royal Institute of Technology
10044 Stockholm, Sweden
aila@polymer.kth.se

Prof. Ruth Duncan
Welsh School of Pharmacy
Cardiff University
Redwood Building
King Edward VII Avenue
Cardiff CF 10 3XF, UK
DuncanR@cf.ac.uk

Prof. Karel Dušek
Institute of Macromolecular Chemistry,
Czech
Academy of Sciences of the Czech Republic
Heyrovský Sq. 2
16206 Prague 6, Czech Republic
dusek@imc.cas.cz

Prof. W. H. de Jeu
FOM-Institute AMOLF
Kruislaan 407
1098 SJ Amsterdam, The Netherlands
dejeu@amolf.nl
and Dutch Polymer Institute
Eindhoven University of Technology
PO Box 513
5600 MB Eindhoven, The Netherlands

Prof. Jean-François Joanny
Physicochimie Curie
Institut Curie section recherche
26 rue d'Ulm
75248 Paris cedex 05, France
jean-francois.joanny@curie.fr

Prof. Hans-Henning Kausch
Ecole Polytechnique Fédérale de Lausanne
Science de Base
Station 6
1015 Lausanne, Switzerland
kausch.cully@bluewin.ch

Prof. Shiro Kobayashi
R & D Center for Bio-based Materials
Kyoto Institute of Technology
Matsugasaki, Sakyo-ku
Kyoto 606-8585, Japan
kobayash@kit.ac.jp

Prof. Kwang-Sup Lee
Department of Polymer Science & Engineering
Hannam University
133 Ojung-Dong
Daejeon 306-791, Korea
kslee@hannam.ac.kr

Prof. L. Leibler
Matière Molle et Chimie
Ecole Supérieure de Physique et Chimie Industrielles (ESPCI)
10 rue Vauquelin
75231 Paris Cedex 05, France
ludwik.leibler@espci.fr

Prof. Timothy E. Long
Department of Chemistry and Research Institute
Virginia Tech
2110 Hahn Hall (0344)
Blacksburg, VA 24061, USA
telong@vt.edu

Prof. Ian Manners
School of Chemistry
University of Bristol
Cantock's Close
BS8 1TS Bristol, UK
ian.manners@bristol.ac.uk

Prof. Martin Möller
Deutsches Wollforschungsinstitut an der RWTH Aachen e.V.
Pauwelsstraße 8
52056 Aachen, Germany
moeller@dwi.rwth-aachen.de

Prof. Oskar Nuyken
Lehrstuhl für Makromolekulare Stoffe
TU München
Lichtenbergstr. 4
85747 Garching, Germany
oskar.nuyken@ch.tum.de

Prof. E. M. Terentjev
Cavendish Laboratory
Madingley Road
Cambridge CB 3 OHE, UK
emt1000@cam.ac.uk

Prof. Brigitte Voit
Institut für Polymerforschung Dresden
Hohe Straße 6
01069 Dresden, Germany
voit@ipfdd.de

Prof. Gerhard Wegner
Max-Planck-Institut für Polymerforschung
Ackermannweg 10
Postfach 3148
55128 Mainz, Germany
wegner@mpip-mainz.mpg.de

Prof. Ulrich Wiesner
Materials Science & Engineering
Cornell University
329 Bard Hall
Ithaca, NY 14853, USA
ubw1@cornell.edu

Advances in Polymer Science
Also Available Electronically

For all customers who have a standing order to Advances in Polymer Science, we offer the electronic version via SpringerLink free of charge. Please contact your librarian who can receive a password or free access to the full articles by registering at:

springerlink.com

If you do not have a subscription, you can still view the tables of contents of the volumes and the abstract of each article by going to the SpringerLink Homepage, clicking on "Browse by Online Libraries", then "Chemical Sciences", and finally choose Advances in Polymer Science.

You will find information about the

- Editorial Board
- Aims and Scope
- Instructions for Authors
- Sample Contribution

at springeronline.com using the search function.

Preface

For a long time, chemical industry was focused on polymers mainly from the viewpoint of obtaining advanced construction materials, such as plastics, rubbers, fibers, polymer composites. These materials provided a number of important benefits, including improved strength and long-term durability, light weight, environmental resistance, and design flexibility. Starting from about the early 1980s, the main focus of interest shifted to functional polymers. Among these are superabsorbents, nanoporous rate-controlling membranes, reversible adhesives, electro-conductive polymers and nanowires. In the 1990s, the scientific and industrial polymer community started to discuss "smart" or "intellectual" polymer systems (e.g., soft manipulators, polymer systems for controlled drug release, field-responsive polymers, shape memory networks, and self-healing coatings); the meaning behind these terms is that simply the functions performed by polymers become more sophisticated and diverse. The line of research concentrating on polymer systems with more and more complex functions will certainly be in the mainstream of polymer science in the 21st century.

One of the ways to obtain new polymers for sophisticated functions is connected to the synthesis of novel building blocks – monomer species – where the required function is linked to the chemical structure of these blocks. However, the potential of this approach is rather limited because complicated and diverse functions of polymeric materials would then require a very complex structure of monomers, which normally means that the organic synthesis is more expensive and less robust. An alternative approach is to use known building blocks and to try to design a copolymer with a given sequence of these units. At the present time, there are many synthetic and theoretical strategies directed towards varying the chemical sequences of copolymers: from the variation of their composition and blocky structure to more sophisticated features like "tapered" and gradient structures. In a broad sense, most conventional chemical syntheses, especially polymer syntheses, can be regarded as *bottom-up nanotechnology* leading to the assembly of building blocks into the final macromolecules. Unfortunately, in most conventional polymerization processes, the physical control of assembly during the reactions is practically impossible.

With these difficulties in mind, it is instructive to look at main biological macromolecules – proteins, DNA, and RNA – that have precise and specific structures. These polymers in living systems are responsible for functions, which are incomparably more complex and diverse than the functions that we

normally discuss for synthetic copolymers. The molecular basis for this ability to perform sophisticated functions is associated with the primary sequences of biopolymers. In particular, the unique functions of proteins reflect their molecular structure, so that the sequence of amino acids in a protein defines its secondary and tertiary structure (fibrous versus globular, for example) as well as its function. Therefore, the study of biopolymers at the molecular level may point to new directions in materials design and construction – not just actually using biomolecules themselves to construct novel materials, but mimicking the specific primary sequences of biological polymers. Indeed, by taking this biomimetic route, significant and path-breaking achievements may be made by materials scientists and engineers. Thus, a promising path related to the design of new synthetic copolymers is to learn the rules of biologically driven controlled synthesis and directed assembly in vivo and eventually to apply these rules to the creation of engineered synthetic polymer systems from cheap and commonly available building blocks.

Original ideas connected with the biomimetic design of sequences in synthetic functional copolymers were formulated by us in 1998. They were based on the simple and well-known fact that the function of all globular proteins depends on two main factors: (1) they are globular and (2) they are soluble in aqueous medium. The combination of these two factors is nontrivial, e.g., for homopolymers and random copolymers the transition to globular conformation is usually accompanied by the precipitation of globules from the solution. Protein globules are soluble in water because of the special primary sequence: in the native conformation most of hydrophobic monomer units are in the core of the globule while hydrophilic monomer units form the envelope of this core. Keeping the biomimetic approach described above in mind, one can formulate the following problem: is it possible to design such a sequence of synthetic HP copolymer (copolymer consisting of monomer units of two types, H and P) that, in the most dense globular conformation, all hydrophobic H-units are in the core of this globule while the hydrophilic (polar) P-units form the envelope of this core? The corresponding bio-inspired two-letter HP copolymers generated on a computer were called *protein-like* copolymers. Of course, the degree of function complexity that we hope to achieve for designed copolymers, is much less than current biopolymers, but the behavior of copolymers with designed sequences can exhibit many useful features distinguishing them from the "scratch" (e.g., statistically random) sequences.

The approach formulated in 1998 is based on the assumption that a copolymer obtained under some preparation conditions is able to "remember" features of its original conformation from which it was built and to store the corresponding information in the resulting sequence. Therefore, this approach may be called *conformation-dependent sequence design*.

Most of the contributions collected in volumes 195 and 196 are dedicated to the review of the results obtained recently in this direction, i.e., dealing with the conformation-dependent sequence design of copolymers and the study of

their properties. The contributions collected present the up-to-date research results on most of the topics related to this approach. Surface and interfacial phenomena are also major topics of these volumes. The individual chapters are diverse in purpose and in style. Some of them paint the field in broad, conceptual strokes, others in fine methodical detail. Some present information, others arguments or interpretation. Some summarize past activities, others point to future potential.

Volume 195 begins with a chapter by Khalatur and Khokhlov that gives a survey of the simulation methods as applied to the design of nontrivial sequences in synthetic copolymers aimed to achieve desired functional properties. Several new synthetic strategies allowing for the synthesis of copolymers with a broad variation of their sequence distributions are reported. Synthetic copolymers exhibiting long-range statistical correlations, large-scale compositional heterogeneities, and physical complexity are the focal point of this review. Roughly speaking, the physical complexity of a sequence is understood as the amount of information that is stored in that sequence about a particular environment.

Zhang and Wu review the experimental results on the folding of different hydrophilically or hydrophobically modified copolymers in extremely dilute solutions. The focus is on the formation of stable and soluble mesoglobules made of several amphiphilic copolymers and on the folding of single copolymers – both linear and grafted – into core-shell nanostructures that have various applications. All these features are directly related to the unique chemical sequence of the copolymer chains under discussion. The authors discuss the insights that can be obtained by the analysis of the data of laser light scattering and the use of this method as a potential probe of fine molecular structures, including the so-called "molten" globule state. Emphasis is put on the most recent achievements, although important historical contributions are also mentioned.

A concept of amphiphilicity, as applied to single monomer units of designed water-soluble polymers, is presented in the third chapter by Okhapkin, Makhaeva, and Khokhlov. The concept is relevant to biomolecular structures and assemblies in aqueous solution. The authors consider the substantial body of information obtained experimentally and theoretically on surface molecular chemical structures, including those that are prospective for surface catalysis. Unusual conformational behaviors of single amphiphilic polymers recently observed in simulations are also discussed in detail.

The problems related to the colloidal stability of amphiphilic polymers in water are reviewed by Aseyev, Tenhu, and Winnik in the first chapter of volume 196. The focus is on the derivatives of thermally responsive smart macromolecules – both on copolymers and homopolymers – which are present in a solution as stable micelles potentially having various applications.

One of the promising synthetic strategies of conformation-dependent sequence design is based on direct copolymerization under unusual conditions.

此为试读,需要完整PDF请访问: www.ertongbook.com

This strategy was first realized by Lozinsky et al., who studied the redox-initiated free-radical copolymerization of thermosensitive N-vinylcaprolactam with hydrophilic N-vinylimidazole at different temperatures, as well as by Chi Wu and coworkers. Lozinsky presents an extensive review of the experimental approaches, both already described in the literature and potential new ones, to chemical synthesis of protein-like copolymers capable of forming core-shell nanostructures in a solution.

Continuing along the chemical theme, Kuchanov and Khokhlov review comprehensively the diffusion-controlled polymer-analogous reactions and free-radical copolymerization. The field of polymer chemistry today is distinguished by its depth of mathematical and quantitative rigor in the pursuit of a wide array of challenging new subjects. These ingredients are present in full in this chapter, where the quantitative theory of solution and interphase free-radical copolymerization is discussed from the viewpoint of statistical chemistry and statistical physics of polymers. It is shown that the interaction of these two disciplines has significant impact on the development of new synthetic strategies and technologies in polymer chemistry, including those related to the conformation-dependent design of nontrivial copolymer sequences.

The final short historical review by Grosberg and Khokhlov is devoted exclusively to the discussion of fundamental ideas initially formulated in polymer physics by the outstanding Russian scientist I.M. Lifshitz and especially to today's development of his ideas. Major attention is focused on the statistical theory of heteropolymers covering such areas as protein folding and the sequence design both of protein macromolecules and of synthetic copolymers mimicking some protein properties. In particular, the ideas of sequence design in functional copolymers were originated within the school of Lifshitz; thus, in volume 196, it seems natural to give a review of the achievements along the lines of all major ideas initially formulated by Lifshitz in the field of polymer science.

All of the selected contributions that are present in these special volumes are good representatives for manifesting the importance of the concepts based on conformation-dependent sequence design. It has been our intention to provide the scientific and industrial polymer community with a comprehensive view of the current state of knowledge on designed polymers. Both volumes attempt to review what is currently known about these polymers in terms of their synthesis, chemical and physical properties, and applications. We will feel the volumes have been successful if some of the chapters presented here stimulate readers to become interested in and solve specific problems in this rapidly developing field of research.

Moscow, November 2005 *Alexei R. Khokhlov*

Contents of Volume 196

Conformation-Dependent Design of Sequences in Copolymers II

Volume Editor: Alexei R. Khokhlov
ISBN: 3-540-29515-1

Temperature Dependence of the Colloidal Stability of Neutral Amphiphilic Polymers in Water
V. O. Aseyev · H. Tenhu · F. M. Winnik

Approaches to Chemical Synthesis of Protein-Like Copolymers
V. I. Lozinsky

Role of Physical Factors in the Process of Obtaining Copolymers
S. I. Kuchanov · A. R. Khokhlov

After-Action of the Ideas of I. M. Lifshitz in Polymer and Biopolymer Physics
A. Y. Grosberg · A. R. Khokhlov

Contents

Computer-Aided Conformation-Dependent Design of Copolymer Sequences
P. G. Khalatur · A. R. Khokhlov 1

Folding and Formation of Mesoglobules in Dilute Copolymer Solutions
G. Zhang · C. Wu 101

Water Solutions of Amphiphilic Polymers: Nanostructure Formation and Possibilities for Catalysis
I. M. Okhapkin · E. E. Makhaeva · A. R. Khokhlov 177

Author Index Volumes 101–195 211

Subject Index 237

Adv Polym Sci (2006) 195: 1–100
DOI 10.1007/12_049
© Springer-Verlag Berlin Heidelberg 2005
Published online: 13 December 2005

Computer-Aided Conformation-Dependent Design of Copolymer Sequences

Pavel G. Khalatur[1,2] (✉) · Alexei R. Khokhlov[1,2,3]

[1]Institute of Organoelement Compounds, Russian Academy of Sciences, 117823 Moscow, Russia
khalatur@germany.ru

[2]Department of Polymer Science, University of Ulm, 89069 Ulm, Germany
khalatur@germany.ru

[3]Physics Department, Moscow State University, 119899 Moscow, Russia

1 Introduction: Two Paradigms in Sequence Design 5

2 New Synthetic Strategies in Sequence Design 8
2.1 Preliminary Remarks 8
2.2 CDSD Via Polymer-Analogous Modification 10
2.2.1 Protein-like Copolymers: Structure Dictates Sequence 10
2.2.2 Long-Range Correlations and Their Measure 14
2.2.3 Hydrophobic Modification of Hydrophilic Polymers 19
2.2.4 Adsorption-Tuned Copolymers 23
2.2.5 Design as a Simulation of Evolutionary Process 25
2.3 CDSD Via Copolymerization 31
2.3.1 Conditions for CDSD 31
2.3.2 Copolymerization with Simultaneous Globule Formation 32
2.3.3 Emulsion Copolymerization 36
2.3.4 Copolymerization Near a Selectively Adsorbing Surface 39
2.3.5 Copolymerization Near a Patterned Surface 43
2.4 Design of Monomeric Units 48
2.4.1 Amphiphilic Polymers 48
2.4.2 HA Model 49

3 Properties of Designed Copolymers 51
3.1 Single Chains 51
3.1.1 Coil-to-Globule Transition 51
3.1.2 Kinetics of the Collapse Transition 54
3.2 Phase Behavior: The Sequence-Assembly Problem 57
3.2.1 The Polymer RISM Theory 58
3.2.2 Field-Theoretic Calculation 63
3.2.3 Molecular Dynamics Simulation 64
3.2.4 Evolutionary Approach 67
3.3 Charged Hydrophobic Copolymers 70
3.3.1 Solution Properties 71
3.3.2 Designed Copolymers in the Presence of Monovalent Counterions 72
3.3.3 Effect of Multivalent Counterions 74
3.3.4 Stabilization Mechanism 76
3.3.5 Experimental Results 78

3.4 Hydrophobic-Amphiphilic Copolymers 79
3.4.1 Single Amphiphilic Chains 81
3.4.2 Coil-Globule Transition Versus Aggregation 86
3.5 Adsorption Selectivity 90
3.5.1 Adsorption-Tuned Copolymers 90
3.5.2 Molecular Dispenser 91

4 Conclusion 93

References 95

Abstract A survey is given of the simulation methods as applied to the design of nontrivial sequences in synthetic copolymers aimed at achieving desired functional properties. We consider a recently developed approach, called conformation-dependent sequence design (CDSD), which is based on the assumption that a copolymer obtained under certain preparation conditions is able to "remember" features of the original conformation in which it was built and to store the corresponding information in the resulting sequence. The emphasis is on copolymer sequences exhibiting large-scale compositional heterogeneities and long-range statistical correlations between monomer units. Several new synthetic strategies and polymerization processes that allow synthesis of copolymers with a broad variation of their sequence distributions are reported. We demonstrate that the CDSD polymer-analogous transformation is a versatile approach allowing various functional copolymers to be obtained. Another synthetic strategy is the CDSD step growth copolymerization which is carried out under special conditions. It includes the intrinsic possibilities of exploiting the heterogeneities of the reaction system to control the chemical microstructure of the synthesized copolymers, making possible new paradigms for synthesis and production of polymeric materials. In both cases, we try to show how the preparation conditions dictate copolymer sequences. Also, we discuss advances that have recently been achieved in the computer simulation and theoretical understanding of designed copolymers in solution and in bulk. The focus is on amphiphilic protein-like copolymers and on hydrophobic polyelectrolytes. Here, we demonstrate how copolymer sequence dictates structure and properties.

Keywords Charged heteropolymers · Copolymers · Phase behavior · Polyamphiphiles · Sequence design · Simulation · Solution properties

Abbreviations

A	amphiphilic group (monomer, monomeric unit)
α^2	chain expansion factor
$[A_M]$	mole fraction of intermolecular aggregates of size M
ATC	adsorption-tuned copolymer
ATRP	atom transfer radical polymerization
b	bond length
$\boldsymbol{C}$	symmetric matrix of direct correlation functions
χ	Flory–Huggins interaction parameter
$\widetilde{\chi}$	effective interaction parameter
C_α^0	bulk concentration of monomer species α
$C_\alpha(\boldsymbol{r})$	instant local concentration of monomer species α
$C_\alpha(z)$	equilibrium concentration profile of monomer species α
$c(r)$	direct site-site pair correlation function

CRP	controlled radical polymerization
DCTT	degenerative chain transfer technique
CDSD	conformation-dependent sequence design
DF	density functional
DFA	detrended fluctuation analysis
ΔG	change in association free energy
D_{L}	block length dispersion
D_λ	dispersion within a sliding window of length λ
$\Delta\mu_{\mathrm{s}}$	solvation free energy
$\Delta(q)$	determinant of matrix integral equation
ΔT^*	change in transition temperature
ε	energy parameter
$\boldsymbol{E}$	unit diagonal matrix
ε^*	critical adsorption energy
$\varepsilon_{\mathrm{PP}}$	attraction energy between hydrophilic (polar) segments
f	fraction of charged monomers
$\boldsymbol{\Phi}$	volume fraction of macromolecules
φ_α	average fraction of monomer species α in copolymer chain
ϕ_α	volume fraction of monomer species α
$\varphi_\alpha^{(i)}$	intrachain composition profile of monomer species α
$\phi_\alpha(\boldsymbol{r})$	volume fraction field of monomer species α
$F_D(\lambda)$	detrended local fluctuations within a window of length λ
$f(\lambda)$	block length distribution function
F_{s}	sequence free energy
γ	solvation parameter
h	Shannon's entropy
H	hydrophobic monomer (monomeric unit)
$\boldsymbol{H}$	symmetric matrix of total site-site correlation functions
HA model	hydrophobic-amphiphilic (side-chain) model
HPE	hydrophobic polyelectrolyte
HP model	hydrophobic-hydrophilic(polar) model
$h(r)$	total site-site pair correlation function
JS	Jensen–Shannon divergence measure
K	association equilibrium constant
k_{B}	Boltzmann constant
ℓ	block length
L	average block length
λ	length of sliding window along copolymer sequence
L_{H}	average length of hydrophobic blocks
L_{P}	average length of hydrophilic (polar) blocks
LRC	long-range correlation
m	average number of copolymer chains per aggregate
MAST	macrophase separation transition
MFPT	mean first passage time
MIST	microphase separation transition
N	total chain length, number of repeat units
N_α	number of repeat units of type α (α = A, B) in the chain
NIPA	poly(*N*-isopropylacrylamide)
n_{J}	number of crosslinks
N_τ	current chain length

此为试读,需要完整PDF请访问: www.ertongbook.com