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Topology of Polymers

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Preface

There is a growing awareness of the importance of topology in various fields, including *polymer chemistry*. We discuss the *topology of polymers* from both mathematical and chemical viewpoints via a close collaboration of topology (Shimokawa and Ishihara) and polymer chemistry (Tezuka). We cover fundamental and selected topology topics as applied to polymers with the goal to provide novel insights revealed through the unique interaction between mathematics and polymer materials science.

We apply graph theory to analyze structures of multicyclic polymers and use terminologies to define their nomenclature. We discuss the types of multicyclic polymers, such as *spiro*, *bridged*, *fused* and *hybrid* forms, and constitutional isomers; the enumeration of multicyclic polymers is also provided. Using knot theory, we also discuss *topological isomers* and *chirality* of multicyclic polymers. In addition, we discuss the graph-theoretical and knot-theoretical properties of multicyclic polymers in practice.

With regard to polymer chemistry, we discuss the nomenclature based on the classification of mono- and poly-cycloalkanes. We then demonstrate the chemical synthesis of topologically unique multicyclic polymers via *electrostatic self-assembly and covalent fixation* protocols.

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Chapter 1
Topology meets polymers: Introduction

In this chapter, we introduce polymers, long-chain molecules with diverse chemical compositions and structures. Topology can provide fundamental insights into the principle properties of polymers via their segment structures. We also present a brief description of the following chapters with respect to topological geometry and polymer chemistry.

1.1 Polymer constructions by topology insights

Polymers are ubiquitous long-chain molecules that are fundamental in biological as well as in industrial synthesis. Examples include DNA, proteins, and cellulosic compounds, as well as plastics, films, fibers, rubbers, and other common materials. There has been continuous progress in both the fundamental scientific understanding and the applications of polymers. In particular, a number of formidable breakthroughs in synthetic polymers have extended the range of structures from linear or randomly branched forms toward a variety of precisely controlled topologies, including an essential class having cyclic and multicyclic forms[1, 2]. These developments now offer opportunities to design unprecedented properties and functions via computational modeling/simulation of their forms, i.e., topologies, followed by experimental verification[3].

Because the long-chain form of polymers can be represented as a geometrical line construction, the topological (soft) geometry provides a fundamental basis to elucidate basic structural properties of flexible and randomly coiled polymers having diverse structures, in contrast to small molecules modeled on Euclidian (hard) geometry principles[4, 5]. So far, topological geometry and graph theory have successfully elucidated unique properties of DNA with cyclic, knot, and link topologies, relevant to their evolution for diverse biofunctions[6, 7]. Notably, any branching of single-stranded DNA is inherently circumvented, presumably because its principal biological function is to store and read out genetic information. In contrast, frequently encountered branching/folding structures in proteins and polypeptides are

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