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Perspective on Polymer Chemistry

Heidari A

Department of Chemistry, California South University, Irvine, California, USA

Perspective

Polymer chemistry is a sub-discipline of chemistry that focuses on the chemical synthesis, structure, and chemical and physical properties of polymers and macromolecules. The principles and methods used within polymer chemistry are also applicable through a wide range of other chemistry sub-disciplines like organic chemistry, analytical chemistry, and physical chemistry. Many materials have polymeric structures, from fully inorganic metals and ceramics to DNA and other biological molecules.

In 1884 Hilaire de Chardonnet started the first artificial fiber plant based on regenerated cellulose, or viscose rayon, as a substitute for silk, but it was very flammable. In 1907 Leo Baekeland invented the first polymer made independent of the products of organisms, a thermosetting phenol-formaldehyde resin called Bakelite. Around the same time, Hermann Leuchs reported the synthesis of amino acid N-carboxyanhydrides and their high molecular weight products upon reaction with nucleophiles, but stopped short of referring to these as polymers, possibly due to the strong views espoused by Emil Fischer, his direct supervisor, denying the possibility of any covalent molecule exceeding 6,000 daltons. Cellophane was invented in 1908 by Jocques Brandenberger who treated sheets of viscose rayon with acid.

Polymer chemistry is adept at producing a wide range of polymeric materials tailored to a variety of applications. Unfortunately, the human eye is unable to see atoms, so the beauty of the molecular architecture of these materials often goes unnoticed. Molecular modeling is able to solve this problem and enables the visualization of these complex structures along with an insight into their physical and mechanical properties.

Polymer modeling is the counter part of the modeling used on a daily basis in the pharmaceutical industry. The vast sums of money and time that have to be invested to get a new drug to market have stimulated the field of pharmaceutical modeling, with protein homology modeling, protein-ligand docking, and computational design of combinatorial libraries commonplace these days. This is interesting as the average protein is a polymer of up to 20 monomers (amino acids), whereas the average synthetic polymer contains maybe one or two monomers. Hence, synthetic polymer modeling ought to be conceptually simpler than protein modeling but there has been less research into its applications.

Polymer modeling is rapidly advancing to the stage where the modeling is quicker than the synthesis, and so computational screening of new potential polymers can be carried out prior to synthesis for desired properties. Therefore, we are embarking on the age of computer-aided polymer design.

There are a variety of ways to address the modeling of polymers, the most conceptually simple being to build a model of every atom in the polymer. This, however, is also the most computationally intensive method and requires a good knowledge of the system and software. A quicker method is to add parameters together to produce the desired property, from knowledge of the chemical groups in the polymer. This is termed QSPR (quantitative structure property relationships) and is the counter part of QSAR (quantitative structure activity relationships) in drug design. These QSPR methods are quick and easy to apply but lack the insight that the atomic detail can provide. We concentrate here on atomistic modeling and provide some examples of what can be produced for a cross-linked polymeric system.

Organic polymers play a crucial role in living things, providing basic structural materials and participating in vital life processes. For example, the solid parts of all plants are made up of polymers. These include cellulose, lignin, and various resins. Cellulose is a polysaccharide, a polymer that is composed of sugar molecules. Lignin consists of a complicated three-dimensional network of polymers. Wood resins are polymers of a simple hydrocarbon, isoprene. Another familiar isoprene polymer is rubber.

Other important natural polymers include the proteins, which are polymers of amino acids, and the nucleic acids, which are polymers of nucleotides—complex molecules composed of nitrogen-containing bases, sugars, and phosphoric acid. The nucleic acids carry genetic information in the cell. Starches, important sources of food energy derived from plants, are natural polymers composed of glucose.

Polystyrene can be coloured any shade and is used in the manufacture of toys and other plastic objects. In modern organic polymer chemistry, the main focus is on the environmental impact of novel applications of polymers that are basically derived from monomers based on carbon–carbon bonds. Still, we have one class of polymers that differs significantly from the carbon chemistry: siloxanes where the polymeric backbone is mainly free from carbon and consists of alternating silicon and oxygen. The further substitution pattern at the silicon may vary; still dominating the methyl group, leading to polydimethyl siloxanes (PDMSs), a polymeric class with unique properties and high economic importance.

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***Address for Correspondence:** Heidari A, Department of Chemistry, California South University, Irvine, California, USA, E-mail: heidari.a@gmail.com*

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