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Editorial

Modeling of Chain Conformations and Spatial Configurations

It is a pleasure for me to be the guest editor for the series of papers in this issue on the topic of Modeling of Chain Conformations and Spatial Configurations. I thank the Editor Dr J. E. Mark for giving me this opportunity.

Atomistic simulation of polymers dates back several decades. Even before the invention of computers (or calculating machines), the conformation of the cellulose chain in the crystalline state deduced by Meyer and Misch [1], using ball and stick models, remains valid to date, but for the details. Similarly, the model constructed by Watson and Crick for the DNA conformation, was as tall as Crick [2]. Using a plumb line on a graph paper to determine the coordinates of the atoms was a practice in those days. Then came the 'contact distance' criterion introduced by Ramachandran [3], to estimate the accessible conformations of polymer chains. At the same time, methods such as the 'virtual bond analysis' were introduced [4] for determining the conformations of polymers based on X-ray diffraction data. This phase was quickly followed in the mid 60's by the introduction of potential functions, or force fields. Today, we are able to perform detailed atomistic simulation of complex structures and the dynamics of polymer systems.

Some of the pioneering contributions of Flory include the rotational isomeric state formalism for the analysis of the spatial configurations, polymer chain folding and rubber elasticity. In this issue on Chain Conformations and Spatial Configurations, the papers cover these topics, in various aspects. In the sequence of papers, the effect of tacticity is discussed by Helfer, Mattice, and Soldera, Grohens. The RIS treatment of the mean square dipole moment is described by Zhou, Abe. The description of chain conformations of a polyelectrolyte (Marcelo, Tarazona, Saiz), with geometry relaxation (Chakraborty, Lagowski), and with confinement in channels (Hunt, Jung, Shamsheer, Uyar, Tonelli), and the solubility parameters (Zhao, Choi) follow. Then the aspects of chain folding (Yamamoto) and interpenetration of globules (Liang, Zhang, Li, Yang) are discussed. The paper by Ijantkar and Natarajan deals with the thermodynamic properties of polymer surfaces derived from simulations. Finally, the effects of elongational flow and deformation are discussed by Liu, Ashok, Muthukumar; Capaldi, Boyce, Rutledge; and Roberge, Prud'homme, Brisson.

Publishing focussed articles of this nature periodically, helps the researchers to follow the progress and steer the field to new frontiers. I express my appreciation to the authors for their participation in this project and their support.

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