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Computational Materials Science of Polymers

By Andrey Aleksandrovich

Viva Books Private Limited, 2009. Hardcover. Book Condition: New. First edition. An approach to the quantitative analysis of the effect of the chemical structure of linear and network polymers on their properties is described. The approach is based on the representation of the repeating unit of the polymer in the form of a set of anharmonic oscillators which describe the thermal motion of atoms in the field of intra- and intermolecular forces, including weak dispersion forces, dipole-dipole interactions, hydrogen and valency bonds. Computer programs based on this approach are also presented. They can be used for calculating more than 50 fundamental physical and chemical constants of linear and network polymers as well as low molecular liquids. The programs make it possible to solve a direct problem, i.e. quantitative evaluation of the physical properties of polymers based on their chemical nature, and a reverse problem, i.e. computer synthesis of polymers with the prescribed physical properties. Contents: Introduction ? Brief information on types of polymers and their chemical structure ? Packing of macromolecules and polymers density ? Increments method and basic physical assumptions ? Relationship between free volume of polymers, coefficient of molecular packing and porous structure ? Temperature coefficient of volumetric...



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