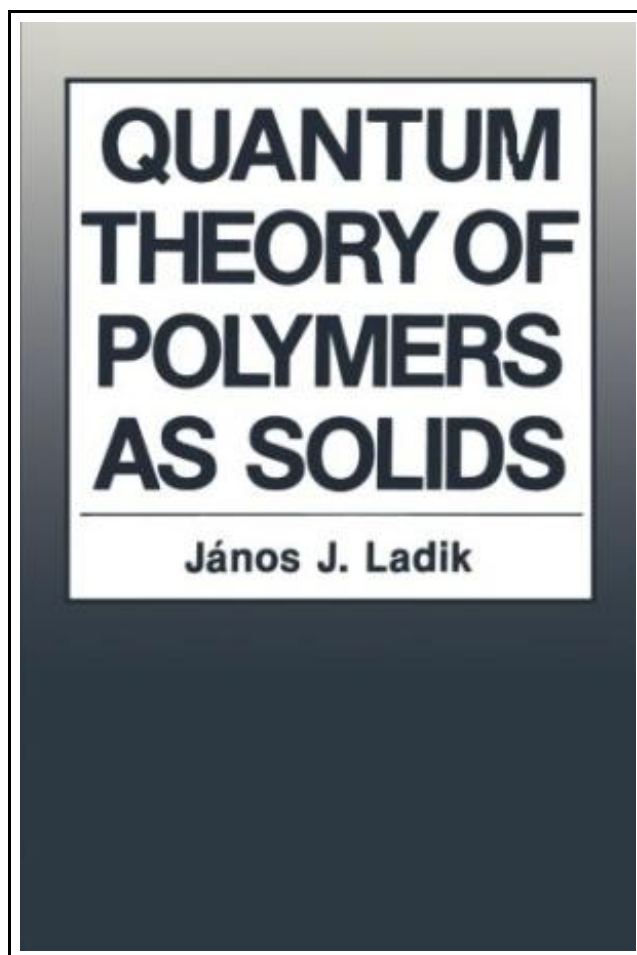


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Springer, United States, 2012. Paperback. Book Condition: New. 1988 ed.. 229 x 152 mm. Language: English . Brand New Book ***** Print on Demand *****.The goal of this monograph is to summarize the different quantum mechanical methods developed in the last 20 years to treat the electronic structure of polymers. Owing to the nature of the problem, these methods consist of a mixture of quantum-chemical and solid-state physical techniques. The theory described in Part I treats, besides the Hartree-Fock problem, the electron correlation, and it has also been developed for disordered polymeric systems. Though for obvious reasons the book could not include all the existing calculations, each new method described is illustrated by a few applications, with a discussion of the numerical results obtained. Far more details see the Introduction to Part I. The second part contains the theoretical calculation of different properties of polymers based on the methods systematically introduced in the first part. The properties calculated include the electronic and vibrational spectra of polymers, and the computation of their transport, magnetic, and mechanical properties. In cases where reliable experimental data are available, the theoretical results are compared with them.



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