

Book Reviews

Quantum Theory of Polymers
*Edited by Jean-Marie Andre,
Joseph Delhalle and Janos Ladik*
D. Reidel Publishing Company,
1978, 376 pp., Dfl. 85

This volume contains the proceedings of the NATO Advanced Study Institute on Electronic Structure and Properties of Polymers held at Namur, Belgium from 31st August to 14th September 1977.

The papers are almost exclusively concerned with the electronic properties of polymers and for the most part with the basic energy level structure. The chapter by VERBIST provides a useful resumé of the principles of X-ray photoelectron spectroscopy and its relationship with calculated electronic structures. All the other articles are contributions to the theory.

Over the past decade or so the Belgian group, André, Delhalle, Leroy *et al.* have made many valuable contributions to the theoretical study of electronic energy bands in polymers. Their method has consisted of applying the well tried and reasonably successful semiempirical and *ab initio* methods of molecular quantum chemistry to linear polymers with one dimensional translational symmetry. (The treatment is of a three-dimensional monomer repeated regularly in one dimension). Single electron energy bands are then calculated in the one dimensional Brillouin zone – in exact analogy with solid state energy bands. Since the coupling between adjacent 'unit cells' is covalent the bands are wide, as in semiconductors, and might reasonably be expected to give an adequate overall view of the electronic density of states. It is this approach to the electronic structure which forms the basis of many of the articles in this volume.

The opening chapter by André and Delhalle describes the theoretical method. The difficulties in the way of obtaining unambiguous comparisons between the theory and the experimental densities of states obtained from photoelectron spectroscopy are discussed by Verbist. The articles by Veillard on the evaluation of electronic repulsion integrals and by Harris on Fourier representation methods are concerned with the details of computational techniques. Two articles by Ladik describe band structure calculations in biopolymers and in highly conducting polymers, respectively.

Most of the remaining chapters are devoted to discussions of general theoretical approaches in crystalline and disordered solids which might presumably be expected to find some application in polymeric systems in the future. Although the articles are of a high quality it has to be said that their correction with polymer science as it exists at present is often tenuous.

There are a number of chapters on electron correlation, treated by diagrammatic and other techniques (March, Collins, Cizek, Brandow). These articles are often innovative and are certainly pedagogically useful, but they rarely discuss the specific features of polaron and exciton structures which might be expected in polymers.

Two chapters by Csavinsky are devoted respectively to quantum mechanical treatments of transport properties in semiconductors and of electronic effects on the mechanical properties of semiconductors. Possible applications to polymers are given a very brief mention. A treatment of transport properties much more specifically oriented towards polymers is attempted by Suhai.

In rather a different vein there are interesting articles by McCubbin and by Martino on electronic states in structurally disordered chains, by Del Re on chemisorption on polymers and by Schuster on hydrogen bonding.

D. Pugh

**Advances in Polymer Science, 28;
Polymerisation reactions**
Springer-Verlag, Berlin-Heidelberg-New York, 36\$

This book is the latest in a long running and highly valued series devoted to reviews on all aspects of polymer science. It is subtitled Polymerisation Reactions, but is concerned principally with ionic, and in particular, cationic processes. Three topics are discussed: 'Random and Block Copolymers by Ring Opening Polymerisation' by Y. Yamashita; 'Ring Opening Polymerisation of Bicyclic Acetals, Oxalactone and Oxalactam' by H. Sumitomo and M. Okada; and 'Cationic

Olefin Polymerisation Using Alkyl Halide – Alkyl Aluminium Initiator Systems', by J. P. Kennedy and P. D. Trivedi. The last topic has been divided into two sections, the first concerning itself with reactivity studies and the second with molecular weight studies.

The review by Yamashita is very comprehensive and covers a wide field. The general features of the homopolymerisation of cyclic monomers are first discussed, and these are applied in subsequent sections to the formation of various types of copolymers. Although mechanisms detailed are principally cationic in character, anionic and coordinate processes are also considered, and examples given of their application to the production of copolymers. A full bibliography of over 400 references is provided and the article should be of value to all polymer chemists with synthetic interests. The reviewer has, however, one minor criticism on the layout of the review. The monomers described are, after their introduction, referred to by abbreviations; to readers unfamiliar with these terms it would have been very useful to have provided a glossary for ease of reference.

The review by Sumitomo and Okada is more restricted in scope, and is confined to the polymerization of bicyclic compounds in which the authors have taken an active interest over recent years. The article considers in detail the polymerisation of about a dozen classes of compounds under the three headings given in the title. The accounts are thorough with stress laid on the structural conformations of the products. The physical properties of selected polymers are also listed.

The contributions by Kennedy and Trivedi has been given too general a title as it is exclusively concerned with the polymerization of isobutylene by alkyl halide – alkyl aluminium initiators – a topic which has long occupied the attention of the former author and his research team. Nevertheless, the survey given makes fascinating reading since it involves a lucid description of systematic investigations in which virtually every relevant technique in the armoury of the polymer scientist was used to unravel the mechanistic complexities of these systems.

All the articles in this volume meet the high standards that are now expected of this series, and the book, whilst being of general interest, will be of particular value to investigators in the field of ionic polymerizations.

D. H. Richards