

Book Review

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds, LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

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Lecture notes in chemistry. Vol. 9. Crystals as giant molecules. By A. JULG. Pp. vii + 135. Berlin, Heidelberg, New York: Springer, 1978. Price: DM 18, US \$ 9.00.

The aim of the author, in this volume of a series whose purpose is to report new developments in chemical research and teaching, is to explore the possibilities of using quantum-chemistry methods to describe crystal structure by regarding crystals as extended assemblies of atoms forming giant molecules. As might be expected from such an approach, the principles are set out with the style and economy of a mathematician, but the larger part of the book is essentially descriptive and there are many delightful free-hand illustrations.

The first chapter is a review of the localized molecular-orbital approach, *i.e.* the use of hybridized atomic orbitals, to rationalize observed molecular geometry and the polarization of electron charge in bonds within molecules. Chapter 2 applies these ideas to crystals, where it becomes necessary to distinguish between molecular crystals and the more extended lattices containing networks of bonding orbitals. Chapter 3 considers methods of calculating charge distribution and bond ionicity in crystals and describes some new work relating ionicity parameters to calculations of hardness. Chapter 4 describes progress made towards

directly predicting crystal structure using energy-minimization calculations. *Ab initio* calculations for the alkali-metal halides show the expected trend towards increased stability of the CsCl structure for the heavier cations, but the work is not complete. The crystal arrangements found in some metals are analysed, but energy bands and electric and magnetic properties are not considered. The remainder of the chapter gives descriptions in hybrid-orbital terms of a wide range of structures including metal oxides, complex halides and molecular crystals. The final two chapters deal with perturbations arising from the presence of crystal faces, and preliminary attempts to describe the external shapes of crystals through surface-energy calculations.

The book is reproduced from a typed manuscript, and contains few errors. The notation used for hybrid orbitals is unfamiliar, *e.g.* sp_3 for sp^3 , and the use of the abbreviation bcc for the CsCl structure is unfortunate.

In this different approach to the description of the crystalline state, the author has presented some interesting new ideas and may well initiate further directions for research to his readers.

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