there is an obvious relationship between surface band structure and LEED calculations and hence that the programs provided could be used for either. The methods used are based on a dynamical formulation of the scattering problem and use approaches due to J. B. Pendry.

The set of programs provided comprise almost 200 of the 278 pages of the volume. They are most complete and an offer is made to send a magnetic-tape copy of these programs to interested parties. In fact, one of the members of our laboratory (Dr A. Smith) has made use of this offer and has used such a tape. This experience has shown that the programs work quite well to the extent that the authors claim although, as stated in the book, since there are so many different types of problems, exhaustive tests of the programs have not been carried out.

The book cannot be used without reference to the work of J. B. Pendry, *Low energy electron diffraction* (Academic Press, 1974). This is acknowledged by Van Hove and Tong. Pendry's book contained a set of programs that could deal with simple substances. In the volume under review a significant new method has been introduced, the 'combined space method', which, together with further developments, allows a much wider range of real crystals to be dealt with. It is a pity that the detailed formulation of symmetry lacks contact with the treatments of symmetry in dynamic diffraction that have occurred in other areas of diffraction and crystallography such as electron diffraction and X-ray diffraction. It is clear from reported work in the literature, as well as the many results displayed in this volume, that surface structure analysis, using the methods described in this text, is now a common activity. In addition to the coordinates of atoms at real surfaces, the thermal vibration amplitudes of these atoms are also being estimated. At present this is done at the level of a simple Debye–Waller factor.

This book is an invaluable tool for those research groups which are involved in the study of atomic and electronic surface structure. There is a useful summary of results in these areas which is reasonably complete to the year 1978. The book is not truly a book in the traditional sense but rather a brief review of LEED theory combined with a detailed instruction manual for the use of a set of computer programs for the calculation of LEED intensities and some other surface properties.

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**Superionic solids: principles and applications.** By S. CHANDRA. Pp. xi + 404. Amsterdam: North Holland, 1981. Price US $78.00, Dfl 160.00.

Although the field of superionic conductors, preferably referred to as solid electrolytes or fast ion conductors, has attracted an intense research effort over the last decade or so, a good teaching text was hitherto unavailable. Chandra's book represents, in the first place, a welcome effort to take the reader with little knowledge of solids through a descriptive and well illustrated course to a well rounded understanding of this area. Even for the specialist, the description extends to include comprehensive compilations of up to date data digested in a very satisfying fashion.

In the second place, the chapters on *Experimental probes* and *Applications* provide a uniquely wide-ranging coverage ideal for those entering the field or diversifying their interests within the field.

Finally, there are two chapters which more formally and extensively develop the theoretical description of *Ion transport in point defect type ionic and superionic solids* and *Ion transport in molten sublattice type superionic solids.*

The book will be valued by teachers, students and research workers alike for its unified yet detailed approach which only a single author could bring to a work such as this.

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**Crystal cohesion and conformational energies.** Part 26 of **Topics in current physics.** Edited by R. M. METZGER. Pp. ix + 154. Berlin–Heidelberg–New York: Springer Verlag, 1981. Price DM 54.00, US $23.00.

This book contains four chapters devoted to the calculation of cohesive energies in organic crystals and dimers and of energies in larger biomolecules.

In the first chapter D. E. Williams reviews his approach to the calculation of lattice energies of organic crystals by means of the empirical atom–atom potential method, using transferable parameters. He discusses various types of interaction-energy contributions and amply describes methods for the derivation of the parameters and point charges needed for the potentials. Detailed results are shown and discussed for 18 hydrocarbon crystals. Special attention is paid to the tedious formulation of the analytical expressions for the matrix elements used in the least-squares formalism for the refinements of the parameters.

F. A. Momany shows in the second article how conformational analysis can aid in polypeptide drug design. After a brief introduction of the method used for the calculation of the conformational energy of a polypeptide (*viz* using empirical potentials and the computer program *ECEPP*) he illustrates it with a number of examples. These include peptide backbones and modifications of these [*e.g.* *N*-methyl analogs, depsipeptides, carbazic acid (α-aza) analogs], aspects of bond types, chain reversal and direction reversal, disulfide bonds and modification of side chains (*e.g.* α,β dehydro analogs). For these examples a number of isoenergetic contour diagrams is given, from which favorable conformations can be deduced. The author also discusses

connections between conformational analysis and drug activity.

In the third part R. M. Metzger contributes on the calculation of cohesion energy and on ionicity in organic semiconductors and metals. He first discusses Löwdin's formalism for the calculation of crystal cohesive energy with its various energy contributions. Expressions for Madelung, charge-dipole, dipolar, polarization and dispersion energies are elaborated. A number of lattice-energy calculations are then described for compounds like TTF–TCNQ, TTF–$Br_{0.74}$ *etc.*, using atomic charges derived from *ab initio* or semi-empirical MO calculations. The calculations are compared with experimental data derived from Born–Haber cycles. It appears that the simplest Madelung–uniform lattice model does not satisfactorily describe the cohesive energy for organic partially ionic quasi-one-dimensional metals. In these crystals special attention is therefore paid to contributions other than pure Madelung, *e.g.* charge-dipole, dispersion and polarization terms, to the Wigner lattice model and to a nonlinear dependency of the polarization energy on the charge transfer.

The closely related fourth contribution of B. D. Silverman deals with dimers of tetrathiafulvalene (TTF) and of tetracyanoquinodimethane (TCNQ). He studies the energies of isolated dimers as a function of the relative positions of the two molecules (slipped *versus* eclipsed) in order to understand the stacking of the molecules in the crystals. On the semi-empirical MO level (extended Hückel or CNDO/2) the calculated energies do not lead to satisfying geometries. Empirical atom–atom parameters yield results only in qualitative agreement with the observed crystal structure for TTF. The Gordon–Kim procedure, using semi-empirical or minimal basis wave functions for the monomers, leads to a dimer interaction energy for $(TTF)_2$ which has a minimum near the position in the neutral crystal. The influence of ionization (charge transfer) is also studied.

The book as a whole thus deals with three different rather specialized topics. Each of the valuable contributions emphasizes the author's approach and work, although in each chapter a large number of references to recent related work are included. The contents are well organized and the typesetting is simple but clear, with few misprints.

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**Ordering in two dimensions.** Edited by S. K. SINHA. Pp. xix + 497. Amsterdam: North Holland, 1980. Price US $70.75, Dfl 145.00.

The contents of this book are the papers presented at an international conference at Lake Geneva, Wisconsin, USA, May 1980, with 200 participants, 90% coming from the USA. From the 98 publications of experimental and theoretical work, about 85% are from the United States; no scientist from the UK or Japan is to be found in the list of participants or authors. So the name international conference seems to be inappropriate.

The volume is divided into the following chapters: *Invited papers* (27), *Physisorbed and chemisorbed systems* (28), *2D Wigner crystals and computer simulation studies* (8), *Theory of 2D phase transitions* (11), *Intercalated materials* (4), *2D magnetism* (4) and *Molecular monolayers, bilayers, membranes and liquid crystals* (16). This shows the wide spectrum of the subject matter of the papers, so, for instance, one contribution is entitled *Phase transition of the membrane associated with the blood–brain barrier via interaction with drugs.*

But there are many papers with the same method (*e.g.* ten papers using LEED), or with a particular system (*e.g.* graphite as a substrate). Besides the papers in the chapter *Theory of 2D transitions*, there are about 50 papers with the keywords transitions or melting in the index, and there are phase diagrams in about 15 papers. For the experimental methods, investigations with X-rays and neutrons (seven papers each) must be mentioned also. It is a sign of the times that ten papers are connected with computer simulations, and it is not surprising that a book with the word ordering in its title contains about 25 papers with figures or sketches of structures, or models of structures. From the title of one paper, *Preparation of surface films far from thermodynamic equilibrium by surface chemical reactions*, it can be seen that the reader is also informed of highly sophisticated preparative methods by this book.

Fortunately, remarks from the discussion are also printed. The print of the type-written manuscripts, with line drawings, is of good quality. The volume contains only a few half-tone pictures of moderate quality. The book is an important source of information for the specialist and it gives a good overview of the state of the art and the science of 2D systems for the beginner too, even if it is a pity that contributions from a lot of laboratories outside the USA are missing. Besides this, 3D scientists also can find interesting stimulation in this book.

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## Books Received

*The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.*

**Traditional ornamentation** (in Azeri). Pp. 48 + pp. 52 of figures. Asarnashr, Baku, 1981. Price 50 kopeks, and **Crystallographic ornaments** (Russian summary of the above). Pp. 32. Baku, 1982. Price 4 kopeks. Both by Kh. S.