

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.