

Book reviews

Fractals, quasicrystals, chaos, knots and algebraic quantum mechanics. Amann, A., Cederbaum, L., Gans, W. (eds.) NATO ASI Series C: Mathematical and physical sciences, Vol. 235. Kluwer Academic Publishers, Dordrecht 1988, 331 pp.

This collective volume represents the proceedings of a workshop on “New Theoretical Concepts in Physical Chemistry” which took place in October 1987 in Italy. The 21 individual contributions focus on the five subjects given in the title which originate from the intersection of chemistry, physics and mathematics. The first four articles are about fractals, selfsimilarity and related concepts applied to problems of physical chemistry. After an introductory review written for the physical chemist, with many pictures and references, specific problems of reaction kinetics and diffusion in heterogeneous media as well as coagulation are addressed. The next five contributions deal with quasicrystals. The two theoretical papers, in essence, approach the problem of that kind of irregularity by embedding structures into a space of dimension greater than 3. In addition there are two experimental papers and a computer simulation on the growth of icosahedral phases.

Chaos in classical and quantum mechanics is the subject of five papers. The notion of chaos and the most relevant properties of classical chaotic systems are briefly reviewed. Most noticeable is the survey on the celebrated results on the ionization of highly excited hydrogen atoms. The other interesting contributions address the kicked rotator as a model, the statistics of energy levels and finally a numerical study of the ro-vibrations of a weakly bound state.

The following three papers present knot theory and its application to biomolecules, essentially to DNA, and catenanes. In particular the contribution about the mathematics of knots and link polynomials is very instructive. The last four talks, finally, are about “algebraic quantum mechanics”. They all address interesting but rather different problems.

The present book might be appealing to theoretical chemists because the interesting mixture of mathematics, physics and chemistry is rather stimulating and it presents problems, concepts and results which do not belong to the standard knowledge of theoretical chemists yet, some of them probably will never do so. On the other hand the volume is rather expensive and most of the relevant literature on these topics is available already in research journals — if one knows where to look.

T. Hoffmann-Ostenhof and P. Schuster, Vienna

Hoffmann, R.: Solids and surfaces. A chemist's view of bonding in extended structures. Verlag Chemie, Weinheim Basel Cambridge New York 1988. 142 p., 177 figs. (ISBN 3-527-26905-3; 089 573-709-4) DM 48.00; £16.25

There are several ways to study solids or surfaces ranging from the many-body treatment with complicated formalism often used by physicists to a molecular orbital description chemists prefer. Roald Hoffmann tries a typical chemist's view to understand solids and surfaces, with the most

chemical notion, i.e., the solid is a large molecule. Hardly any formula is presented, but there are many diagrams and figures which illustrate the essence of bonding in a set of selected examples. Firstly, this book teaches chemists the basic concepts of the electronic structure in extended systems: terms as Bloch functions, band width, Fermi level, density-of-states etc. are discussed where the analogy to simple molecules is often used. One starts out with one-dimensional systems and quickly reaches the three-dimensional case. Instead of using the details of band structure calculations Hoffmann shows that a qualitative picture is enough to understand certain aspects of solids in a frontier orbital perspective. Whenever there is (covalent or metallic) interaction the (partly) delocalized electrons determine the structure and reactivity of such systems, but one can still speak of bonds, i.e. one knows where the electrons are. The band filling or the position of the Fermi level is stressed since it plays an important role in many examples as well as the characterization of bonding and antibonding states. Even phenomena such as the Peierls distortion are explained in simple terms for a linear hydrogen chain. The author makes one believe that even for a more complicated system it is almost trivial for any chemist to draw a qualitative band structure from which he can derive properties of solids. Although certain prerequisites (e.g., a good background about symmetries and molecular orbitals in molecules or clusters) are needed to do that, it is demonstrated how one can have a qualitative reasoning about orbital interactions especially on surfaces. Other examples are forces which control dissociation or deformations. No attempt is made to describe other theoretical models which focus on an understanding of solids. It is not even mentioned how the band structures shown in the book are obtained or under which assumptions or approximations they are computed. The emphasis is on concepts. In comparison to many other publications in this field Hoffmann's book provides a different approach to understand solids and surfaces and is an excellent introduction for chemists in relevant aspects of solid states physics, but it could be equally useful for physicists if they wish to learn more about descriptive tools to interpret the electronic structure of extended systems. Such books can help to bridge the gap between chemistry and physics in an exciting field.

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