

**Quantum chemistry of solids: The chemical bond and energy bands in tetrahedral semiconductors.** By A. LEVIN. Pp. xii + 249. Moscow: Khimiya Press, 1974 (in Russian); New York: McGraw-Hill, 1977 (in English). Price £14.10, US\$24.00.

'All matter is made of atoms'. Richard Feynman, in his famous lectures on physics, regards this statement as the most important and informative piece of present scientific knowledge. If just one sentence could be passed to the next generation, this should be the one, he says. The previous generation still disputed seriously about the real existence of the atom. Now it is a well established fact. We have many means, well known by all crystallographers, that make the detailed atomic structure of matter concretely visible. Still, the quantitative significance of this statement poses some problems.

The idea of atomic constituents of matter involves identification of the basic structural units of matter with free atoms. Of course, we get free atoms when we decompose matter, and matter when we put free atoms together; we can even recognize the atomic species in our density maps. However, a conclusive physical proof of the idea requires derivation or at least understanding of the measurable properties of matter on the basis of the measurable properties of free atoms and of their mutual interactions. This is easy for many mechanical' and thermal properties, but as soon as we turn to phenomena, where basic electronic properties enter the scene, difficulties arise.

The band calculations, on which our understanding of electronic properties are based, preferably ignore the atoms. Many attempts to derive band structures from the properties of constituent atoms by tight binding or LCAO methods have sadly failed. There has grown the general belief that reasonable results can be reached by some plane-wave methods only, where the atomic properties have no role. This is the situation where this book enters the game.

This book is the first extensive and quantitative apology of the chemical or atomic view on band theory. It boldly opposes the general opinion of solid-state physics. True, dating from 1974, it is no longer quite up to date in its details. However, it still deserves attention today. In the present hasty times one seldom meets books which are so carefully considered in their structure and all details. The book starts with an introduction to the basic theory at a level which brings it within the reach of a

newcomer. It proceeds logically, explains every step clearly and thoroughly and displays honestly the physical argumentation, motivation and consequences of the assumptions and approximations, which are so often omitted and left to the headache of the reader.

The book is concentrated merely on elements with diamond structure and on the related partially-covalent crystals with ZnS structure. In spite of this restriction it is instructive in a general sense. It gives a coherent presentation of the methods and ideas followed and may thus give impulses to new applications and developments.

The main approach is the 'equivalent orbital' or EO LCAO method. The bonds are described in terms of symmetry-related local orbitals, and the band structure resulting from the corresponding Bloch functions is discussed. Band widths, gaps and other critical measures of the band structure are expressed in terms of several Coulomb and resonance integrals, which - on the assumption that 'matter is made of atoms' - are related to spectroscopic and thermodynamic data on the atoms and structurally-related molecules. This makes the treatment both semiempirical and semiquantitative, but, on the other hand, it gives a simple and astonishingly consistent explanation of many known properties of the crystals. It is able to produce, in a simple parametric form, plausible explanations for both the systematic behaviour and the lack of it, either horizontally as a function of ionicity or vertically as a function of the atomic masses.

As minor points of criticism, one may note some unconventional use of terms *e.g.* 'self consistent' instead of 'self adjoint' or 'Hermitian' and 'associated' instead of 'augmented' plane waves for APW; also some non-standard notations are used. The list of references is impressive. It gives a good view also of the Russian literature in the field. It is also interesting to see how many western books are available in Russian translation, although in case of real need a western reader might prefer a reference to the original.

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