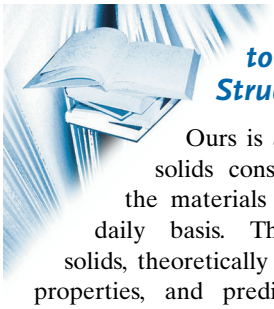

Orbital Approach to the Electronic Structure of Solids

Ours is a material(s) world, and solids constitute at least 90% of the materials useful to humans on a daily basis. Therefore, understanding solids, theoretically modeling their essential properties, and predicting the behavior of those not yet synthesized is an essential task in modern theoretical solid state science. A silent revolution has been taking place in this field, as more and more powerful computers have been put at our disposal. In the 1980s, *Gaussian*, which is a program for ab initio calculations on isolated molecules, made it possible to apply quantum-mechanical methods on a large scale for calculations on molecular systems. In a similar fashion, the advanced codes now available for computing the properties of extended organic and inorganic solids—usually based on density functional theory—are used to model the properties of millions of important materials, sometimes with astonishing accuracy when one considers the simplifications and assumptions that are made in the underlying theory. Even beginner chemists can now reproduce, model, and even predict materials. But what about understanding? Chemists and materials scientists rely on computational packages written by physicists and, just as in the case of *Gaussian*, they sometimes use these tools as black boxes which somehow produce results. One major difficulty for chemists who play with their atomic toys in real space is the important fundamental concept of band structure theory, that of reciprocal space. The complexity of the band structures for most real materials is hidden in the spaghetti of bands running almost unpredictably between various k-points. Who has the patience to eat pasta one spaghetto at a time?

The book *Orbital Approach to the Electronic Structure of Solids*, by Enric Canadell, Marie-Liesse Doublet, and Christophe Iung, helps you enjoy the meal. The authors build upon excellent teaching traditions that have been set by R. Hoffmann, J. Goodenough, J. K. Burdett, M.-H. Whangbo, and others, patiently showing how to understand and make use of the band structures of solids by looking at their real-space representations, the crystal orbitals, while relentlessly shuttling between the two. The theoretical tools that are used extensively in the book—molecular orbital theory and the extended Hückel method—are taught to young chemists throughout the world. MO theory is quite intuitive at the molecular level, and is therefore applied to model crystalline systems in 1, 2, or 3 dimensions. The authors build understanding slowly, often dividing more complex systems into chemically meaningful molecular fragments or functional groups, and then showing you how their symmetry-adapted orbitals interact. Frequently looking at orbital loops and drawing them by hand comes with a bonus: not only does it allow you to discover insightful qualitative explanations, but also you build your intuition about what the chemical system will or won't do.

The authors know well that one good figure is better than 10 written pages, so the book is rich in simple illustrations (typically two per page), and there are a number of good exercises at the end of each chapter.

Orbital Approach to the Electronic Structure of Solids is an example of qualitative thinking in the age of numerical quantum chemistry. To my personal taste it would benefit from semi-quantitative analyses, for example analyzing the relationship between the partial density of states of a system and the electronegativities of its constituent elements. Illustrations of band dispersion along various directions in k-space in relation to interactions between crystallographic unit cells in various directions would be useful. Some readers might complain that the crystal orbital overlap population (COOP) tool is not used more often, and much can be learned from comparing the band structures and densities of states of related systems side by side (as in the children's game "spot the difference"), but all these features could be improved in the next edition. Overall, this is a great book. Ask your students if they enjoyed the pasta—their response will best inform you of its didactic aspects.

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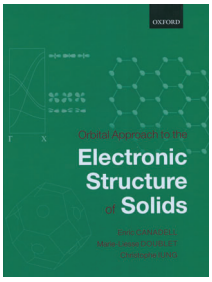

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