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Book Reviews

Computational Chemistry of Solid State Materials

by R. Dronskowski,
Wiley-VCH Verlag GmbH Co. KGaA,
Weinheim, Germany, 2005,
pp 300. ISBN: 3-52731410-5,
Price: EUR 105.00

When I go on holiday I always take a large selection of books to read, some for pleasure others for review on the rainy days. My mistake was in not taking this book since it would have fallen into both categories, as it is an excellent text, well written and a book that has been needed for many years.

Richard Dronskowski holds the Chair of Solid-State and Quantum Chemistry at RWTH Apache University and he wrote this book while at Tohoku University (Sendai) in the summer of 2004. I wish he had taken a visiting position sooner then maybe we would not have had to wait until 2006 for this book.

This is a much-needed volume as it brings together the real world of the practical chemist and the theoretical world of the quantum-theoretical approach to solid state and materials chemistry. The author says the book is targeted at an intelligent reader, chemist or physicist and I think it should be read by all chemists who wish to understand more about chemical bonding and asking the basic questions of theoretical approaches that can explain existing structures of materials and discover new materials. However, the book does far more than this, it proves a very good platform for anyone wanting to understand the basic concepts in computer programs used in theoretical chemistry.

The book is very well written and addresses key points that bring together the concepts of practical and theoretical chemistry we have all been taught and tries to identify the myths that have developed in our understanding of the chemical bond. For example, the oversimplification that chemical bonding in molecules is due to spin pairing of formerly unpaired electrons. It also addresses the myth of the relationship between bond length and bond strength; it is a common rule of thumb that shorter bonds are stronger bonds. Examples are given showing how this rule cannot be generalised. The myth of relating chemical bond formation with a decrease in kinetic energy is also explored and dismissed.

The book has only three main chapters. The first dealing with the classical approach to solid-state chemistry e.g. ionic radii, electrostatics and Pauling's Rules. I think those key words will make many of you think about your undergraduate days and maybe shudder a little, but the concepts are well described and undergraduates would be well advised to read the accounts of them written here. In Chap. 2 the quantum-chemical approach is described and of course has to start from the beginning with the Schrödinger wave equation before developing into the Hartree-Flock and Slater's orbital approximations. I enjoyed reading this chapter; as someone who has an interest in computational chemistry it filled in some of my misunderstandings.

Each chapter starts with a couple of very well sourced quotations. One such quotation is given at the start of Chap. 2. It is a quotation by John Cage "I can't understand why people are frightened of new ideas. I am frightened of the old ones" How true that is for anyone with vision. Chap. 2 is the longest chapter in the book and you have to think, go back a few pages and read it again, or at least I did to understand and get the full benefit. It is not a chapter you are going to read in one afternoon, especially if you have had a good lunch and maybe a drink!

The final chapter is on using the computational machine and predicting various chemical and physical properties of materials. But again I must share with you one of the quotations given at the start of this chapter from one of my boyhood heroes, Winston Churchill "However beautiful the strategy, you should occasionally look back at the results" Any experimental and theoretical chemist will relate to that quotation. I was amazed in reading this chapter to find out how close modern computational functions are to the real world, but then again in some cases how there are still large differences. However, as opposed to just leaving this as a problem the author attempts to analysis and explain the differences.

If I had to pick a fault then it must be the inclusion of the tables of ionic radii, bond-valence parameters for oxides, extended Hückel energy parameters, absolute electro-negativities and absolute hardness of atoms. I do not think they are required in this book, if I need them I can look them up in a reference book or even on the web. Moreover, references to the tables are also given in the excellent bibliography and items can be found very easily in the index.

I hope you have gained the impression that I like this book, I do and I would recommend it to any chemist.

P. Myers

Ewing's Analytical Instrumentation Handbook

by J. Cazes (ed.),
CRC Press (Thomson Publishing Service),
Andover, UK, 2005,
pp 1064. ISBN 0-8247-5348-8,
Price: GBP 145.00

The *Analytical Instrumentation Handbook* is intended to serve as a guide for workers in analytical chemistry needing a starting place for information about a specific instrumental technique, either as a basic introduction or as a means of finding