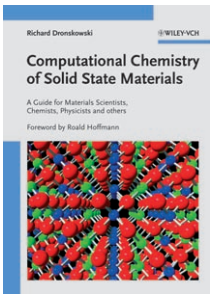
## Computational Chemistry of Solid State Materials




A Guide for Materials Scientists, Chemists, Physicists and Others. By *Richard Dronskowski*. Wiley-VCH, Weinheim 2005. 294 pp., hardcover € 99.00.—ISBN 3-527-31410-5

Even before interdisciplinary scientific research activities came into vogue, the solid state was already a field in which chemists, physicists, materials scientists, and engineers came together to manipulate the chemical elements in ways to generate new basic science and new technologies. Nevertheless, even within this arena, the distinctions between these scientific disciplines are real—each discipline has developed its own ways of thinking, working, and understanding, and has created its own language. But real scientific advances occur when language barriers are broken down and ideas that cross between disciplines are blended or pushed in new directions. In his foreword to this monograph, Roald Hoffmann comments about this with regard to chemistry and physics: "So it is interesting when two mature sciences are forced by the facts of nature and a shared subject to confront each other's ways of thinking, both of them productive and yet, and yet … seemingly incommensurate". He goes on to state that the "contemporary solid state" is the "shared subject", and that the future is "shaped by *computational techniques* … that are respectful of both chemistry and physics". One could extend this concept to different scientific approaches: experiment versus theory. The two approaches work together for the advancement of science—experiments provide data from which theories are constructed, and are then verified, modified, or eliminated. Theory provides guiding hypotheses for further experiments. An individual scientist is often categorized as either an "experimentalist" or a "theorist", but experimentalists often develop new theories, and theorists suggest experiments. Moreover, times are changing, as more scientists are combining experiment and theory directly in their own work, through *computation*.

This "pocket book" has been written to provide a common language by which chemists, physicists, and materials scientists can use theory and computation to help understand and predict phenomena in the solid state. It is a clearly written monograph, which begins with some classical and quantum-mechanical background, then moves on to descriptions of various computational methods, and finishes with a cascade of examples taken from the author's own research activities, on topics concerned with structure, composition, physical properties, thermodynamics, and predictions. It is a superb resource by which students and researchers who are unaccustomed to the theoretical and computational literature of the solid state can gain entrance into this arena. For the experienced theoretician or computational scientist, the diversity of examples provides a broad sweep of ideas that may stimulate further theoretical developments.

Chapter 1 addresses classical ideas that come essentially from the chemical literature—atomic and ionic sizes, the ionic model of chemical bonding, Pauling's rules, bond-valence methods, and volume increments. The tables of data for the elements in relation to these various classical models are especially useful. Chapter 2 moves onto quantum-mechanical approaches. Through a combination of essential mathematics and figures, the principles of the tight-binding (molecular orbital) approach for crystalline solids are explained. That is followed by methods for generating densities of states, the partitioning of the total energy, and analysis in terms of overlap populations. The discussion is then extended to include exchange and correlation, before describing density functional theory. The chapter continues by discussing the applications of pseudopotentials, cellular methods, linear methods, and modern developments, and concludes with molecular dynamics. A particularly significant section is the summary of existing computer implementations at the end of this chapter. Chapter 3, the final chapter, applies these methods to a variety of problems, which are concerned with optimizations, explanations, failures, and—ultimately—predictions. This chapter begins by optimizing and explaining observed structures of metal oxides and nitrides, rationalizing structural distortions in elements such as tellurium, discussing the magnetic properties of transition metals and their compounds, and exploring composite materials by molecular dynamics. Next, a section on carbodiimides and cyanamides focuses on limitations and potential failures. The chapter ends with attempts to predict new materials, which range from oxynitrides to intermetallics and magnetic materials.

Chapters 1 and 2 contain a synergistic mixture of mathematics and illustrations to explain and evaluate the various classical and quantum-mechanical approaches. The various case studies in Chapter 3 rely significantly on illustrations. Many literature references are provided, so that readers can explore aspects of special interest in greater depth.

In summary, *Computational Chemistry of Solid State Materials* is an excellent desktop reference source for students and researchers who use, or are looking to use, computational approaches to study the solid state. It is well organized, with just enough detail to provide insight into various techniques and applications. As Roald Hoffmann concludes, "This book … provides a passport of a common language for creative excursions in this fertile middle ground" (between chemistry and physics). The monograph also comes at an appropriate time, for as computational methods become accessible to many different researchers, an understanding and assessment of the strengths and

weaknesses of the various models is needed.

*Gordon J. Miller*
Department of Chemistry
Iowa State University
Ames (USA)

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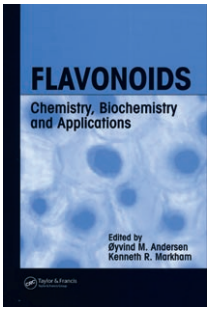
## *Flavonoids*




Chemistry, Biochemistry and Applications. Edited by *Øyvind M. Andersen* and *Kenneth R. Markham*. CRC Press/Taylor & Francis 2006. 1237 pp., hardcover $ 249.95.—ISBN 0-8493-2021-6

8150, and counting…! This still increasing figure is the number of flavonoids that have been reported to date. *Flavonoids* consists of 1237 pages of text, divided into 17 chapters, on all there is to know about these natural products, from their biogenesis and role in plants to their implications and applications in human food and health! This large collection of chapters, written by experts in the field, each one a specialist in a class of flavonoids, covers most aspects of the chemistry of these plant metabolites: isolation, structural identification, physicochemical properties, reactivity, and synthesis. Flavonoids are secondary metabolic hybrids that are biogenerated through a combination of the shikimate/phenylpropanoid pathway, which produces their aromatic $C_6$-$C_3$ moiety, and the "polyketide" acetate/malonate, which gives the second aromatic $C_6$ moiety. One can consider the resulting $C_6$-$C_3$-$C_6$ skeleton to be generated combinatorially by plants and their various enzymatic machineries, to lead to the different subclasses of flavonoids, which include flavones, flavanones, flavonols, flavanols, anthocyanidins, isoflavones, and others. In all of these compounds, the two aromatic $C_6$ rings are joined through the $C_3$ unit in a characteristic chromane cyclic structure. The extent of hydroxylation and *O*-methylation, the level of oxidation/dehydrogenation, and the degrees of freedom for regio- and stereochemical variations, further complicated by conformational restrictions, are the main sources of the remarkable structural diversity of this molecular system. But nature does not stop there; it allows the system to undergo various glycosidations, as well as dimerization and oligo/polymerization processes, and, most importantly from a basic structural point of view, ring-opening and ring-contracting transformations leading to chalcones and aurones. Most, but not all, of these molecular entities bear two mono-, di-, or trihydroxyphenyl units, and as such they belong to the polyphenol family of natural products, which are the subject of current media hype because of their occurrence in plant-derived foods and their claimed benefits for human health. I am sure that you are all aware of the necessity to include at least five servings of fruits and veggies in your daily diet!? That recommendation is partly based on the presence of flavonoids—widely valued for their antioxidant properties—in significant amounts in all common plant-derived food products, as well as in beverages such as wine and tea. Well, I reckon many of you still have lots of questions about these so-called and precious flavonoids, but don't ask me—rather get this book! This is, of course, not the first book on this important topic of natural products chemistry; however, the previous one, edited by J. B. Harborne, was published a decade ago. A lot has happened since then…

The excellent first chapter of this book, written by A. Marston and K. Hostettmann, constitutes in itself an extremely valuable handbook on flavonoids. It describes the different techniques for extracting, separating, purifying, quantifying, and characterizing flavonoids, with useful information on the different types of chromatographic stationary phases and solvent systems that are most appropriate for separating different subclasses of flavonoids at the preparative level. Analytical methods based on high-performance liquid chromatographic techniques, coupled with mass-spectrometric (MS), ultraviolet (UV), spectrophotometric, and nuclear magnetic resonance (NMR) spectroscopic detection methods, are discussed. The imposing second chapter, written by T. Fossen and Ø. M. Andersen, one of the editors of this book, is in the same vein, and describes in detail all the spectroscopic techniques that are used for characterizing flavonoids. This chapter focuses on NMR-spectroscopic and mass-spectrometric analyses, and is nicely laced with numerous tables filled with lots of highly practical information, including NMR chemical shifts in various solvents and MS ionization modes. Vibrational spectroscopic techniques (infrared and Raman spectroscopies), including two-dimensional IR studies, are also reviewed in the context of flavonoid analysis. Of course, in view of the authors' particular interest in anthocyanins, UV-visible absorption-spectroscopic and colorimetric studies on these flavonoid-based pigments are given special attention in this chapter. Of particular note is the tabulated description of colors of pure anthocyanins based on the specification parameters of the "Commission International de l'Eclairage".

The third chapter, written by K. M. Davies and K. E. Schwinn, addresses a more fundamental aspect of flavonoids by focusing on the recent advances in the biochemistry and genetics of these secondary metabolites. All the main enzymes that are involved in the construction and diversification of the basic flavonoid structural skeleton, and for which genes or cDNAs have been identified, are reviewed. Regulation of gene transcription and approaches to genetic modification of flavonoid biosynthesis are also discussed and well referenced.

The following four chapters deal with the occurrence of flavonoids and other phenols and polyphenols in plant-derived foods and beverages, and their contribution to human health. In their chapter, J. A. M. Kyle and G. G. Duthie present a rigorously built database of flavonoids in foods, and discuss factors affecting the flavonoid content of food and dietary intake. Almost all that anyone wants to know about the structures and reactivities of the various types of native and (bio)chemically modified flavonoids found in wine, as well as the influence of these com-