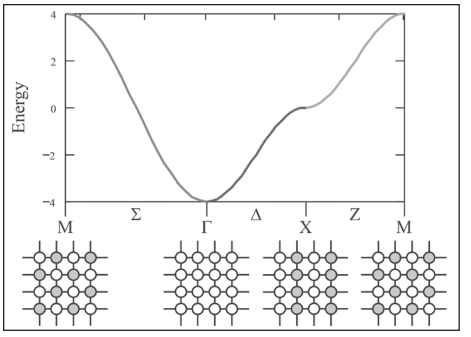
edited by
Theresa Julia Zielinski
Monmouth University
West Long Branch, NJ 07764-1898

Introduction to Basic Terms of Band Structures: BandStructure2001i.zip, BandStructure.pdf, InstructorNotes.pdf

Marc Meyer, Stephan Glaus, and Gion Calzaferri, Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH-3012 Bern, Switzerland;
gion.calzaferri@iac.unibe.ch



A screen showing the band structure diagram for the 2s(C) orbitals of a square carbon lattice. At the k-points Γ, X, and M of reciprocal space the crystal orbitals are real, and the corresponding crystal orbital (CO) schemes are shown in the lower part of the figure. Σ, Δ, and Z are lines of high symmetry in reciprocal space connecting the k-points. There the COs are not real.

In this document you will find an explanation of the concepts and applications of band structures, translational symmetry, crystal orbitals, Bloch functions, wave vectors, the Peierls distortion, density of states (DOS), crystal orbital overlap population (COOP), and Brillouin zones.

Although extended structures starting from molecules as building blocks have been well elucidated in the literature *(1–4)*, the concept of energy bands with their related terms and ideas is often unfamiliar to chemistry students. This Mathcad document, which has been successfully used for several years, acts as an introduction to the theory of band structures.

This document is best used if the students interactively learn and practice individually or in small groups until they master the topic with teacher assistance. The worksheet consists of a main document containing the indispensable parts of the theory, while more involved, more detailed, and more mathematical contents are included in files that can be opened as popups using hyperlinks within the main document. The problems range from simple visualizations to challenging exercises.

The level of the document flows from elementary quantum mechanics to research-level topics such as the quantum-chemical description of three-dimensional crystalline systems. At the end of the course the student is therefore capable and encouraged to use our research-level tight binding program package, BICON-CEDiT, which includes oscillator strength calculations and many more options. It is available with examples free of charge *(5)*. After working with these documents students should also be able to understand and to benefit from the research that will still deepen and broaden their understanding. The document cites useful references.

Literature Cited

1. Hoffmann, R. *Solids and Surfaces;* VCH: New York, 1988.
2. Lowe, J. P. *Quantum Chemistry;* Academic: San Diego, 1993.
3. Duke, B. J.; O'Leary, B. *J. Chem. Educ.* **1988,** *65,* 319; *J. Chem. Educ.* **1988,** *65,* 379; *J. Chem. Educ.* **1988,** *65,* 513.
4. Pisanty, A. *J. Chem. Educ.* **1991,** *68,* 804.
5. Brändle, M.; Rytz, R.; Glaus, S.; Meyer, M.; Calzaferri, G. *BICON-CEDiT* (tight binding program package, including oscillator strength calculations); available at *http://www.dcb.unibe.ch/groups/calzaferri/* (accessed Aug 2003).