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Digital Learning in Physical Chemistry

Using symbolic software in the chemistry curriculum depends on the readiness of the students and the availability of useful documents. For first-year physical chemistry students who have no prior programming experience, a stepwise approach using templates fosters mastery of chemistry concepts and promotes software skill development. More complex concepts in more sophisticated templates challenge advanced students. Well-crafted documents also can move portions of the curriculum out of the classroom or provide enrichment beyond what is in the traditional curriculum. This month we present two such documents.

Kinetics by eBook

ABC Kinetics by J. A. Carrazana Garcia is an eBook collection of Mathcad worksheets that can be used in the traditional undergraduate physical chemistry curriculum. Students will need some introduction to chemical kinetics concepts and some familiarity with Mathcad before using the eBook. If undergraduate students are expected to use the materials independently or in small groups, the instructor may want to provide guidance for the more difficult derivations.

The goal of the ABC Kinetics eBook is to provide a systematic and interactive study of the kinetics of the ABC system. Starting from the analytic solutions to the first-order irreversible ABC system the author develops expressions for the velocity and initial rates for the component species. The global variable definitions permit students to explore other values for the parameters in the rate expressions and observe changes that appear in kinetics plots. The situation where $k_1 = k_2$ is treated by more general expressions that avoid division by zero. Several alternative ABC schemes are left for the students to explore on their own. These can be used as independent projects for determining student mastery of kinetics concepts and Mathcad techniques. The table of contents provides links directly to any part of the eBook and definitions of the symbols used. Embedded links ease navigation throughout the eBook. ABC Kinetics is an excellent package of Mathcad worksheets with a well-conceived organization. Each section of the eBook contains specific references for further study and several exercises for challenging students. The eBook requires Mathcad7 or Mathcad2001i.

Band Structure Basics

Introduction to Basic Terms of Band Structures, by Meyer, Glaus, and Calzaferri, is geared to the advanced undergraduate or graduate students studying solid-state physical chemistry. Before using this document students should have mastered the basic terms and concepts of quantum chemistry. They will need moderate skill with Mathcad and know about the ZDO approximation, Bravais lattices, and reciprocal lattices. The last two are reviewed briefly in the document. This Mathcad worksheet could stand alone as an excellent special topics course for study at the undergraduate or graduate level.

The Band Structure document provides students with an opportunity to study the basic concepts of translational symmetry, crystal orbitals, Bloch functions, wave vectors, the Peierls distortion, density of states, crystal orbital overlap population, and Brillouin zones. The document utilizes the hyperlink capabilities of Mathcad by providing links to supplementary information. This avoids lengthy stretches of tangential information that would distract the reader from the flow of the main discussion in each section of the worksheet. The authors provide a complete index using hyperlinks from which each section of the document can be reached and at the end of each page a HOME link returns one to the table of contents. Double clicking opens both the table of contents links and supplementary links. The document contains many student exercises and provides key references for further work. The Band Structures document requires Mathcad 2001i or higher.

The ABC Kinetics eBook and the Introduction to Basic Terms of Band Structures are excellent examples of how symbolic mathematics software can be constructed. Both make optimal use of the hyperlink feature of Mathcad.

Supplemental Material

Fully interactive Mathcad files along with static PDF files are available on *JCE Online* at *http://jchemed.chem.wisc.edu/JCEWWW/Features/McadInChem.*

ABC Kinetics: ABC_Kinetics11.zip, ABC_Kinetics7.zip, ABC_Kinetics (HTML), ABC_Kinetics.pdf, InstructorNotes.pdf

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The system formed by three chemical species "A", "B", and "C" related to each other by elementary reactions, reversible or not, is broadly used in chemical kinetics as a first step in the study of the so-called complex reactions. This model presents an appropriate combination of mathematical complexity and chemical applicability that transforms it into a didactic resource of great educational value at various levels of chemical kinetics, physical chemistry, or even basic general chemistry, where reaction rates and mechanisms are of interest. In this collection of worksheets, a step-by-step study of the "ABC" system is accomplished with the aid of Mathcad. Working with real mathematics notation, interactive graphs, and symbolic processing allows useful equations to be obtained, transformed and applied live, with the result of clarifying the study goals and objectives. Perturbing the parameter values and observing the effect per-

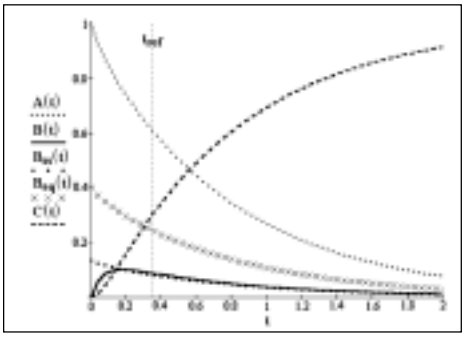

Figure 1. Comparison of the concentrations of [A], [B], and [C] (mole/L) as functions of time using the exact analytic solution, and the steady state, $[B]_{ss}$, and pre-equilibrium $[B]_{eq}$ concentration approximation predictions in the $A \rightleftharpoons B \rightarrow C$ system where $k_1 = 2$ sec^{-1}, $k_{-1} = 5$ sec^{-1}, and $k_2 = 10$ sec^{-1}. t_{ref} is the twice the time required to reach $[B]_{max}$.

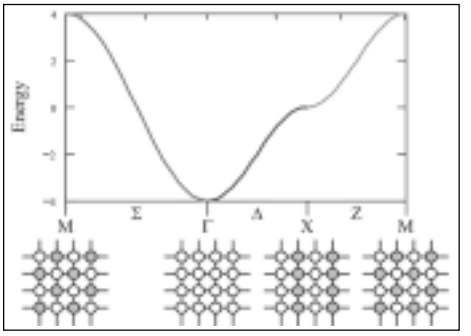

Figure 2. Band structure diagram for the 2s(C) orbitals of a square carbon lattice. At the k-points Γ, X, and M of reciprocal space the crystal orbitals are real, and the corresponding crystal orbital (CO) schemes are shown in the lower part of the figure. Σ, Δ, and Z are lines of high symmetry in reciprocal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

mits visual determination of the significance of the different model parameters. The proposed exercises not only consolidate the concepts and skills but also extend the analysis by applying the models and methods to other similar systems.

The organization of all the material into a Mathcad electronic book makes it user friendly. Users can learn by working with the interactive models and can annotate the book while conserving the original information. The "live" book can be used with versions 7 and 11 of Mathcad. Non-interactive images in PDF and HTML formats are also available.

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

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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).