

A ToolBook Front-End for a Molecular Modeling Program

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Five years ago we purchased three copies of the molecular modeling software package, HyperChem, for our General Chemistry and Physical Chemistry courses. HyperChem is running on three 486 PCs in one of our laboratories. As part of a five-week laboratory-based project on organic chemistry and spectroscopy, the General Chemistry students in my sections sign up in pairs to use the computers. In one assignment, the students use molecular mechanics to model organic molecules as part of an introduction to organic chemistry. In another they do semi-empirical molecular orbital calculations as part of an exercise teaching about molecular orbital theory.

This hands-on approach with HyperChem

seemed to be a good way to teach these concepts and to introduce our students to molecular modeling. It was not without difficulties, however. One problem was upper-level students, who were using HyperChem for other purposes, leaving it in a nonstandard configuration that sometimes confused the introductory students. We also found that the General Chemistry students spent one to two hours learning how to use the program, which was undesirable since our main goal was to help the students learn about organic chemistry, spectroscopy, and MO theory -- not how to use the program.

HyperChem is a Windows 3.1 program that can be linked to other Windows applications, such as ToolBook and Excel. We have written several previous applications with ToolBook 1.5, and decided to use it to develop a front-end program that controls HyperChem. The ToolBook and HyperChem programs run in two windows displayed simultaneously on the screen. The students can transfer control to either program by clicking on that program's window with the mouse. This has the advantage of always starting HyperChem in the same configuration. It also decreases the learning time significantly, because the only HyperChem tools that

The image shows two overlapping windows from a Windows 3.1 environment. The left window, titled "Molecular Orbital Theory", features a dark header with the word "Oxygen" in a white box. Below this, there is a text area with a "Do a molecular orbital calculation for the O₂ molecule" prompt and an "Oxygen" button. A central section displays an energy level diagram with a vertical axis labeled "Energy" and several horizontal lines representing energy levels. Text to the left of the diagram reads: "This is the MO theory energy level diagram for the oxygen molecule. Click on each energy level to see the corresponding molecular orbital". At the bottom of this window are three buttons labeled "Question 1", "Question 2", and "Question 3", and a row of navigation buttons: a left arrow, a right arrow, "Menu", "Index", and "Exit".

The right window, titled "HyperChem - oxygen.hin", has a menu bar with "File", "Edit", "Build", "Select", "Display", "Databases", "Setup", "Compute", "Script", "Cancel", and "Help". The main area of this window displays a 3D contour plot of a molecular orbital, showing two lobes of electron density on either side of a central node. A vertical toolbar on the left side of this window contains icons for zooming in/out, rotating, and other viewing functions. At the bottom of the HyperChem window, a status bar displays the text: "Alpha: Orbital Index = 5 Orbital Energy = -17.304726[eV]".

the students must use are the rotation tools that rotate the molecule and the selection tool with which they can see the calculated bond lengths and bond angles. All other HyperChem operations, such as building the molecule, setting up calculations, doing the calculations, and observing the molecular orbitals are controlled by buttons in the ToolBook program.

We have written two ToolBook front-end programs -- one for molecular mechanics and the other for molecular orbital theory. The MO program is constructed as a series of pages that lead students through a Molecular Orbital Theory lesson. One page in this lesson covers the oxygen molecule. In this page, clicking on the Oxygen button in the ToolBook window prompts the construction of the oxygen molecule in the HyperChem window, followed by an AM1 calculation. The students can rotate the molecule using the HyperChem rotation tool or select the bond to observe the calculated bond length. They also can click on an energy level in a molecular orbital energy level diagram shown in the ToolBook window and see the contour of the corresponding HyperChem MO.

An additional advantage of using a ToolBook front-end program is the ability to include buttons that pop up "question windows" on the screen. For instance, three questions are included on the Oxygen page. The first question asks the students to sketch the eight valence electron MOs of oxygen and identify them as σ or π and bonding or antibonding (a ToolBook reference page, which introduces these labels, is included in the program). The students next are asked to feed the oxygen electrons into the energy levels and to predict if molecular oxygen would have unpaired electrons. They then predict whether the molecule would be diamagnetic or paramagnetic, and observe a video of liquid oxygen in a magnetic field. The ability to ask questions such as these and to supply reference information in the same program that controls the molecular modeling software turns the ToolBook program into more than just a simple front-end. It also is being used as a teaching tool.

We have found that the ToolBook-HyperChem combination has several advantages. It has furnished us with an efficient way to introduce molecular modeling in conjunction with our laboratory program. It also has given us the opportunity to use molecular modeling to teach about organic chemistry and molecular orbital theory. The present ToolBook program is not totally satisfactory, however, because of one remaining problem that we have not been able to solve. The ToolBook program is set up so that it loads first as a window that occupies around 40% of the screen. After the ToolBook front-end has loaded, it automatically runs Hyperchem. Unfortunately, we have not found a way to get the

HyperChem window to fill the other 60% of the screen. Because of this we must load the programs in at the beginning of the day, or when the programs have been shut down during the day, in order to manually bring the HyperChem window to the proper shape and size. This has not prevented us from using the program, but has been an annoyance that we would like to eliminate. We are in the process of pursuing a solution to this problem.

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Multimedia - Are we all speaking the same language?

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It's 11pm once again! For the last 4 weeks no one gets to leave before midnight. The programmer has been glued to the computer to the point that he can't see straight and my assistant and I have been burning (writing) CD-ROMs and testing them furiously mimicking all the varied things that students may do to the product once it's in their hands. Once again it's product deadline time. Sound glamorous? Well, it really is not, but it is the reality of larger scale multimedia productions. For the last 18 months, this large scale CD-ROM project has come in and out of my life, and if I'm lucky it will be done within the next six months. This is what happens when you have virtually no budget and a staff that until recently is mostly volunteers. On the upside, I have learned a tremendous amount (directly propor-