MOLECULAR MODELING
IN
UNDERGRADUATE INSTRUCTION

A Workshop Held at
The University of Lethbridge
April 30, 2001

Program

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Integrated Strategies for Molecular Modeling

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At The King's University College we are trying to use molecular modeling as an integrated tool across much of the chemistry curriculum, as well as in our course for non-science students. We introduce HYPERCHEM 5.1 in two courses required of all biology and chemistry majors, and then build on this foundation in many senior courses. This presentation describes our use of molecular modeling to:

- Understand molecular structure, bonding and reactivity
- Understand how models function in science and chemistry (strengths and limitations)
- Visualize the dynamic character of molecules
- Support investigative approaches
- Accommodate different learning styles

Examples of models and animations used to teach non-majors chemistry, introductory chemistry, organic chemistry, environmental chemistry and spectroscopy will be demonstrated, with an emphasis on examples from organic chemistry.

There are some interesting recent initiatives in science education to bring together chemists and social scientists with backgrounds in areas such as learning styles, perception, and misconceptions; to explore how to best use visualization tools for learning chemistry. We are involved in these discussions and are trying to take them into account in our approach.

Electronic Models of Crystal Structures for the Introductory Course in Inorganic Chemistry

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Almost all text-books of inorganic chemistry, whether aimed at the beginner in the discipline or at advanced students, contain sections dealing with the structures of the common metals as well as the structures of the common (usually monoatomic) ionic salts. Only a very few texts deal in a more extensive manner with solid state chemistry, although a Renaissance of sorts is occurring in this area. The approach that we have used at the University of Lethbridge, based on our recently used texts of inorganic chemistry (those by Wulfsberg and by Shriver/Atkins), starts with metallic lattices and holes in metallic lattices, then develops ionic solids using the holes-in-close-packed-lattices analogy.

Over the course of several years we have experimented with the use of two novel computer programs designed for modeling simple metallic and ionic crystal lattices: CRYSTALDESIGNER and CARINE 3.1. We have recently obtained a multi-user license for CARINE 3.1 so that students can use the software during directed tutorials and on their own in studying the class material. In this presentation I will demonstrate the use of our crystal models as teaching/learning aids. Some of the topics that will be mentioned are: closest-packed layers; metallic lattices of lower density than CP; location, shape and size of holes in metallic lattices; the unit cell and its relationship to the extended crystal lattice; common ionic salt unit cells (the rock salt, CsCl, sphalerite or zinc blende, fluorite, antifluorite, nickel arsenide, wurtzite, rutile and perovskite lattice types); ideal and real radius ratios; the holes in CP analogy; estimating Madelung constants.

The CARINE software is also quite capable of supporting advanced courses in solid state chemistry, including the simulation of powder X-ray diffraction patterns, construction of reciprocal lattices, *hkl* labelling of planes and r.l. points, etc. If time permits I will demonstrate some of these advanced features of the software. Workshops attenders who work in a MacOS environment may also be interested in some general comparisons between CARINE and CRYSTALDESIGNER since the latter is only available for the Mac.

Using CHIME to Facilitate Learning in Organic Chemistry

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CHIME is a free, downloadable web browser plug-in capable of displaying chemical structures as 3D-images that can be manipulated by the user. These images can be based on static structures or as animations of molecular processes such as reactions or conformational changes. Our experiences using CHIME in lectures, on-line tutorials and on-line assessments will be presented.

Escaping from Multiple Choice when On-Line

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On-line questions are typically fundamentally glorified (or not) multiple choice. Though this has its place, it is a distinct disadvantage over the more traditional writing on paper, but this isn't always possible with large classes. In the Fall 2000 we started using a browser drawing applet with the ability to generate SMILES strings (Simplified Molecular Input Line Entry Specification), for example 2-bromobutane = CCBrCC. These strings can be used to text match answers and so allow an escape from multiple choice and allow the computer screen to become a virtual piece of paper.

Modeling Software Used in Introductory Biochemistry Courses

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As part of the laboratory work in introductory biochemistry students are introduced to two modeling programs: SWISS-PDBVIEWER and GEPASI. The SWISS-PDBVIEWER software is used to introduce protein structures. After having worked through a detailed tutorial, students are assigned a protein for which they have to create a series of views that illustrate secondary structure, ligand binding, distances and angles between particular amino acids, surface properties and other important features. These views are submitted to the instructor either as files to be viewed with SWISS-PDBVIEWER, or in a Microsoft POWERPOINT presentation. The metabolic control analysis software GEPASI is used to illustrate the dynamic aspect of metabolic pathways. Using a series of metabolic pathways of increasing complexity, students investigate the effect of changes in the kinetic parameters of enzymes on the metabolic flux through the pathways.

Teaching Molecular Simulation: Molecular Dynamics

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Over the last decades, computer simulation techniques have advanced from a method to study hard spheres to a powerful and widely applied method to study complex models of biological systems. Molecular dynamics simulations of proteins in water are now feasible on desktop PCs for teaching purposes. For research purposes, a cluster of cheap Pentium or Athlon machines allows a wide variety of problems to be studied. In molecular dynamics simulations, equations of motion are solved for a large number of atoms simultaneously, resulting in a movie of the motions of all atoms in a model. I will give a brief overview of the development of molecular dynamics simulations, demonstrate the use of a molecular dynamics program and discuss the hardware and software requirements for using simulations in a course on molecular simulation and modeling. I will also give a few examples of relatively simple research projects for summer and project students in my field of interest, biological membranes.

Homology Modeling: A Comparatively Useful Technique in Protein Structure Prediction

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This lecture will focus on the technique of comparative protein modeling by which a target protein is predicted based on the known three dimensional coordinates of another template protein sharing significant sequence identity. Important considerations discussed will include sequence alignments, using families of template structures, refinement of the models, and pitfalls in the interpretation of the final structures. Practical examples of homology modeling will be provided from the calmodulin and calmodulin-like domain protein kinase proteins from the calcium-binding EF-hand superfamily. Time permitting, two software packages with modeling capabilities will be discussed, namely the free SWISS PDBVIEWER linked to SWISS-MODEL and the commercial INSIGHT package (MSI Inc.).

Visualization Techniques Using MAPLE, HYPERCHEM and EXCEL in an Undergraduate Chemistry Quantum Mechanics Course

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Chemistry undergraduate courses in quantum mechanics are challenging. Frequently students are less well-prepared in electrostatics, magnetism, kinematics and mathematics than their physics counterparts; however, they frequently have well-developed (but occasionally erroneous) qualitative notions related to orbitals, quantization of energy, etc. introduced in earlier courses. In our course we have used MAPLE, HYPERCHEM and EXCEL in an integrated fashion to aid visualization. We feel that such an approach helps alleviate the parallel problems often encountered of conceptual understanding coupled with mathematical complexity.

Design of a Modern Quantum Chemistry Course

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Chemists don't necessarily need to be experts in quantum chemistry, but they do need to understand the underlying concepts. Modern computer-based tools make it possible to teach the theory relatively thoroughly while minimizing the mathematical burden on students. In my quantum chemistry course, I start by teaching the fundamentals of wave mechanics using the computer algebra system MAPLE. In this module of the course, the students learn the machinery of quantum chemistry (including approximate solution methods) by studying the classical problems (particle in a box, harmonic oscillator, etc.). Once students become comfortable with the concepts, we turn to molecular quantum mechanics. In this second part of the course, we use the molecular modeling package HYPERCHEM to reinforce the lecture material. Since this is a quantum chemistry course, we focus exclusively on the ab initio calculation capabilities of the program. The students learn both the strengths and weaknesses of the various ab initio methods available in HYPERCHEM. Throughout this part of the course, I emphasize the practical consequences of various theoretical issues raised. For instance, we discuss basis set effects both from a theoretical perspective and through practical exercises. Although this is a first course in quantum mechanics, software-supported instruction makes it possible to discuss advanced topics such as electron correlation.

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