

7-11 June 1998 Northeast Regional Molecular Modeling Workshop Tentative Schedule

All Meetings will be held in the Chemistry Resource Center (CRC), room 152, Goessmann Laboratory.
All meals will be served in the Campus Center, 10th floor.

Sunday, June 07

- 2:00PM Checkin anytime after this time at CRC in 152 Goessmann Laboratory
- 4:00PM Welcome gathering. Campus Center
- 5:00PM Dinner
- 7:00PM Introductory session on use of UMass modeling software at the CRC

Monday, June 08

- 7:30 Breakfast
- 8:30 Introduction and Overview
Group tutorial: Graphical interfaces for computational chemistry -- preparing structures for use
Manipulation and display options.
- 10:00 Break
- 10:15 Work session: Hands-on session with exercises in building, displaying, modifying, and saving
molecular structures. Measurement and modification of bond lengths and angles
Advanced building and visualization techniques.
- 11:15 Discussion: Instructional Applications. Problems encountered, solutions
- 12:15 Lunch
- 1:30 Introduction to Force Field Methods: Strengths, Weaknesses, Limitations
Selection of a Force Field: Choices and Parameters
Validation methods. Selected useful comparisons with experiment
- 2:30 Break
- 2:45 Work Session: Force Field Optimizations for various molecules
Interpreting the output. Establishing trends to maximize confidence in computed results
- 4:15 Discussion of ways to incorporate force field calculations into the curriculum
Problems encountered and solutions
- 5:30 Dinner
- 7:00 Free Lab. Further testing of force field methods and software
Examples include ChemOffice, Spartan, Hyperchem, Cerius², PCModel

Tuesday, June 09

- 7:30 Breakfast
- 8:30 Lecture/Presentation. Molecular Orbital Methods Part I.
Advantages of having electronic information and what you can do with it
Limitations: practical (size) and theoretical (neglect of electron correlation)
Semiempirical vs. *ab initio* methods
- 10:00 Break
- 10:15 Laboratory. Examples to illustrate the following: geometry optimization, heat of
formation, dipole analysis, molecular orbital display, charge/spin population analysis
- 11:15 Discussion. Possibilities for curricular integration. Effective strategies for introducing students to computational modeling of
molecules. Optional formation of interest groups.
- 12:15 Lunch

- 1:30 Presentation/Group Tutorial. Molecular Orbital Methods Part II.
Understanding terminology in MO theory (MNDO vs. AM1 vs. PM3 vs. ZINDO)
How to choose the best semiempirical method. Choosing appropriate hamiltonian methods
Molecular orbital display options. Electronic and vibrational spectra. Animation of vibrational modes
- 2:30 Break
- 2:45 Laboratory/work session. Further exploration of semiempirical methods. Calculation of experimentally measurable quantities for comparison with experiment. Validation methods. Trouble- shooting strategies.
- 4:15 Discussion and progress report. Ways to access on-line help and WWW sites for discussion of practical problems.
- 5:30 Dinner
- 7:00 Free format lab. Attendees encouraged to formulate their own problems in MO computation and to experiment with various software packages.
- 8:00 Free format discussion of incorporating test problems into teaching curricula.

Wednesday, June 10

- 7:30 Breakfast
- 8:30 Lecture/Presentation. Advanced Topics. A brief introduction to *ab-initio* methods.
Basis set nomenclature, choosing an appropriate basis set.
Configuration interaction and the concept of post-Hartree Fock methods
- 10:00 Break
- 10:15 Demonstration and group tutorial.
Dipole moment of CO at different levels of theory, comparison with experiment.
Ultraviolet absorption spectrum of conjugated molecules. Individual projects.
- 11:15 Discussion. Computational chemistry as an experimental tool in the laboratory.
- 12:15 Lunch
- 1:30 Prof. Vernon G. S. Box (CCNY) "New Trends in Molecular Modeling and Molecular Mechanics"
- 2:30 Break
- 2:45 Round table discussion. Selected vendors available to discuss their companies' viewpoints and recent initiatives
- 5:00 Reception with industrial participants
- 6:00 Dinner
- 7:30 Open session in CRC

Thursday, June 11

- 7:30 Breakfast
- 8:30 Prof. Eric Martz (UMass-Amherst) "What is CHIME and how does one use it?"
- 9:30 Break
- 9:45 Dr. Robert A. Lancashire (UWI-Mona) "Linking Graphics and Molecular Spectra with CHIME"
- 10:45 Large molecules. Databases. Visualization shareware and freeware. Internet, World Wide Web Resources. Free lab/ discussion/ wrap-up. Evaluation.