COURSE SYLLABUS

CEM 888

Computational Chemistry: A Hands-On Primer

Spring 2009

Faculty: R. I. Cukier, M. Feig, J. F. Harrison, J. E. Jackson, P. Piecuch

Lectures: MWF 9:10-10:00, Room 183
Lab Period, Room 337, TBA

Grading: 75% homework
25% final project

Course Description:

The objective of this course is to acquaint scientists—in chemical, biological, physical, and engineering fields—with the wide variety of computer-based tools for molecular modeling and simulation and, simultaneously, to expose students to the range of computing options available in the chemical-research environment at Michigan State University. Strengths and weaknesses of the most generally used theoretical models will be discussed, and students will be introduced to some of the most widely used software packages for molecular modeling. We will outline the approximations that give rise to the various molecular-modeling techniques: *Ab Initio* and semi empirical electronic structure methods, Molecular Mechanics, and Molecular Dynamics. The models will be presented with particular emphasis on their practical application to modern research problems in chemistry and biochemistry. They will be selected to demonstrate advantages and pitfalls of the various approximations, in order to give students some critical insight into the literature, as well as their own potential applications. Assigned work will include a large component of hands-on calculation in the context of currently available high-performance computer hardware.