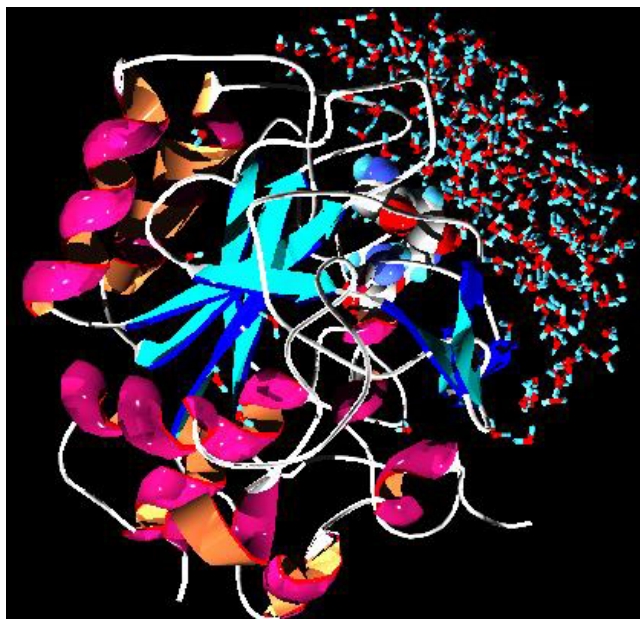


SPRING 2004

**CHEM 550: Special Topics
in Chemical Physics**
(4 units)



Computer Simulations of Chemical and Biological Systems

Professor Arie Warshel

SGM 429 Tues., Thurs. 12:00 – 1:30

warshel@usc.edu
<http://futura.usc.edu/>
(213)-740-4114

CHEM 550: Special Topics in Chemical Physics (4 units)

SPRING 2004

“Computer Simulations of Chemical and Biological Systems”

Professor Arie Warshel

SGM 429 Tues., Thurs. 12:00 – 1:30

The course will cover key aspects of the rapidly growing field of computer simulation of molecular systems in general and biological molecules in particular. Basic concepts will be reviewed with the help of simple computer programs and then demonstrated by the use of modern molecular modeling packages. The course will involve term papers on simulations of biological molecules or chemical processes in condensed phases.

Textbooks:

- 1) Computer Simulation of Chemical Reactions in Enzymes and Solutions, A. Warshel, John Wiley & Sons, (1991).
- 2) Molecular Modeling: Principles and Applications, Andrew Leach, Prentice Hall, 2001

The topics that will be cover include:

(I) Molecular Forces and Potential Surfaces

- A review of the nature of molecular forces.
- Semiempirical approaches for evaluation of potential surfaces.
- *Ab-initio* approaches for calculations of potential surfaces.
- Modeling chemistry in condensed phased in general and solution in particular.
- QM/MM energy surfaces of complex molecules

(II) The Use of Potential Surfaces in Simulating Thermodynamic Properties

- Evaluation of partition functions by simulation approaches.
- Evaluation of free energies and entropies of chemical processes (e.g. free energy perturbation approach).
- Reaction rates and activation free energies.
- Calculation of solvent effects.

(III) Molecular Dynamics (MD) of Processes in Condensed Phases

- Running MD trajectories of isolated molecules.
- Dynamics of pure solvents (radial distribution functions, etc.)
- Diffusion processes.
- Dynamics of macromolecules.
- Dynamics of ultrafast processes.

(IV) Simulating Biomolecular Properties

- Modeling electrostatic effects in proteins and other macromolecules.
- Simulating chemical reactions in enzymes.
- Computer aided drug design.
- Simulating protein folding.
- Simulating photochemical and photobiological processes.
- Simulating ion channels.
- Simulating protein-protein interaction.