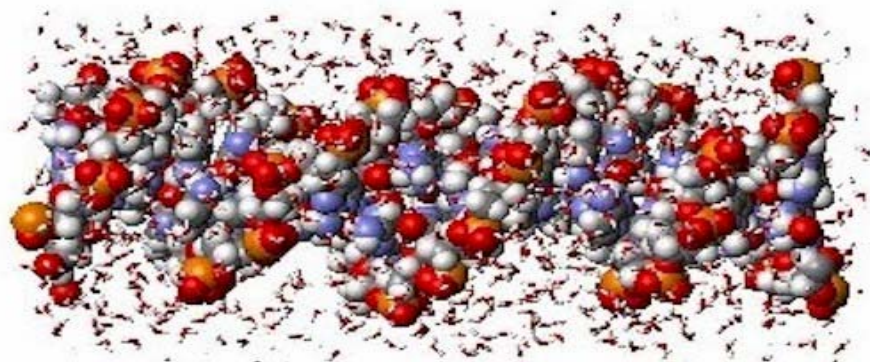


# MAE 715: ATOMISTIC MODELING OF MATERIALS

Spring 2007, MW 4:30 – 5:45 PM, Rhodes 178 (4 credits)



**Instructor:** Nicholas Zabarar, 188 Rhodes Hall, zabarar@cornell.edu

**Course description:** The course is aimed at graduate students in engineering, physics and chemistry with interests in understanding the fundamentals behind the methods and software (e.g. Moldy, Gaussian, Gulp, Quantum Espresso, Abinit) for computing electronic structure based properties of materials. Emphasis is given to physical models of interatomic forces from Lennard-Jones models to self-consistent all-electron solution of the quantum mechanical problem.

**Course requirements:** The course material is self-contained but an earlier exposure to quantum mechanics and solid state physics is desirable.

**Recommended references:** The course material is addressed in a number of recent books such as: (1) *Electronic structure of materials*, A. P. Sutton, (2) *Methods of Electronic Structure Calculations*, M. Springborg (3) *Electronic structure: Basic theory & practical methods*, R. M. Martin, (4) *Atomic and Electronic Structure of Solids*, E. Kaxiras, (5) *Essentials of Computational Chemistry*, C.J. Cramer, and (6) *Computational Physics*, J.M. Thijsen. Notes and literature material will be provided.

## SYLLABUS

1. Essential QM (the variational principle, the matrix eigenvalue problem, spin orbitals, molecular orbital theory, valence bond theory, many body problem).
2. Hartree-Fock approximation, mean field theory, the charge density, pseudopotentials, solution of H-F equations, basis sets selection, correlation, perturbation theory.
3. Density functional theory, Kohn-Sham equations, exchange-correlation functionals, the plane-wave pseudopotential method, LDA/GGA approximations.
4. Periodicity and band structures, applications to crystal structure and property prediction in solids, band gap calculations, finite temperature DFT calculations, phonons.
5. Energetics & structure from empirical potentials, pair-wise potentials, pseudopotentials, cluster expansions. Molecular dynamics, Car-Parrinello, first-principles MD.
6. Statistical thermodynamics and MC, applications of ab-initio based MC to adsorption.
7. Ab-initio thermodynamics and structure prediction.
8. Accelerated MD, kinetic MC, coarse graining methods, mesoscale calculations.