**Molecular Structure & Energetics II**

**MWF 10-10:50am, BW125A (small computer room in Boettcher West)**

**Instructor:** Andrei Kutateladze, SGM 230, x1-2995. Office hours: Friday 12-2pm

**Text:** J. B. Foresman, A. Frish, "Exploring Chemistry with Electronic Structure Methods", Second Edition, Gaussian, Inc.

**QM Software package:** Gaussian 03 (Gaussian, Inc.)

**Introduction**

* Overview of computational methods (molecular mechanics, Hückel, semi-empirical and ab initio). Introduction to the Hückel theory.
* Molecular geometry specification: Cartesian coordinates, internal coordinates, Z-matrix input; redundant coordinates, constraining molecular symmetry, "ghost" atoms;

**Electronic Structure of Small Molecules**

* Single point energy computations: choosing the level of theory (Hartree-Fock, electron correlation/post HF methods, Møller-Plesset perturbational treatment, configuration interaction methods, CI, MCSCF, the Density Functional Theory), basis set (Slater orbitals, minimal bases, split valence, polarized, diffuse functions); locating results in G03 output
* Geometry optimizations (locating minima on potential energy hypersurfaces, convergence criteria)
* Studying chemical reactions (potential energy surface scans, reaction path following)
* Frequency calculations, predicting IR and Raman spectra (input/output, normal modes, thermochemistry, zero-point energy)
* Excited States (input/output, CIS, CASSCF, excited state optimizations, triplet-singlet energy gaps and spin-orbit coupling)

**Grading:**

Final Exam: 35% (March 12, 10am-noon, BW125A)

Weekly Quizzes: 30% (two lowest scores are dropped, no make-up quizzes)

Homeworks:10%

Class Project: 25%

**Web page:**

loki.nsm.du.edu/mse2