Ch 460 – Statistical Mechanics and Computational Chemistry - Spring 2022

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REQUIRED TEXTS:

(1) Statistical Mechanics by D.A. McQuarrie, Univ. Sci. Press, 2000.
http://www.uscibooks.com/mcqstatm.htm [alternatively you may purchase **Statistical Thermodynamics by McQuarrie, 1973** - it appears to be identical for the chapters I plan to cover and may be available at lower cost]
(2) Introduction to Molecular Simulation and Statistical Thermodynamics by T.J.H. Vlugt et al., 2009. **(FREE at http://homepage.tudelft.nl/v9k6y/imsst/)**
(3) Various Handouts will be provided, online and/or in hardcopy.

OVERVIEW: This course introduces and develops statistical mechanics, which bridges the gap between molecular and thermodynamic properties of complex systems. A reasonably detailed study of intermolecular forces will also be developed. The use of molecular dynamics and Monte Carlo methods in statistical mechanics calculations will be explored. Project work will include Monte Carlo simulated annealing calculations of nanoparticles.

PLANNED TOPICAL UNITS (the order may change):
Unit #   Unit Title

1   The Big Idea: A Connection between Quantum Mechanics and Thermodynamics
2   The Microcanonical and Canonical Ensembles
3   Other Ensembles and Fluctuations
4   Boltzmann, Fermi-Dirac, and Bose–Einstein Statistics
5   Ideal Monatomic and Diatomic Gases
6   Introduction to Lagrangian and Hamiltonian Classical Dynamics
7   Principles of Classical Statistical Mechanics
8   Ideal Polyatomic Gases and Gas-Phase Chemical Equilibria
9   Intermolecular Forces and "Molecular Mechanics"
10 Liquids and Condensed Matter
11 Crystalline Solids and Phonons
12 Introduction to Monte Carlo Methods
13 Simulated Annealing Calculations of Nanoparticles
14 Introduction to Molecular Dynamics Methods

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OFFICE HOURS: Will be posted on the Moodle for this course.

GRADES: Your grade will be calculated using projects (50%), homework (40%) and participation in class discussions and activities (10%). Projects will include either a writeup or a brief class presentation. Your final grade will be assigned according to the scale A=90-100, B=80-89, C=70-79, D=60-69, F=below 60.
All grading opportunities will be available to all students.

ORGANIZATION AND REQUIREMENTS: Homework, projects and reading assignments will be posted on the Moodle. Homework and projects will be collected and reviewed. You should attempt all problems and show all your work to receive full credit. Plots must be generated using professional plotting software; hand-drawn sketches and screen shots are not accepted for credit.

I will be glad to help you with questions before or after the assignment or report or presentation is due. You must do your own work on individual assignments, but you may of course consult with other students.

Missed projects or assignments will merit a grade of zero unless lateness is approved in advance, typically due to a documented medical emergency or other unforeseeable circumstances. Please note that documentation from a relative is not acceptable.

Documenting Data, Figures, and Data Analysis - Project data must be presented in neat, well-organized tables. Tables must have a title which clearly explains the contents of the table. Units must be clear and symbols must be defined either in the text or in a table caption. Figures must also have a title. Units must be clear. A figure caption or title is always necessary to explain the figure's contents or meaning. All calculations must be fully explained in an attachment and a sample calculation must be given to illustrate a complicated data analysis. Plots must have a title and have clear labels on the X and Y axes which include the units of X and Y as well as the variable names. Please consult the ACS Style Guide for more information.

STUDENTS WHO NEED ACCOMMODATIONS: Students with disabilities who need special accommodations for this class are encouraged to meet with me and the Dean of Students as soon as possible in order to receive accommodations. Students will not be afforded any special accommodations for academic work completed prior to disclosure

and documentation of the disability. A minimum of two weeks advance notice must be given for accommodations requiring extra time on exams.

STATEMENT ON ACADEMIC HONESTY: This is a graduate course, and everyone is expected to know what plagiarism is (see http://www.plagiarism.org for a good set of definitions). You may not present someone else's work as if it were your own or there will be severe penalties. If you do your own work with integrity and give credit to others where credit is due, all will be well.