CHEMISTRY 1480 COURSE INFORMATION 2019

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Syllabus – CHM1480, 2019

The course will cover basic aspects of equilibrium and nonequilibrium statistical mechanics. The following topics will be discussed from both quantum and classical perspectives:

Introduction: relation between statistical mechanics and thermodynamics; microscopic versus macroscopic quantities; average values in statistical mechanics

Ensemble theory: time averages versus ensemble averages; microcanonical, canonical and grand canonical ensembles; fluctuations in different ensembles

Applications to liquids and condensed phases: discussion of reduced distribution functions; radial distribution function; potential of mean force; physical content of these quantities.

Nonequilibrium statistical mechanics: Brownian motion theory; Langevin and Fokker-Planck equations; correlation function expressions for transport properties; linear response theory.

Applications: transport properties such as diffusion coefficients and reaction rate constants.

Recommended Text: Tuckerman, Statistical Mechanics: Theory and Molecular Simulation, Oxford; or any other standard statistical mechanics texts.

Tentative marking scheme for the course:

marked problem set – date due February 7; 20 marks
term test 1 – February 28; 25 marks
marked problem set – date due March 21; 25 marks
term test 2 – April 4; 20 marks
term paper – due at end of course; 10 marks

Problem sets will be assigned regularly but only two of them, indicated above, will be marked. Notes for the solutions to the problem sets will be provided.