CHEM 6755: Theoretical Chemistry of Polymers
MW Room: Molecular Sciences & Engineering Building (MoSE) 1224
T Room: Molecular Sciences & Engineering Building (MoSE) G021

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I. Course Abstract

CHEM 6755. Theoretical Chemistry of Polymers
`3-0-3. Prerequisite: CHEM 6471 And (CHE/CHEM/MSE/TFE 6751)`
`Thermodynamics and microscopic dynamics of polymers. Fundamental concepts, including scaling concepts, governing anisotropy of polarizability, phase transitions, morphology, time-dependent correlations, etc. are discussed. Crosslisted with MSE and TFE 6755.`

NOTE: CHEM 6471 is "Chemical Thermodynamics and Kinetics," and CHEM 6751 is "Physical Chemistry of Polymer Solutions."

II. TextBooks

The course uses a combination of the textbooks: "Introduction to Modern Statistical Mechanics," by David Chandler (Oxford, New York, 1982), and "Introduction to Polymer Physics," by Masao Doi (Oxford, New York, 1996). Book chapters from these books will be referred to below as SM and PP, respectively.

The text, "The Theory of Polymer Dynamics," by Masao Doi and Sam F. Edwards (Oxford, New York, 1986) will not be required but may serve as a valuable reference for advanced topics.

III. General Outline of Topics

Week	Material to be covered	Description
1	Introduction & Preliminaries	motivation & classical mechanics
2	SM 1, Thermodynamics	review
3	SM 2, Equilibrium & Stability	review
4-5	SM 3, Statistical Mechanics	general ensembles: fundamentals & thermodynamic connections
5-6	SM 4, Ideal Systems	
6-7	SM 5, Phase Transitions	Ising systems, mean field & renormalization group theory
10	PP 1, Isolated Polymers	Equilibrium Models, Excluded Volume
11	PP 2, Solutions and Melts	Flory-Huggins, Scaling Theory
12	SM 6, Monte Carlo Methods	
12-13	PP 3, Polymer Gels	
13	SM 8, Non-Equilibrium Systems	Fluctuation-dissipation theorem, and Brownian Motion
14-15	PP 4, Dynamics of Dilute Polymers	Rouse & Zimm Models, Dynamic scaling
15-16	PP 5, Dynamics of Entangled Polymers	

Week	Dates M	T	W	Material to be covered	Comment
1	Aug. 17,	W: 19,	F: 21	Intro/Math/Classical Mechanics	(ACS Meeting)
2	Aug. 24,	25,	26	SM 1	Thermodynamics
3	Aug. 31,	Sept. 1,	$\boxed{2}$	SM 2	Equilibrium & Stability
4	Sep. ~~7~~,	8,	9	SM 3	Labor Day
5	Sep. 14,	15,	$\boxed{16}$	SM 3-4	
6	Sep. 21,	22,	23	SM 4-5	
7	Sep. 28,	29,	$\boxed{30}$	SM 5	
8	Oct. 5,	6,	<u>**7**</u>	Review	**Mid-Term Exam**
9	Oct. ~~12~~,	~~13~~,	14	Test Recap	Fall Break
10	Oct. 19,	20,	21	PP 1	
11	Oct. 26,	$\boxed{27}$,	~~28~~	PP 2	
12	Nov. 2,	3,	4	SM6 & PP 3	
13	Nov. 9,	$\boxed{10}$,	11	SM 8	
14	Nov. 16,	17,	18	PP 4	
15	Nov. 23,	$\boxed{24}$,	~~25~~	PP 4-5	Thanksgiving Holiday
16	Nov. 30,	Dec. 1,	<u>**2**</u>	PP 5 & Review	**Papers due**
	Dec. <u>**7**</u>,			Period 2 : 11:30AM-2:20PM	**Final Exam**

Grading: 18% Problem Sets
30% Higher of Two Exam Grades
20% Lower of Two Exam Grades
32% Paper

PS: Problem sets will be handed out one week before they are due, and they are due at the beginning of class. The expected due dates are $\boxed{\text{boxed}}$ on the schedule above. Late problem sets will not be accepted. Collaboration on problem sets is permitted, but you must hand in your own hand-written solutions.

Problems sets will be graded on a scale from 0 to 4 with:

+1 = anything with your name handed in
+1 = a reasonable attempt was made to complete all the problems, with most being correct.
+2 = for the graded first problem.

Exams: The term exams on October 7th and December 7th will be closed book and closed notes. But you will be allowed one and two single crib sheets —a single letter-sized sheet of paper hand-written on **one side only**— for the first and second exams, respectively. The term exams should take no more than 50 minutes to complete. The tested material will include topics discussed until and including the last lecture prior to the exam.

Exam Absences: In the event that you miss an exam because of a university-approved absence, you will be given an oral exam at a mutually agreed date and time.

Paper: A 3-page paper will be due on December 2nd. You will choose a paper from the Journal of Chemical Physics or Macromolecules published in 2015 that is significantly relevant to this course. You will discuss the important findings in the paper, and provide and justify a proposal extending the work. (The chosen paper should not be one that you have been exposed to as part of your coursework or that has been published by a group you have worked with.)

You should expect to have a question on the Midterm Exam asking you to provide the literature citation of your chosen **and approved** paper, and a justification of your choice in terms of the criteria above.

Attendance: Required. You will be responsible for any material covered in class irrespective of whether or not it is to be found in the assigned texts.

Office Hours: One hour/week, to be scheduled. Additional time may be requested by appointment, but standing appointments will be discouraged.

I. LEARNING OBJECTIVES

After successful completion of this course, students should be able to:

- understand the fundamentals of statistical mechanics;
- understand the fundamentals of the underlying statistical mechanics of polymer physics;
- use statistical mechanics to obtain information about equilibrium properties of large collections of interacting particles and polymers;
- use statistical mechanics to predict relaxation and reaction time scales of large collections of interacting particles and polymers;
- read and understand articles in the chemistry literature that use the language and tools of statistical mechanics and polymer physics.