

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



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	SM 3, Statistical Mechanics	general ensembles: fundamentals & thermodynamic connections
5	SM 4, Ideal Systems	
5-6	SM 5, Phase Transitions	Ising systems, mean field & renormalization group theory
7-8	PP 1, Isolated Polymers	Equilibrium Models, Excluded Volume
9-10	PP 2, Solutions and Melts	Flory-Huggins, Scaling Theory
11	SM 6, Monte Carlo Methods	
12	PP 3, Polymer Gels	
13	SM 8, Non-Equilibrium Systems	Fluctuation-dissipation theorem, and Brownian Motion
14	PP 4, Dynamics of Dilute Polymers	Rouse & Zimm Models, Dynamic scaling
15	PP 5, Dynamics of Entangled Polymers	
16	Current topics in nonequilibrium dynamics	

Week	Dates			Material to be covered	Comment
	M	W	F		
1	Aug. 22,	24,	26	Intro/Math/Classical Mechanics	Thermodynamics
2	Aug. 29 ,	31 ,	Sep. 2	SM 1	
3	Sep. 5,	7		SM 2	Labor Day
4	Sep. 12,	14,	16	SM 3	
5	Sep. 19,	21 ,	23	SM 4-5	
6	Sep. 26,	28	30	SM 5	
7	Oct. 3	5 ,	7	PP 1.1-2	
8	Oct. 10, Oct. <u>12</u>			Review & Exam	Mid-Term Exam
9	Oct. 17 ,	19 ,	21	PP 1.3-4	Fall Break
10	Oct. 24 ,	26	28	PP 2	Oct.30 is Drop Day
11	Oct. 31, Nov. 2		4	SM 6	
12	Nov. 7,	9	11	PP 3	
13	Nov. 14,	16		SM 8	
14	Nov. 21,	23 ,	25	PP 4	Thanksgiving Holiday
15	Nov. 28,	30, Dec. 2		PP 5.1-3	
16	Dec. 5,	7,	<u>9</u>	Review	Papers due
	Dec. <u>12</u>			Period 1 : 8:00AM-10:50AM	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 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 12th and December 12th 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 1.5 hours to complete. The tested material will include topics discussed until and including the last lecture prior to the exam. (Note that our class meets across the 10:00AM MWF and 11:00AM MWF course schedule. These correspond to exam periods 14 and 1 respectively. Given this choice, the instructor has chosen period 1 for the exam date.)

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 9th. You will choose a paper from the Journal of Chemical Physics or Macromolecules published in 2011 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, immediately following Monday lectures from 11:30AM to 12:30AM. Additional time may be requested by appointment, but standing appointments will be discouraged.