MSE 598

"Molecular and Ion Transport in Polymers", 4 Credit hours

Instructor: Prof. Christopher Evans, cme365@illinois.edu

Spring Semester 2024

MWF, 1-1:50 pm, 214 Ceramics

web page: Canvas

Primary Textbook:

There is no assigned text. We will be using journal articles and select chapters of various texts for this course. "Diffusion" by E. L. Cussler is good for macroscopic concepts. "Molecular Driving Forces" by Dill is better for microscopic concepts. Then it will be largely journal articles.

Office Hours, TA, and instructor information

Instructor: Prof. Evans
e-mail: cme365@illinois.edu
Office: 202A Materials Science and Engineering Building
Office hours: Wednesdays, 10-11 am

Prerequisites:

Introductory polymers course MSE 450, CHBE 456, or equivalent
Undergraduate kinetics or diffusion course is helpful

Credit hours:

Commensurate with other graduate programs in the department, this course will require substantial effort outside of course, hence the 4 credit hours.

Grading

The grade for this course will consist of a midterm exam (15%), literature report (40%) journal club participation (25%), and a final presentation (20%). Homework will be assigned but not graded. Midterm exam will be in-class, no open notes or books. It will involve solving qualitative and quantitative aspects of transport problems discussed in the first 20 Lectures of the course.

Learning Objectives:

1. Understand the molecular structure and basic synthesis of polymers used in separations
2. Solve quantitative problems related to diffusion and selective permeation of molecules through rubbers, glasses, and polymeric liquids.
3. Calculate conductivities for ions in polymers using real experimental data
4. Determine how molecular structure impacts both ion transport and mechanical properties
5. Qualitatively describe the impact of nanoconfinement on mass and ion transport

Syllabus for MSE 598: Molecular and Ion Transport in Polymers

Lecture	Topic
Lecture 1	Introduction, Fick's Laws
Lecture 2	Thin films and Boundary Conditions
Lecture 3	Semi-infinite slab, unsteady diffusion
Lecture 4	Diffusion in glassy and rubbery polymers
Lecture 5	Case II diffusion in polymers
Lecture 6	**Journal club 1: Case II and solution-diffusion in polymers**
Lecture 7	Gas separations in polymers
Lecture 8	Methods to measure diffusion and solubility
Lecture 9	**Journal club 2: Separation membranes**
Lecture 10	Types of membranes and methods of synthesis
Lecture 11	Water purification
Lecture 12	**Journal club 3: RO membranes and water purification**
Lecture 13	Reaction-diffusion problems
Lecture 14	Coupled transport
Lecture 15	**Journal club 4: Facilitated and coupled transport**
Lecture 16	Random walk diffusion
Lecture 17	Solubility from microscopic concepts
Lecture 18	Basics of polymer dynamics
Lecture 19	Coupling of mass transport to polymer dynamics, decoupling phenomena
Lecture 20	Polymer dynamics in confinement
Lecture 21	Diffusion in nanoconfinement
Lecture 22	**Journal club 5: Molecular diffusion in bulk and confined polymers**
Lecture 23	**Midterm Exam**
Lecture 24	Ion exchange membranes (macroscopic picture and chemistries)
Lecture 25	Swelling of ionic and neutral networks (hydrogels)
Lecture 26	Controlled release and diffusion
Lecture 27	Diffusion in biomaterials
Lecture 28	**Journal club 6: Diffusion in hydrogels**
Lecture 29	Conductivity, transference numbers, and impedance
Lecture 30	Dual vs single ion conductors
Lecture 31	Coupling of ion transport to polymer dynamics
Lecture 32	Polymerized ionic liquids
Lecture 33	Nanoconfined ion transport: block copolymers and thin films
Lecture 34	**Journal club 7: Polymer electrolytes**
Lecture 35	Nanoparticle diffusion in polymers
Lecture 36	Single particle tracking experiments, Gaussian vs Fickian behavior

Lecture 37	Diffusion in polymer networks
Lecture 38	**Journal club 8: Nanoparticle diffusion in polymers**
Lecture 39	Transport in dynamic polymer networks
Lecture 40	**Final Presentations**
Lecture 41	**Final Presentations**
Lecture 42	**Final Presentations**
Lecture 43	**Final Presentations**

Literature project for MSE 598

This project will consist of a 15-page, double spaced research proposal regarding some key aspect of transport in polymers. This could be polymers for gas separations, RO membranes, liquid separations, ion conducting membranes, etc. Your proposal should contain the following sections:

1. **Background**. What is the current state of the art? Where are the knowledge gaps?
2. **Intellectual Merit**. What are you proposing to do? How will this advance our understanding of the field?
3. **Research Plan**. How will you do the proposed research. This could involve synthesis of new polymers, characterization methods for transport analysis, computer simulations, model studies on idealized systems, etc.
4. **References**. Make sure to appropriately reference papers in the fields. Likely 30+ references will be appropriate.

You will also want to include figures, largely taken from the literature, which illustrate why your research would be impactful and advance the field. Feel free to run ideas by me before starting. This proposal will be due on the last day of class. Please send an electronic version.

Journal Club
Throughout the semester, we will periodically break from traditional lectures and have a discussion of 2-3 papers relevant to the class. I will provide the papers 1 week in advance, and each student will lead the discussion of 1 paper throughout the semester. Everyone is expected to read the papers before class, and the discussion leader with provide guiding questions and moderate the dialogue.

Absence Policy

Student attendance during each class is important and will be a prerequisite for success. If you know that you will be absent from class for religious or other reasons that can be known in advance, please let me know. A set of lecture notes will be posted on the website but are not intended to substitute for the lecture presentation itself nor will they include every detail discussed in class.

All examinations must be taken in this course. Make-up exams are discouraged and will be given ONLY under extraordinary circumstances. Missed exams will be allowed only if written notice of a conflict or illness is given to the instructor 24 hours prior to the exam. There will be NO early final exams given in this course.

Academic Integrity

Students should pay particular attention to Article 1, Part 4: Academic Integrity. Read the Code at the following URL: http://studentcode.illinois.edu/. Academic dishonesty may result in a failing grade. Every student is expected to review and abide by the Academic Integrity Policy: https://studentcode.illinois.edu/article1/part4/1-401/. Ignorance is not an excuse for any academic dishonesty. It is your responsibility to read this policy to avoid any misunderstanding. Do not hesitate to ask the instructor(s) if you are ever in doubt about what constitutes plagiarism, cheating, or any other breach of academic integrity.

Mental Health

Significant stress, mood changes, excessive worry, substance/alcohol misuse or interferences in eating or sleep can have an impact on academic performance, social development, and emotional wellbeing. The University of Illinois offers a variety of confidential services including individual and group counseling, crisis intervention, psychiatric services, and specialized screenings which are covered through the Student Health Fee. If you or someone you know experiences any of the above mental health concerns, it is strongly encouraged to contact or visit any of the University's resources provided below. Getting help is a smart and courageous thing to do for yourself and for those who care about you.

- Counseling Center (217) 333-3704
- McKinley Health Center (217) 333-2700
- National Suicide Prevention Lifeline (800) 273-8255
- Rosecrance Crisis Line (217) 359-4141 (available 24/7, 365 days a year)

If you are in immediate danger, call 911.

*This statement is approved by the University of Illinois Counseling Center

Community of Care

As members of the Illinois community, we each have a responsibility to express care and concern for one another. If you come across a classmate whose behavior concerns you, whether in regards to their well-being or yours, we encourage you to refer this behavior to the Student Assistance Center (217-333-0050 or http://odos.illinois.edu/community-of-care/referral/). Based on your report, the staff in the Student Assistance Center reaches out to students to make sure they have the support they need to be healthy and safe. Further, we understand the impact that struggles with mental health can have on your
experience at Illinois. Significant stress, strained relationships, anxiety, excessive worry, alcohol/drug problems, a loss of motivation, or problems with eating and/or sleeping can all interfere with optimal academic performance. We encourage all students to reach out to talk with someone, and we want to make sure you are aware that you can access mental health support at McKinley Health Center (https://mckinley.illinois.edu/). Or the Counseling Center (https://counselingcenter.illinois.edu/). For urgent matters during business hours, no appointment is needed to contact the Counseling Center. For mental health emergencies, you can call 911.

Students with Disabilities

To obtain disability-related academic adjustments and/or auxiliary aids, students with disabilities must contact the course instructor and the as soon as possible. To ensure that disability-related concerns are properly addressed from the beginning, students with disabilities who require assistance to participate in this class should contact Disability Resources and Educational Services (DRES) and see the instructor as soon as possible. If you need accommodations for any sort of disability, please speak to me after class, or make an appointment to see me or see me during my office hours. DRES provides students with academic accommodations, access, and support services. To contact DRES you may visit 1207 S. Oak St., Champaign, call 333-4603 (V/TDD), or e-mail disability@illinois.edu. http://www.disability.illinois.edu/.

Disruptive Behavior

Behavior that persistently or grossly interferes with classroom activities is considered disruptive behavior and may be subject to disciplinary action. Such behavior inhibits other students' ability to learn and an instructor's ability to teach. A student responsible for disruptive behavior may be required to leave class pending discussion and resolution of the problem and may be reported to the Office for Student Conflict Resolution (https://conflictresolution.illinois.edu; conflictresolution@illinois.edu; 333-3680) for disciplinary action.

Emergency Response Recommendations

Emergency response recommendations can be found at the following website: http://police.illinois.edu/emergency-preparedness/. I encourage you to review this website and the campus building floor plans website within the first 10 days of class. http://police.illinois.edu/emergency-preparedness/building-emergency-action-plans/.

Religious Observances

Students should complete the Request for Accommodation for Religious Observances form should any instructors require an absence letter in order to manage the absence. In order to best facilitate planning and communication between students and faculty, we request that students make requests for absence letters as early as possible in the semester in which the request applies.

Sexual Misconduct Reporting Obligation

The University of Illinois is committed to combating sexual misconduct. Faculty and staff members are required to report any instances of sexual misconduct to the University's Title IX and Disability Office. In turn, an individual with the Title IX and Disability Office will provide information about rights and options, including accommodations, support services, the campus disciplinary process, and law enforcement options.

A list of the designated University employees who, as counselors, confidential advisors, and medical professionals, do not have this reporting responsibility and can maintain confidentiality, can be found here: wecare.illinois.edu/resources/students/#confidential.