

Nanoscale Transport
ECH 6937/ ECH 4905
Class Periods: M,W,F | Period 4 (10:40 AM - 11:30 AM)
Location: WEIL 0234
Academic Term: Spring 2022

Instructor

Prof. Sergey Vasenkov
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392-0315

Office Hours: TBD (2 hours weekly)

Course Description

(3 credits) Introduction to theoretical concepts and approaches that describe nanoscale mass diffusion and its relevance to chemical engineering problems.

Course Pre-Requisites / Co-Requisites

N/A

Course Objectives

Problems involving molecular transport on small length scales often cannot be solved using relations derived for macroscopic displacements when effective diffusivity remains independent of diffusion time and the corresponding displacement. This course will introduce students to concepts and approaches used to analyze, describe, and quantify mass transport on small length scales when the relevant transport rates can be a function of the displacement length scale. Students will learn how to approach such nanoscale transport problems using random walk and other formalisms. Several case studies including diffusion in cell membranes, nanoporous membranes, and catalysts will be considered in detail.

The goal is to provide students with the knowledge and skills allowing them to formulate ideas, explore these ideas, and solve problems related to such mass transport. By the end of this course, students will be able to:

- Develop understanding of the relationship between normal (i.e., Fickian) mass diffusion and mass diffusion on small length scales;
- Develop a description of mass diffusion in the framework of the random walk approximation;
- Apply knowledge of the origins and types of anomalous diffusion to solve problems;
- Develop skills that allow analyzing and formulating ideas related to nanoscale transport; and
- Develop presentation skills.

Materials and Supply Fees

N/A

Required Textbooks and Software

N/A

Recommended Materials

- 1) Jörg Kärger, Douglas M. Ruthven, Doros N. Theodorou (2012), Diffusion in Nanoporous Materials, 2 Volume Set: Wiley-VCH Verlag GmbH & Co. KGaA, doi:10.1002/9783527651276
- 2) Oliver C. Ibe (2013), Elements of Random Walk and Diffusion Processes: Wiley Publishing, doi:10.1002/9781118618059
- 3) Ben-Avraham, D., & Havlin, S. (2000), Diffusion and Reactions in Fractals and Disordered Systems. Cambridge: Cambridge University Press, doi:10.1017/CBO9780511605826
- 4) Rudnick, J., & Gaspari, G. (2004), Elements of the Random Walk: An introduction for Advanced Students and Researchers. Cambridge: Cambridge University Press, doi:10.1017/CBO9780511610912

- 5) Regier, M.; Schuchmann, H. P. Monte carlo simulations of observation time-dependent self-diffusion in porous media models. *Transport in Porous Media* 2005, 59, 115-126.
- 6) Oliver C. Ibe (2013), *Elements of Random Walk and Diffusion Processes*: Wiley Publishing, doi:10.1002/9781118618059

Course Schedule

- Week 1: Review of normal (i.e. Fickian) diffusion with examples
- Week 2: Relationship between transport diffusion and self-diffusion
- Week 3: Presentation of diffusion as a random walk
- Week 4: Introduction to anomalous diffusion
- Week 5: Continuous-time random walk (CTRW) approach
- Week 6: Lévy walks
- Week 7: Introduction to fractals
- Week 8: Diffusion in fractal systems, percolation
- Week 9: Examples of percolation
- Week 10: Probability density distribution in fractal systems
- Week 11: Lateral diffusion in cell membranes
- Week 12: Diffusion in porous materials
- Week 13: Single-file diffusion
- Week 14: Experimental techniques to study diffusion on small length scales
- Week 15: Computational approaches to study diffusion on small length scales

Attendance Policy, Class Expectations, and Make-Up Policy

Excused absences must be in compliance with university policies in the Graduate Catalog (<http://gradcatalog.ufl.edu/content.php?catoid=10&navoid=2020#attendance>) and require appropriate documentation.

Evaluation of Grades

Grades will be based on in-class quizzes and two projects.

Assignment	Percentage of Final Grade
Quizzes (2-3)	30%
Project 1: Presentation of a review of a published research article related to molecular/ion transport on small length scales and participation in discussions of such reviews	30%
Project 2: Preparation of an NSF-style proposal related to molecular/ion transport on small length scales	40%

Grading Policy

Percent	Grade	Grade points
90.0 - 100	A	4.00
87.0 - 89.9	A-	3.67
84.0 - 86.9	B+	3.33
81.0 - 83.9	B	3.00
78.0 - 80.9	B-	2.67
75.0 - 77.9	C+	2.33
72.0 - 74.9	C	2.00
69.0 - 71.9	C-	1.67
66.0 - 68.9	D+	1.33
63.0 - 65.9	D	1.00
60.0 - 62.9	D-	0.67
0 - 59.9	E	0.00

More information on UF grading policy may be found at:

<http://gradcatalog.ufl.edu/content.php?catoid=10&navoid=2020#grades>

Students Requiring Accommodations

Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the Disability Resource Center (352-392-8565, <https://www.dso.ufl.edu/drc>). It is important for students to share their accommodation letter with their instructor and discuss their access needs, as early as possible in the semester.

Course Evaluation

Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at

<https://gatorevals.aa.ufl.edu/students/>.

Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via

<https://ufl.bluera.com/ufl/>. Summaries of course evaluation results are available to students at <https://gatorevals.aa.ufl.edu/public-results/>.

University Honesty Policy

UF students are bound by The Honor Pledge which states, "We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code." On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied:

On my honor, I have neither given nor received unauthorized aid in doing this assignment.

The Honor Code (<https://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/>) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class.

Software Use

All faculty, staff, and students of the University are required and expected to obey the laws and legal agreements governing software use. Failure to do so can lead to monetary damages and/or criminal penalties for the individual violator. Because such violations are also against University policies and rules, disciplinary action will be taken as appropriate. We, the members of the University of Florida community, pledge to uphold ourselves and our peers to the highest standards of honesty and integrity.

Student Privacy

There are federal laws protecting your privacy with regards to grades earned in courses and on individual assignments. For more information, please see:

<http://registrar.ufl.edu/catalog0910/policies/regulationferpa.html>

Campus Resources:

Health and Wellness

U Matter, We Care:

If you or a friend is in distress, please contact umatter@ufl.edu or 352 392-1575 so that a team member can reach out to the student.

Counseling and Wellness Center: <http://www.counseling.ufl.edu/cwc>, and 392-1575; and the University Police Department: 392-1111 or 9-1-1 for emergencies.

Sexual Assault Recovery Services (SARS)

Student Health Care Center, 392-1161.

University Police Department at 392-1111 (or 9-1-1 for emergencies), or <http://www.police.ufl.edu/>.

Academic Resources

E-learning technical support, 352-392-4357 (select option 2) or e-mail to Learning-support@ufl.edu.

<https://lss.at.ufl.edu/help.shtml>

Career Resource Center, Reitz Union, 392-1601. Career assistance and counseling. <https://www.crc.ufl.edu/>.

Library Support, <http://cms.uflib.ufl.edu/ask>. Various ways to receive assistance with respect to using the libraries or finding resources.

Teaching Center, Broward Hall, 392-2010 or 392-6420. General study skills and tutoring.

<https://teachingcenter.ufl.edu/>.

Writing Studio, 302 Tigert Hall, 846-1138. Help brainstorming, formatting, and writing papers.

<https://writing.ufl.edu/writing-studio/>.

Student Complaints Campus: https://www.dso.ufl.edu/documents/UF_Complaints_policy.pdf

On-Line Students Complaints: <http://www.distance.ufl.edu/student-complaint-process>.