Course Syllabus

CHEM 542 (Special Topics): *Advanced topics in physical chemistry: modern applications*

Darrin M. York

Tue/Thu 10:55am-12:15pm ET

Zoom link: **https://rutgers.zoom.us/j/99530411282?pwd=SzdHV253RnNYM0FxQWdNSHEyZnBlZz09** **(https://rutgers.zoom.us/j/99530411282?pwd=SzdHV253RnNYM0FxQWdNSHEyZnBlZz09)**

Note: the Zoom link requires registration at **https://it.rutgers.edu/zoom/** **(https://it.rutgers.edu/zoom/)**

This is an advanced topics class in modern applications of physical chemistry (broadly defined) presented by a series of world experts in the field. The course builds on the fundamentals of quantum chemistry and statistical thermodynamics and kinetics in order to illustrate how these principles provide deep insight into the natural world and are used to guide the design of new technology with far-reaching impact.

The format of the class is a series of weekly topics, beginning with a brief review of the relevant mathematics, chemistry and physics. Weekly lectures are topical in nature and will be delivered by faculty members expert in the field. A complete schedule of topics and speakers are given below. Review material will be provided prior to the lecture and posted on the class Canvas site. Assignments will be made periodically, and turned in also using the Canvas site.

There is no required textbook, but it is strongly recommended that students obtain a reference mathematical textbook, such as:

“Mathematical Methods for Physicists” by G. B. Arfken, H. J. Weber and F. E. Harris

“Mathematical Methods in the Physical Sciences” by M. L. Boas

There will be no formal in-class exams, but rather grades will be assigned based on:

Class participation: 20%

Homework Assignments: 50%

Capstone project: 30%

Class participation: class participation has two required components - attendance and engagement, and there is no partial credit (i.e. attendance alone is not sufficient). But engagement is easy! All that is required is your attention, participation in homework reflections, quizzes and interactive discussions - and coming up with at least ***one question*** or discussion point at each lecture. Since this is an online class, it is critical that you also have the ability to work interactively using a whiteboard while using Zoom, as some of the discussions will involve whiteboard work. It is suggested that students get access to a writing slate and stylus for this purpose - it is up to you, but expect to be asked to go over a homework or quiz question in class on a virtual whiteboard.

Homework Assignments: assignments will be made approximately each week, although it might vary. Assignments can be worked on collaboratively, but each student must turn in their own individual copy of each assignment electronically on Canvas as a PDF file(*). Assignments are meant to help solidify the concepts, form connections between concepts, and give students additional insight into the topics being taught. Students should complete assignments by explaining their answers to questions and problems such that the assignments themselves become part of personal notes from the class.

**If you do work from digital note-taking app like OneNote, PDFs can be created easily. If you are doing work on paper, there are many scanning apps that can create PDF files from images - one useful one is Genius Scan.*

Capstone project: the last week of class will be reserved for Capstone projects. Capstone projects will be short research-related projects that will be presented in 30-minute virtual talks the last week of class. Students can choose their own projects, but they need to be approved by Prof. York. Examples of projects include: 1) create a program to solve a practical problem, perform data analysis, or illustrate behavior of a simplified analytic model; 2) perform a molecular simulation or quantum chemical calculation to answer an interesting or important question; 3) provide a teaching overview of a cutting-edge experimental or computational/theoretical method.

A 1-page project proposal that describes significance, context and specific aims is due Tue Feb 16. A detailed project outline is due in the first class after Spring Break (Tue Mar 23), and a full draft of the presentation is due Tue Apr 20. The second to last week of class will involve performing dry runs of presentations in groups and providing written and verbal feedback. This feedback will be used for revision before making final oral presentations the last week of class (and turning in presentation material).

Course Schedule

Week	Dates	Topic	Instructor
1	Jan 19/21	Review: Calculus of variations	Darrin York
2	Jan 26/28	Review: Linear response theory, Classical dynamics	Darrin York
3	Feb 2/4	Classical and *ab initio* molecular dynamics	Lu Wang
4	Feb 9/11	Introduction to cell membranes - chemistry, mechanics, and motion	Zheng Shi
5	Feb 16/18	Follow the C-H bond road into a dark and mystical realm: catalysis and energy and climate, Oh my!	Alan Goldman
6	Feb 23/25	NMR: Theory - fundamentals and product operator formalism	Andy Nieuwkoop
7	Mar 2/4	NMR: Practice - pulse sequences and modern protein NMR	Andy Nieuwkoop
8	Mar 9/11	Mesoscale modeling	Wilma Olson
9		**SPRING BREAK**	
10	Mar 23/25	Free energy simulation methods	Darrin York
11	Mar 30/Apr 1	Theory of simple liquids	Rick Remsing
12	Apr 6/8	Structure and dynamics of liquids	Ed Castner
13	Apr 13/15	Structure and dynamics of liquids	Ed Castner

14	Apr 20/22	Presentation preparation/discussion	Darrin York
15	Apr 27/29	Presentations	Darrin York

Course Summary:

Date	Details	
Tue Jan 19, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352819&include_contexts=course_111565)	10:30am to 12:30pm
Thu Jan 21, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352820&include_contexts=course_111565)	10:30am to 12:30pm
Jan 25, 2021	Homework, Week 1 - Calculus of variations (https://rutgers.instructure.com/courses/111565/assignments/1246297)	due by 8am
Tue Jan 26, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352831&include_contexts=course_111565)	10:30am to 12:30pm
Thu Jan 28, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352837&include_contexts=course_111565)	10:30am to 12:30pm
Mon Feb 1, 2021	Homework, Week 2 - Linear response theory, Classical dynamics (https://rutgers.instructure.com/courses/111565/assignments/1246338)	due by 8am
Tue Feb 2, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352838&include_contexts=course_111565)	10:30am to 12:30pm

Date	Details	
Thu Feb 4, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352839&include_contexts=course_111565)	10:30am to 12:30pm
Tue Feb 9, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352840&include_contexts=course_111565)	10:30am to 12:30pm
Thu Feb 11, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352841&include_contexts=course_111565)	10:30am to 12:30pm
Tue Feb 16, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352842&include_contexts=course_111565)	10:30am to 12:30pm
Feb 18, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352843&include_contexts=course_111565)	10:30am to 12:30pm
Tue Feb 23, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352844&include_contexts=course_111565)	10:30am to 12:30pm
Thu Feb 25, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352845&include_contexts=course_111565)	10:30am to 12:30pm
Tue Mar 2, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352846&include_contexts=course_111565)	10:30am to 12:30pm
Thu Mar 4, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352847&include_contexts=course_111565)	10:30am to 12:30pm

Date	Details	
Tue Mar 9, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352848&include_contexts=course_111565)	10:30am to 12:30pm
Thu Mar 11, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352849&include_contexts=course_111565)	10:30am to 12:30pm
Tue Mar 23, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352852&include_contexts=course_111565)	10:30am to 12:30pm
Thu Mar 25, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352853&include_contexts=course_111565)	10:30am to 12:30pm
Mar 30, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352854&include_contexts=course_111565)	10:30am to 12:30pm
Thu Apr 1, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352855&include_contexts=course_111565)	10:30am to 12:30pm
Tue Apr 6, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352856&include_contexts=course_111565)	10:30am to 12:30pm
Thu Apr 8, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352857&include_contexts=course_111565)	10:30am to 12:30pm
Tue Apr 13, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352858&include_contexts=course_111565)	10:30am to 12:30pm

Date	Details	
Thu Apr 15, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352859&include_contexts=course_111565)	10:30am to 12:30pm
Tue Apr 20, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352860&include_contexts=course_111565)	10:30am to 12:30pm
Thu Apr 22, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352861&include_contexts=course_111565)	10:30am to 12:30pm
Tue Apr 27, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352862&include_contexts=course_111565)	10:30am to 12:30pm
Apr 29, 2021	2021SP - SPEC TOPICS PHYS CHM 16:160:542:01 (https://rutgers.instructure.com/calendar?event_id=352863&include_contexts=course_111565)	10:30am to 12:30pm