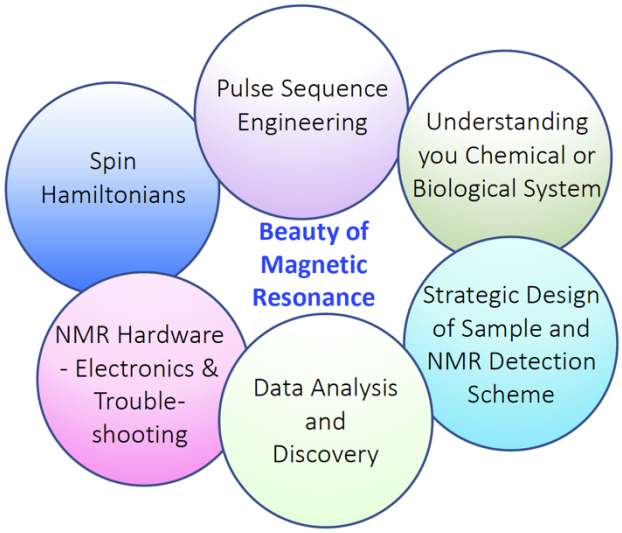
MANIPULATING SPINS: NMR THEORY AND APPLICATIONS

CHEM 277 - SPRING 2024

PROF. LYNETTE CEGELSKI



From the underlying quantum mechanics to isotopic labeling strategies, pulse sequence design, and hardware troubleshooting, students will develop a strong foundation in understanding magnetic resonance and manipulating spins to detect and discover chemistry – the atomic-level structure and dynamics – in diverse biological systems, synthetic polymers, and other organic and inorganic materials and glasses. This course will provide a foundation in magnetic resonance for those interested or engaged in research in magnetic resonance imaging (MRI). We will cover the following foundational material: quantum and classical descriptions of NMR; analysis of pulse sequences and nuclear spin coherences via density matrices and the product operator formalism; NMR spectrometer design; Fourier analysis of time-dependent observable magnetization; relaxation; solid-state NMR; NMR problem-solving strategies and examples. Students will participate through exciting short presentations of NMR applications or topics of interest later in the quarter. The course assumes completion of an undergraduate physical chemistry course that included quantum mechanics; key aspects will be reviewed.

INSTRUCTOR:

Professor Lynette Cegelski
Department of Chemistry
Email: cegelski@stanford.edu

Office Hours (Keck 351): Thursday 1:00PM – 2:30PM

WEBSITE: The class website is on Stanford's Canvas platform and on Prof. Cegelski's website.

LECTURES: Tues and Thurs, 10:30 – 11:50 AM, STLC 118. In the second half of the course, students will present a paper or a focused topic to the class during the final half of the class for some lectures.

TEXTBOOK: Please see suggested reading for each lecture. A suggested reference text for some chapters is Malcolm Levitt's Spin Dynamics. Two copies of this text will be available on reserve in the Chemistry Library. Cavanagh et al. Protein NMR Spectroscopy, 2nd Edition is also **highly recommended** reading and is available online (for free) from Stanford: http://www.sciencedirect.com/science/book/9780121644918. Also **highly recommended** is James Keeler's Understanding NMR Spectroscopy **and** Eichi Fukushima's Experimental Pulse NMR - A Nuts and Bolts Approach. There are many great texts and we will discuss some on the first day. Please see Prof. Cegelski if you would like to borrow or would like help to identify best books for key concepts. Additional references will be posted.

GRADING: Grading will be based on a midterm exam (40%), individual in-class presentations (20%), and the final exam (40%). Exams are closed book except for handouts with product operator multiplication tables that will be provided to you. You can bring a simple calculator. No iPhones or other smart phones allowed. Students may not work together on exams. Four problem Sets (similar to exam format and content) will be given for practice, but will not be graded. These are excellent preparation for exams.

CHEM 277 - SPRING 2024 COURSE SCHEDULE (LECTURES: 10:30-11:50 AM IN STLC 118)

LECTURE #	DATE	TOPIC	SUGGESTED READING/ NOTES
1	4/2	Intro to course; NMR History and Fundamental Experiments	Stern-Gerlach; Rabi; Rigden; Bloch; Purcell
2	4/4	Magnetic Moments; Density Matrix Representations of Spins and Populations; Angular Momentum Operators	Feynman Lect (Vol. I,Ch. 20 torques); Levitt; Cavanagh et al
3	4/9	Sudden Change for Isolated Spin ½; Time-dependent Interactions; Isolated Spin ½ and the Rotating Frame;	Cavanagh et al; Ernst et al
4	4/11	One-pulse Expt; Product Operator Formalism	Cavanagh et al; Levitt
5	4/16	Classical Description of NMR and the Spin Echo	Cavanagh et al; Levitt
6	4/18	Two-pulse Echo Expts and Intro to Carr-Purcell Meiboom Gill	Cavanagh et al
7	4/23	Fourier Transform and NMR Spectra	Levitt; Cavanagh et al; thefouriertransform.com
8	4/25	The Spectrometer	Fukushima
9	4/30	Intro to 2D NMR and CPMG application	
Midterm	5/2	**Midterm Evaluation – *Lectures 1-9 (PS 1 & 2)***	
10	5/7	Coupled I-S Pair (Spin-1/2)	Cavanagh et al
11	5/9	Spin Echo for IS Pair	Cavanagh et al
12	5/14	Product Operator Evaluation of SEDOR	
13	5/16	COSY; 2D INEPT (HETCOR)	
14	5/21	Relaxation I - Bloch Equations, T1 & T2 (classical)	
15	5/23	Relaxation II – Quantitative (non-classical); Autocorrelation & spectral density	
16	5/28	Introduction to Solid-state NMR	Posted reading
17	5/30	Dipolar Couplings in Solution and Solids	Posted reading
18	6/4	NMR for Macrosystems	Posted reading
	TBD	***FINAL EXAM***	

PRESENTATIONS: The presentation schedule will be determined once the class begins and enrollment is determined. Presentations will be 15-30 minutes (depending on enrollment) and will cover a single recent publication that used NMR or MRI as a uniquely enabling problem solving tool and/or a selected topic of interest. A short abstract will be required in advance of the start of class presentations that will be provided to the class.

STUDENTS WITH DOCUMENTED DISABILITIES: Students who may need an academic accommodation based on the impact of a disability must initiate the request with the Office of Accessible Education (OAE). Professional staff will evaluate the request with required documentation, recommend reasonable accommodations, and prepare an Accommodation Letter for faculty dated in the current quarter in which the request is being made. Students should contact the OAE as soon as possible since timely notice is needed to coordinate accommodations. The OAE is located at 563 Salvatierra Walk (phone: 723-1066, URL: http://studentaffairs.stanford.edu/oae).

Important Stanford Spring Quarter 2024 Deadlines relevant to courses.

- **April 19 (Fri, 5 p.m.)** Final Study List deadline. **Last day to add or drop a class**; last day to adjust units on a variable-unit course. Last day for tuition reassessment for dropped courses or units. **Students may withdraw from a course until the Course Withdrawal deadline** and a "W" notation will appear on the transcript.
- **May 13 (Mon, 5 p.m.) Term withdrawal deadline**; last day to submit Leave of Absence to withdraw from the University with a partial refund.
- **May 24 (Fri, 5 p.m.)** Change of grading basis deadline.
- **May 24 (Fri, 5 p.m.)** Course withdrawal deadline.
- **May 31 - June 6 (Fri-Thu)** End-Quarter Period.
- **June 7-12 (Fri-Wed)** End-Quarter examinations.