SYLLABUS – CHM6580, Spring 2025

Introduction to Nuclear Magnetic Resonance in Liquids and Solids
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Office Hours: TBA.
Class meetings: M Periods 8-9 (3:00 – 4:55), W Period 8 (3:00 – 3:50) Leigh Hall 242
Class dates: 01/13/25-4/23/25

OBJECTIVES

Welcome to this course on nuclear magnetic resonance (NMR) spectroscopy, a cornerstone of modern structural and dynamic analysis in chemical, materials and biological sciences. This course is designed to introduce the principles, techniques, and applications of NMR in solids and liquids. The course content will be adapted based on the interests of the registered students.

What You Will Learn

- Fundamental Principles: Learn the density matrix/operator formalism in the Hilbert and Liouville spaces to explore the physics of NMR.
- Techniques and Methods: Understand the key methodologies such as cross-polarization, magic angle spinning (MAS), dipolar decoupling, correlation spectroscopy, and dynamic nuclear polarization.
- Applications: Delve into the role of solid-state NMR in characterizing organic and inorganic materials, polymers, catalysts, and biomolecules.
- Data Analysis and Interpretation: Gain expertise in acquiring and processing complex NMR data and extracting meaningful structural and dynamic information.
- Understand how an NMR spectrometer operates, RF measurements, probe tuning and matching, and pulse programming.

Why Study NMR?

NMR offers unparalleled opportunities to study the local environments and dynamics of atoms in liquids and solids, making it a critical tool in areas spanning chemistry, materials science and pharmaceutical development. UF researchers have access to state-of-the-art NMR facilities located in the National High Magnetic Field Lab. This course aims to elucidate these techniques and empower you with skills to apply them in cutting-edge research.

Course Format

Through a combination of lectures, hands-on experiments, and data analysis tutorials, this course provides a comprehensive and interactive learning experience. Whether you are new to NMR or looking to expand your expertise, this course is tailored to equip you with the theoretical and practical tools essential for success. The experimental labs (enumerated below) will be performed on various instruments available to UF researchers, including those in the UF Chemistry Department, teaching labs, and the National High Magnetic Field Lab.

Join us to unlock the secrets of the solid state with NMR spectroscopy!

PREREQUISITES

An undergraduate level understanding of quantum mechanics is recommended but not assumed. The key principles of quantum mechanics are reviewed. Spin systems provide an unparalleled platform for learning quantum mechanics.

PLACE IN CURRICULUM

This course satisfies the spectroscopy course requirement to qualify for the PhD in the Division of Physical Chemistry.

REQUIRED TEXTS

- Malcolm H. Levitt, Spin Dynamics: Basics of Nuclear Magnetic Resonance (Paperback), Wiley; 2nd edition, ISBN-13: 978-0470511176
- James Keeler, Understanding NMR Spectroscopy (Paperback), Wiley, 2nd edition, ISBN-13: 978-0470746080**. (free e-book).**

SUPPLEMENTAL TEXTS

- Richard R. Ernst, Geoffrey Bodenhausen, Alexander Wokaun, Principles of Nuclear Magnetic Resonance in One and Two Dimensions (Paperback), Oxford University Press, ISBN-13: 978-0198556473
- B.C. Gerstein and C.R. Dybowski, Transient Techniques in NMR of Solids: An Introduction to Theory and Practice, Academic Press, Inc. (1985) ISBN: 0-12-281180-1.
- M. Duer, Introduction to Solid-State NMR Spectroscopy, Wiley-Blackwell, 1st Edition (2005) 978-1405109147.
- Spin Choreography: Basic Steps in High Resolution NMR, Ray Freeman, ISBN-13:978-0198504818.

SOFTWARE PACKAGES

- Wolfram's Mathematica (purchase or access via UFApps)
- Malcolm Levitt's Spindynamica package (free, http://www.spindynamica.soton.ac.uk/)
- Matlab (UF Chemistry site-license available)
- Spinach (free, www.spindynamics.org)
- MestReNova (UF Chemistry site-license)

GRADING

Exams (2 @ 15%), term paper/project (20%), experimental lab writeups (20%), quizzes (15%), homework (15%). Letter grades will be assigned based on the following rubric (subject to change):

>85 %	A	>75 %	B+	>60 %	C+
>80 %	A-	>70 %	B	>55 %	C
		>65 %	B-	>50 %	C-

ATTENDANCE

Please notify the instructor in advance if you expect to miss a lecture. Requirements for class attendance and make-up exams, assignments, and other work in this course are consistent with university policies that can be found at: https://catalog.ufl.edu/ugrad/current/regulations/info/attendance.aspx

HOMEWORK

Completed homework will be collected via Canvas as a single PDF file.

TERM PAPER

The term paper consists of a written report and a 15-minute oral presentation based on the report.

Oral Presentation

clarity 15% quality 20% creativity 15%

Written Report

Format: 5 pages, single-spaced, 11 pt font, 1 inch margins, with references up to 5 figures max code may be included as an appendix, no page limit. Reports will be scanned for AI/plagiarism.

writing and organization 15% creative insight and originality 15%
depth of review 10% inclusion of code 10%

Make-Up Exams

Must be arranged in advance of the scheduled date. No make-up exams are allowed except for emergencies.

Late Submission Policy

Late assignments will receive a late penalty of 10% per day past the scheduled due date. If something arises that prevents you from completing the assignment on time, contact the instructor as soon as possible to request an extension.

GRADING POLICIES:

https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

TENATITIVE SCHEDULE (to be adapted to the interests of the enrolled students)

Part 1: Foundation

1. Dirac notation, Zeeman interaction, two-level systems, spin angular momentum, Eigensystems, Hermitian operators, matrix representation, unitary operators, powers and exponentials of operators, rotation operators.
2. Bloch Equation, time dependent Schrodinger equation, Liouville von-Neumann Equation.
3. Matrix representation, RF pulses, nutation, RF offset effects, ensembles of spins, density operator, populations, coherences, orders of coherence, coherence transfer, thermal equilibrium density operator, Liouville-von Neumann equation, rotating frame density operator, coherence excitation, population inversion, free induction decay.
4. Static and alternating magnetic fields, lab frame Bloch equation, rotating frame Bloch equation, steady-state magnetization, continuous-wave NMR, time-domain NMR, signal calculation.
5. Phase shifts, receiver reference, linear phase shift, Nyquist sampling theorem, Fourier transform, NMR hardware, spectrometer block diagram, probe circuits, duplexer, receiver, transmitter, digitization, signal processing: left shift, baseline correction, zero-fill, apodization, quad-ghosts, phase correction, peak integration, processing real NMR data.
6. Coupled spin systems in liquids, quantum states of coupled spins, diagonalization, singlet/triplet basis, Zeeman basis, signals calculation for arbitrary coupling, tensor product, pure states, entangled states. Multi-spin density operator, master equation, product operator formalism part 1.
7. Product operator formalism part 2: AX_2, AX_3 spin systems, propagators, propagator manipulations, composite pulses, signal calculations

Part II: NMR in Liquids

8. Pulse Sequences INEPT (non-refocused), exchange spectroscopy, phase cycling, coherence transfer pathway selection, homospoil/ field gradients, pure absorption 2D spectra, COSY, TOCSY.
9. Spin interactions in solids: chemical shift, dipole-dipole, electric quadrupole, “secular” vs. “non-secular” interactions, solid-state NMR: chemical shift powder patterns, Pake patterns, quadrupolar powder patterns, principal value extraction.
10. Random field relaxation, fluctuations, spectral density, transition probability, relaxation mechanisms, chemical shift relaxation, homonuclear dipole-dipole relaxation, heteronuclear dipole-dipole, quadrupolar relaxation, relaxation measurements, inversion recovery, CPMG-T2.
11. NOESY spectroscopy, distance measurements, chemical exchange effects, 1D exchange spectroscopy, 2D exchange spectroscopy.
12. DOSY – diffusion ordered NMR
13. Dissolution Dynamic Nuclear Polarization

Part III: Introduction to Solid State NMR

14. Anisotropic Interactions in Solids: Dipolar, Quadrupolar, and Chemical Shielding Anisotropy
15. Single Crystal NMR, CSA Powder Patterns, Pake Pattern, Quadrupolar Powder Pattern
16. Magic angle spinning, Hartmann-Hahn cross-polarization
17. Multiple Pulse Sequences, Dipolar decoupling and recoupling, distance measurements (REDOR).
18. Quadrupolar Nuclei and Electric Quadrupole Interaction, MQMAS NMR.
19. Biological Solid-State NMR (Guest Leture)
20. Dynamic Nuclear Polarization, Surface-Enhanced NMR Spectroscopy

EXPERIMENTAL LABS

#1: RF lab. Oscilloscope and network analyzer operation, measurements on RF components (splitters, mixers, filters, hybrids, directional couplers, attenuators, phase shifters), resonant (LC) circuits.
#2: NMR spectrometer console and probe hardware, signal conditioning and processing, FFT.
#3: Hahn echo, CPMG, solid-echo, stimulated echo experiments, DOSY.
#4: 2D NMR Spectroscopy of Small Molecules
#5: Wide line NMR and Magic Angle Spinning (MAS) of Solids, proton decoupling
#6, Quadrupolar and Multiple Quantum Magic Angle Spinning (MQ-MAS) spectroscopy
#7: Spectroscopy on Student Provided Samples
#8: Grover search on two qubit quantum computer.

Getting Help

- For the quickest response, you might find it useful to post questions to the Canvas Discussion Board. Messaging the Instructor or even a classmate also works.
- For Username/Password issues, such as difficulties logging into any Gatorlink-authenticated site at UF, (including our course website), please contact the UF Help Desk at: helpdesk@ufl.edu, (352) 392-HELP - select option 2.

UF Policies Shaping This Course

This course is aligned with the UF policies below.

- Contact Hours: "Contact Hours" refers to the hours per week in which students are in contact with the instructor, excluding office hours or other voluntary contact. The number of contact hours in this course equals the number of credits the course offers.
- Workload: As a Carnegie I, research-intensive university, UF is required by federal law to assign at least 2 hours of work outside of class for every contact hour. Work done in these hours may include reading/viewing assigned material and doing explicitly assigned individual or group work, as well as reviewing notes from class, synthesizing information in advance of exams or papers, and other self-determined study tasks.
- Accommodation for Student with Disabilities: Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, www.dso.ufl.edu/drc/) by providing appropriate documentation. Once registered, students will receive an accommodation letter which must be presented to the instructor when requesting accommodation. Students with disabilities should follow this procedure as early as possible in the semester
- Statement Regarding Evaluations: Students are expected to provide feedback on the quality of instruction in this course by completing online evaluations at https://evaluations.ufl.edu. Evaluations are typically open during the last two or three weeks of the semester, but students will be given specific times when they are open. Summary results of these assessments are available to students at https://evaluations.ufl.edu/results/.
- Statement Regarding Course Recording: Our class sessions may be audio visually recorded for students in the class to refer back to and for use of enrolled students who are unable to attend live. Students who participate with their camera engaged or utilize a profile image are agreeing to have their video or image recorded. If you are unwilling to consent to have your profile or video image recorded, keep your camera off and do not use a profile image. Likewise, students who un-mute during class and participate verbally are agreeing to have their voices recorded. If you are unwilling to consent to have your voice recorded during class, you will need to keep your mute button activated and communicate exclusively using the "chat" feature, which allows students to type questions and comments live. The chat will not be recorded or shared. As in all courses, unauthorized recording and unauthorized sharing of recorded materials is prohibited.

University Policy on Academic Misconduct

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 (http://www.dso.ufl.edu/sccr/process/student-conduct-honorcode/) 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..

Additional UF Policies and Resources

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/Default.aspx, 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,* 392-1111 (or 9-1-1 for emergencies). http://www.police.ufl.edu/

Academic Resources

- *E-learning technical support*, 352-392-4357 (select option 2) or e-mail to Learningsupport@ufl.edu. https://lss.at.ufl.edu/help.shtml.
- *Career Resource Center*, Reitz Union, 392-1601. Career assistance and counseling. http://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.

DISCLAIMER

All aspects of course operations, including grading scale, points distribution course policy, and policy execution, are subject to change at the discretion of the course instructor at any time without notice.