CHEN E4860 NMR for Biological, Soft, and Energy Materials

Syllabus

Time: Mon/Wed, 5:40–6:55pm, but subject to change
Location: varies
Instructor: Prof. Lauren Marbella
Recommended (but not required) texts: "Spin Dynamics" Malcolm H. Levitt. John Wiley & Sons Ltd, 2008. (on reserve) and "Understanding NMR Spectroscopy" James Keeler. John Wiley & Sons, 2005. (available through Columbia online)
Additional useful texts: "In vivo NMR Spectroscopy: Principles and Techniques" Robin A. De Graaf. John Wiley & Sons, 1998.
"Introduction to Solid-state NMR Spectroscopy" Melinda J. Duer. John Wiley & Sons, 2005.
"NMR Imaging in Chemical Engineering" Seigfried Stapf and Song-I Han. John

Prerequisites: UN1401, CHEE E3010, or instructor's approval

Course Description: This course is for junior/senior undergraduates and graduate (MS) students as well as PhD students interested in applying nuclear magnetic resonance (NMR). The course focuses on the fundamentals of NMR spectroscopy and imaging with applications in fields ranging from biomedical engineering to electrochemical energy storage. Course material covers basic NMR theory, instrumentation (including *in situ*/*operando* setup), data interpretation, and experimental design to couple with other materials characterization strategies. Course grade is based on problem sets, quizzes, participation, and final project presentation.

Course Significance: The design of next generation materials is one of the global challenges facing our society. The ability to engineer solar fuels, batteries, and therapeutics that withstand degradation while simultaneously displaying optimal performance rests on our ability to understand how material structure changes during operation or dynamics in the human body. NMR spectroscopy and imaging has played a crucial role in tracking the evolution of phase transformations, ion dynamics, and interfacial phenomena in real time for these complex materials. Currently, many scientists and engineers participating in these critical research fields are not exposed to NMR in their training and likewise—many NMR experts are not active in materials science applications. This course aims to bridge this gap as the use of NMR in both academics and industry becomes increasingly important in material design, system monitoring, and device fabrication.

Grading

50% Problem sets/quizzes
10% Participation
40% Final Project

Academic Integrity

You are all encouraged to work together at all stages of this course, so there is no need or excuse for cheating, we are a team. "Copying" answers from <u>ANY</u> source is unacceptable. Turning in anything that does not represent your own (or that of your group) work and thought process is considered plagiarism and is subject to the Columbia Policy on Academic Integrity: http://www.studentaffairs.columbia.edu/fysaac/forms/acadinteg.pdfLinks to an external site.

Disability Accommodations
In order to receive disability-related academic accommodations, students must first be registered with Disability Services (DS). More information on the DS registration process is available online at www.health.columbia.edu/odsLinks to an external site.. Please notify Prof. Marbella of registered students' accommodations before the exam or other accommodations will be provided. Students who have, or think they may have, a disability are invited to contact Disability Services for a confidential discussion at (212) 854-2388 (Voice/TTY) or by email at disability@columbia.edu.

Sample Schedule

Date	Topic	Assignment
Sept 9	Syllabus overview Overview of NMR—why is it so powerful?	
Sept 14	Review of physical chemistry/quantum mechanics	
Sept 16	Nuclear spin Energy levels in NMR	
Sept 21	Vector model Pulse sequences	Problem Set 1 assigned
Sept 23	Internal spin interactions: magnitudes and quantum mechanical treatment Magic-angle spinning	
Sept 28	Average Hamiltonian Theory (AHT) Spin Echoes	Problem Set 1 due
Sept 30	Dipolar coupling AHT heteronuclear decoupling	Problem Set 2 assigned
Oct 5	Dipolar coupling—a spectroscopic ruler! REDOR, TRAPDOR Homonuclear dipolar coupling	
Oct 7	Using dipolar coupling to overcome sensitivity issues in NMR CPMAS, DNP	Problem Set 2 due
Oct 12	Internal spin interactions: quadrupolar NMR Quadrupolar techniques, MQMAS	
Oct 14	Internal spin interactions: chemical shift Quantum mechanical description Chemical shift anisotropy	
Oct 19	Isotropic chemical shift assignments Homonuclear and heteronuclear correlations J-coupling	
Oct 21	Relaxation in NMR—physical origin	Problem Set 3 assigned

	Spin-lattice relaxation Spin-spin relaxation Measuring relaxation	
Oct 26	Electron-nuclear coupling in NMR Relaxation enhancement Paramagnetic NMR Knight shifts	
Oct 28	Magnetic Resonance Imaging: Encoding spin position	Problem Set 3 due
Nov 4	NMR equipment Spectrometer, NMR probe Setting up an NMR experiment	
Nov 9	Dynamics in NMR: interpreting relaxation measurements—from polymers to crystalline solids	
Nov 11	Dynamics in NMR: chemical exchange phenomena	
Nov 16	Dynamics in NMR: Translational diffusion	
Nov 18	In situ/operando NMR spectroscopy	
Nov 23	Giving great presentations Final project guidance	
Nov 30	Final project presentations	
Dec 2	Final project presentations	
Dec 7	Final project presentations	
Dec 9	Final project presentations	
Dec 14	Final project presentations	