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
“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 ANY 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.pdf

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/ods.
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

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<th>Date</th>
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| 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                                                             |                  |
<p>| Oct 21 | Relaxation in NMR—physical origin                                     | Problem Set 3 assigned |</p>
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| Oct 26   | Spin-lattice relaxation  
             Spin-spin relaxation  
             Measuring relaxation |                        |
| Oct 28   | Electron-nuclear coupling in NMR  
              Relaxation enhancement  
              Paramagnetic NMR  
              Knight shifts       | Problem Set 3 due      |
| Nov 4    | Magnetic Resonance Imaging:  
              Encoding spin position |                        |
| Nov 9    | NMR equipment  
              Spectrometer, NMR probe  
              Setting up an NMR experiment |                        |
| Nov 11   | Dynamics in NMR: interpreting relaxation measurements—from polymers to  
              crystalline solids    |                        |
| Nov 16   | Dynamics in NMR: chemical exchange phenomena                           |                        |
| Nov 18   | Dynamics in NMR: Translational diffusion                               |                        |
| Nov 23   | In situ/operando NMR spectroscopy                                       |                        |
| Nov 30   | Giving great presentations  
              Final project guidance |                        |
| Dec 2    | Final project presentations                                           |                        |
| Dec 7    | Final project presentations                                           |                        |
| Dec 9    | Final project presentations                                           |                        |
| Dec 14   | Final project presentations                                           |                        |