SYLLABUS - CHM6580 SECTION 1B81 – SPRING 2013

Special Topics in Physical Chemistry: *Introduction to Spin Dynamics and Nuclear Magnetic Resonance*

INSTRUCTOR: Professor Russ Bowers, Division of Physical Chemistry
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COURSE OBJECTIVES AND GOALS: This course is aimed at chemists, physicists and engineers interested in utilizing nuclear magnetic resonance in their research. It will provide the general physical and mathematical background of magnetic resonance, as well as an introduction to digital signal processing, pulse sequence design and spin system analysis. Principles of solid-state NMR and theory of relaxation will also be covered. Computational approaches to spin dynamics and spectral simulation will be integrated into the coursework. Students will learn how to set up calculations using several different software packages, including Malcolm Levitt's Mathematica/Spindynamica and Ilya Kuprov's Matlab/Spinach platform.

REQUIRED TEXTBOOKS AND SOFTWARE:

- Malcolm H. Levitt, Spin Dynamics: Basics of Nuclear Magnetic Resonance (Paperback), Wiley; 2nd edition, ISBN-13: 978-0470511176
- Wolfram's Mathematica (student edition, version 6 or higher)
- Matlab (UF site license available)
- Malcolm Levitt's Spindynamica package (http://www.spindynamica.soton.ac.uk/)
- Ilya Kuprov's Matlab Spinach (http://spindynamics.org/index.php)

SUPPLEMENTAL TEXTS (USED TO PREPARE LECTURES):

- 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.
- Abragam, Principles of Nuclear Magnetism, Eds. W.C. Marshall and D.H. Wilkinson, Oxford University Press, New York,(1985) ISBN 0-19-852014 X Pbk.
- U. Haeberlen, High resolution NMR in solids : selective averaging, Academic Press, New York (1975) ISBN 0-12-0255618.
- M. Duer, Introduction to Solid-State NMR Spectroscopy, Wiley-Blackwell, 1st Edition (2005) 978-1405109147.

GRADING: grade will be based on 1 in-class exam (40%) 1 take-home exam (40%), homework assignments (20%).
ATTENDANCE: 100% attendance is expected. As a courtesy, let the Prof. know in advance if you will miss a class.
MAKE-UP EXAMS: Must be arranged in advance of the scheduled date. No make-up exams are allowed otherwise. Remedy is at the discretion of the Prof.
UF GENERAL INFORMATION A GRADES: https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

Tentative Schedule

Week 1:	Course Organization and Introductory Concepts
	Magnetic moments
Week 2:	Magnetization vector model
	Bloch equations
	Energy levels
	Rotating frame
Week 3:	Fourier transformation and digital signal processing
	Modern NMR Spectrometer architecture
	Probe circuits
Week 4:	Quantum theory of angular momentum
	Quantum mechanics of spin
Week 5:	Nuclear spin Hamiltonian in liquids
Week 6:	Weak and strongly coupled spin systems
	Matrix representation and diagonalization
Week 7:	Density matrix formulation
	Liouville von Neumann equation
	Product operator formalism
Week 8:	Coherence selection pathways, phase cycling and field gradient pulses

Exam 1 (in-class)

Weeks 9:	Pulse sequences for solution state NMR
Week 10-11	Dipole-dipole, quadrupolar and chemical shift interactions in solids
	Rotations and principal axis system
	Powder averaging
Week 12:	Magic angle spinning
	Cross-polarization
	Solid-state NMR pulse sequences
Week 13:	Relaxation basics
	Nuclear Overhauser Effect
Week 14:	Hyperpolarization methods (DNP and PHIP)
Week 15:	Computational examples using Spinach and Spindynamica

Exam 2 (take-home)