NMR spectroscopy of Materials, 7.5 ECTS

1. Course name and extent

NMR spectroscopy of Materials, 7.5 ECTS

2. Course organization

The course is a joint activity by the respective materials-NMR laboratories of KTH Royal Institute of Technology and Stockholm University SU. The two NMR laboratories lead the Material-NMR node of the national infrastructure SwedNMR.

All course developers from the two WISE universities KTH Royal Institute of Technology and Stockholm University with extensive competence in organizing and lecturing at NMR courses at all levels from undergraduate to PhD.

- Prof. István Furó, KTH Royal Institute of Technology
- Prof. Niklas Hedin, Stockholm University
- Prof. Mattias Edén, Stockholm University
- Prof. Sergey Dvinskikh, KTH Royal Institute of Technology
- Dr. Aleksander Jaworski, Stockholm University

3. Course description

Sustainable materials are often very complex and, thereby, difficult to characterize. Hence, there is often a need to subject them to the full assembly of material characterization tools. While diffraction/scattering and (electron-)microscopic techniques are often perceived as the bread-and-butter in that context, NMR spectroscopy is becoming increasingly popular in material characterization. The reason for that lies in its complementary nature – it sees material structure not as a direct or Fourier transformed image of atomic arrangement, but via its imprint on the state of nuclear spins, the omnipresent observers within almost all atoms. The second important difference is that the methodology and theory of NMR is quite distinct from that of all other spectroscopic methods. Finally, characteristic time over which the signal is detected is relative long and therefore NMR observables are more affected by molecular dynamics than do other methods for material characterization. This is both an advantage since it provides into dynamical insights over a broad time scale but also demands attention when analyzing the data.

The course introduces the basic principles of NMR signal generation and treatment including the concept of NMR pulse sequences and multidimensional spectroscopy. What nuclear spins can see depends both on them (spin $I = 1/2$ nuclei can only sense magnetic effects while spin $I > 1/2$ can report also on electric fields within a material) and on the structural and dynamical features of the materials they reside in. The course will present a thorough overview of the various interactions affecting nuclear spins and how they can be exploited in materials. Dynamical features (NMR spin relaxation and diffusion experiments) will be covered together with the basic principles of Magnetic Resonance Imaging MRI. Finally, computational approaches such as quantum chemistry and molecular dynamics will be introduced as tools for interpreting NMR in terms of structure and dynamics. Each course module includes a discussion/flipped classroom session where the course material will be analyzed, interpreted and reviewed.

A 1.5-days practical session at KTH/SU will be held during which the participants will be introduced to basic spectrometer operation, sample handling, and data evaluation and extraction. Experimental demonstrations will be performed on materials/problems selected from the ones suggested by course participants.

4. Course plan incl learning outcomes

4.1 Prerequisites and other conditions for access to the course

The students are expected to have a masters degree in natural science, engineering or equivalent.

4.2 Course content

The course covers how NMR methods techniques can contribute to research for a sustainable society. To that end, the course will provide an introduction to NMR theory and nuclear spin interactions and will illustrate the structural and dynamical features in materials that can be accessed by NMR spectroscopy including examples for materials important for the development towards a sustainable society.

The course also includes a single 1.5-days practical exercise, that will include case studies on materials relevant for sustainability and studied in WISE projects.

4.3 Learning goals

After completing the course the students are expected to:

- explain and describe the basic principles for NMR spectroscopy.
- explain and interpret how the different NMR observables depend on and reflect material properties.
- to compile a minor literature study and use the above listed knowledge to suggest and plan NMR experiments for relevant materials of interest.
- perform and evaluate a laboratory project within the subject area, in group (or individually, depending on the number of participants).

4.4 Education

The education consists of lectures both on-site and via video link, flipped classroom with group exercises and group work, and demonstrations and experiments performed at the NMR labs of KTH and SU.

4.5 Examination

The course is examined in the following way: on-line module quizzes for each module, short written reports/proposals for each flipped classroom session, written laboratory report, and a short written exam at the end of the course.

5. Tentative schedule for 2025

Lunch-to-lunch meetings in Stockholm, April 3-4 and May 21-22. The lectures are 2 × 45 minutes with a 15 min break (except when explicitly stated otherwise). The first practical session for two groups follows the last IRL session.

It is mandatory to participate at the IRL lectures in Stockholm. Zoom lectures are going to be recorded and will be made available after the actual lecture. On-time (camera on, speaker off) participation at least half of the Zoom lectures is mandatory.

Date	Time	Lecture	Lecturer
3/4	13:00-14:10	**Get together, who are we**	All
	14:15-16:00	**Lecture 1: The vector model of NMR 1**	István Furó
	16:00-16:30	Coffee break	
	15:30-18:15	**Lecture 2: The vector model of NMR 2**	István Furó
	18:30-	Dinner	
4/4	8:15-10:00	**Lecture 3: Fourier transformation**	István Furó
	10:00-10:30	Coffee break	
	10:30-12:15	**Lecture 4: Simple pulse sequences and instrumentation**	István Furó

7/4	10:15-12	**Lecture 5: Chemical exchange effects and the concept of multidimensional NMR**	István Furó (Zoom)
8/4	10:15-12	***Flipped classroom/discussion Module 1***	István Furó (Zoom)
11/4	10:15-12	**Lecture 6: Nuclear spin interactions in materials**	Mattias Edén (Zoom)
14/4	10:15-12	**Lecture 7: The concept of anisotropy; NMR on powders and magic-angle spinning**	Mattias Edén (Zoom)
15/4	10:15-12	**Lecture 8: NMR of crystalline and disordered solids**	Mattias Edén (Zoom)
22/4	10:15-12	**Lecture 9: Structural information from NMR**	Mattias Edén (Zoom)
25/4	10:15-12	**Lecture 10: Quadrupolar nuclei**	Mattias Edén (Zoom)
28/4	10:15-12	**Lecture 11: Dipolar recoupling: cross polarization and correlation 2D NMR**	Mattias Edén (Zoom)
29/4	10:15-12	***Flipped classroom/discussion Module 2***	Mattias Edén (Zoom)
6/5	10:15-12	**Lecture 12: Magnetic field gradients and Magnetic Resonance Imaging (MRI)**	István Furó (Zoom)
9/5	10:15-12	**Lecture 13: Diffusion and flow by NMR**	István Furó (Zoom)
12/5	10:15-12	**Lecture 14: Spin relaxation: principles**	Niklas Hedin (Zoom)
13/5	10:15-12	**Lecture 15: Spin relaxation: applications**	Niklas Hedin (Zoom)
16/5	10:15-12	**Lecture 16: Access to NMR parameters with quantum chemistry methods**	Aleksander Jaworski (Zoom)
19/5	10:15-12	**Lecture 17: Molecular dynamics simulations and NMR**	Aleksander Jaworski (Zoom)
21/5	13:15-14	**How and where to perform NMR experiments in Sweden and in Europe?**	All
	14:15-15:00	***Flipped classroom/discussion Modules 3 & 4***	István Furó/Niklas Hedin/Aleksander Jaworski
	15:00-15:30	Coffee break	
	15:30-18:00	***Flipped classroom/discussion Modules 3 & 4***	István Furó/Niklas Hedin/Aleksander Jaworski
	18:15-	Dinner	
22/5	8:15-11:45	***NMR for materials: problem solving workshop***	All

Practical sessions

We will plan for each lab to be given for two parallel groups of 4 students / session. The first practical session will be arranged immediately after last IRL session of the theory part. The practical sessions will be aimed at performing the experiments that were introduced during the theory part of the course.

For each group, the laboratory work involves 1.5 days divided among the NMR labs at KTH and at SU. Students will be topically matched and the practical sessions may, if feasible, involve analysis of actual research samples proposed by the participating students. If necessary, the students may change their preassigned group. The following dates are available for the practical sessions:

22/5, 13:00 – 23/5, 17:00

26/5, 13:00 – 27/5, 17:00

2/6, 13:00 – 3/6, 17:00

9/6, 13:00 – 10/6, 17:00