# Annexe A: New/Revised Course Content in OBTL+ Format

# **Course Overview**

Course over view	·
Expected Implementation in Academic Year	AY2025-2026
Semester/Trimester/Others (specify approx. Start/End date)	Semester 2
Course Author  * Faculty proposing/revising the course	Xue Kai
Course Author Email	kai.xue@ntu.edu.sg
Course Title	NMR Spectroscopy: Methods and Applications
Course Code	PH3606
Academic Units	3
Contact Hours	38
Research Experience Components	Not Applicable

# Course Requisites (if applicable)

Pre-requisites	MH2802 and PH2103
Co-requisites	
Pre-requisite to	
Mutually exclusive to	
Replacement course to	
Remarks (if any)	

## **Course Aims**

This course is designed to introduce you to the principles and applications of Nuclear Magnetic Resonance (NMR) spectroscopy. It will cover key topics including NMR hardware, the underlying physics of NMR, data processing techniques, experimental methods, and real-world applications. If you are pursuing a research career, NMR is a fundamental tool to probe atomic-level molecular structural information. If you are more inclined toward engineering, the course offers insights into the development of an analytical technique—from its physical foundations to its commercialization—helping to build a solid understanding of research and development in scientific instrumentation.

## Course's Intended Learning Outcomes (ILOs)

Upon the successful completion of this course, you (student) would be able to:

ILO 1	Develop a solid understanding of the physical principles and mathematical foundations underlying NMR spectroscopy
ILO 2	Explain and Illustrate the signal processing involved in NMR spectroscopy and the hardware required to generate and analyze NMR signals
ILO 3	Illustrate basic solid-state and solution-state NMR experiments
ILO 4	Explain the methods used in various NMR applications—including clinical imaging, polymer science, and biology—and the insights these methods provide

#### Course Content

#### 1. NMR Physical Background (2h)

Introduction to the fundamental principles of nuclear magnetic resonance (NMR), including key phenomena and observable parameters in NMR spectroscopy.

#### 2. NMR Hardware and Data Processing (2h)

Overview of NMR instrumentation and the mathematical principles underlying signal acquisition, processing, and spectral analysis.

#### 3. Mathematical Description of an NMR Experiment (2h)

Introduction to the formal description of NMR experiments using spin density operators and propagators.

#### 4. Methods in Solution-State NMR (2h)

Coverage of scalar coupling-based experiments, relaxation mechanisms influenced by molecular motion, and solvent suppression techniques.

#### 5. Methods in Solid-State NMR (4h)

Dipolar-based techniques including dipolar decoupling, recoupling, and relaxation methods; quadrupolar-based methods including lineshape analysis, quadrupole echo techniques, and relaxation studies.

#### 6. Applications (14h)

In-depth discussions of NMR applications across various fields, including medical imaging, polymer science, structural biology, and studies of liquid-liquid phase separation.

# Reading and References (if applicable)

Online link: <a href="https://spindynamics.org/?page\_id=18">https://spindynamics.org/?page\_id=18</a>

Spin Dynamics: Basics of Nuclear Magnetic Resonance, 2nd Edition, Malcolm H. Levitt , ISBN: 978-0-470-

51117-6 April 2008 752 pages

Spin: From Basic Symmetries to Quantum Optimal Control (2023), Ilya Kuprov, DOI: https://doi.org/10.1007/978-

3-031-05607-9

Note: The above listing comprises the foundational readings for the course and more up-to-date relevant readings will be provided when they become available.

# **Planned Schedule**

Week or Session	Topics or Themes	ILO	Readings Deli Me		Activities
1	NMR Physical Background	ILO1	https://spindynamics.org/?page_id=18	In-person	Lecture
2	NMR Hardware and Data Processing	ILO 2	https://spindynamics.org/?page_id=18	In-person	Lecture and tutorial
3	Mathematical Description of an NMR Experiment	ILO1	https://spindynamics.org/?page_id=18	In-person	Lecture and tutorial
4	Methods in Solution-State NMR	ILO 3	https://spindynamics.org/?page_id=18	In-person	Lecture and tutorial
5	Methods in Solid-State NMR: Dipolar coupling based methods	ILO 3	https://spindynamics.org/?page_id=18	In-person	Lecture
6	Methods in Solid-State NMR: Quadrupole Based Method	ILO 3	https://spindynamics.org/?page_id=18	In-person	Lecture and tutorial
7	Applications:	ILO 4	https://spindynamics.org/?page_id=18	In-person	lecture and tutorial
8	Applications: Polymer Science mid-term exam	ILO 4	https://spindynamics.org/?page_id=18	In-person	Lecture and a mid- term exam
9	Applications: Polymer Science	ILO 4	https://spindynamics.org/?page_id=18	In-person	Lecture and tutorial
10	Applications: Structural Biology	ILO 4	N.A.	In-person	Lecture and tutorial

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
11	Applications: Structural Biology Lab View	ILO 1, 2, 4	N.A.	In-person	lecture and lab visit
12	Applications: Liquid Liquid Phase Separation by NMR	ILO 1, 2, 3, 4	N.A.	In-person	lecture and presentation
13	Applications: Liquid Liquid Phase Separation by NMR. A viva assessment will also be conducted during the final lecture.	ILO 1, 2, 3, 4	N.A.	In-person	lecture and presentation

# Learning and Teaching Approach

Approach	How does this approach support you in achieving the learning outcomes?
Multi-media resources	You will actively engage with diverse digital materials, such as videos, interactive simulations, and presentations, to enhance your learning.

# **Assessment Structure**

Assessment Components (includes both continuous and summative assessment)

No.	Component	ILO	Related PLO or Accreditation		Description of Assessment Component	Team/Individual	Rubrics	Level of Understanding
1	Continuous Assessment (CA): Test/Quiz(Midterm test, point based, hard assessment)	ILO 1,2,3		25		Individual	Analytic	Multistructural
2	Continuous Assessment (CA): Assignment(Two assignments will be given in the first half and second half of the semester)	ILO 1,2,3		20	10% each assignment	Individual	Analytic	Multistructural
3	Continuous Assessment (CA): Report/Case study(Assessment will include a written report submitted at the end of the semester and a viva examination covering both the report content and the material from the entire course.)	ILO1, 2, 3, 4		50	Viva (20%) and Report (30%)	Individual	Holistic	Relational

No.	Component	ILO	Related PLO or Accreditation		Description of Assessment Component	Team/Individual	Rubrics	Level of Understanding
4	Continuous Assessment (CA): Test/Quiz(Quiz, learning catalytics, class activities)			5	questions asked in during the lecture and is supposed to be answered online	Individual	Holistic	Relational

#### Description of Assessment Components (if applicable)

#### CA1 - Midterm Exam (25%)

CA1 will be a midterm examination designed to assess students' understanding of the fundamental concepts of NMR spectroscopy. The scope will cover material from Week 1 to Week 6. A set of questions will be provided during class, and students are expected to complete and submit their answers within the session for grading.

#### CA2 - Assignments (20%)

CA2 consists of two individual assignments. For each, a set of questions will be given as homework, and students are expected to work independently and submit their solutions for grading. Each assignment contributes 15% to the final grade.

#### CA3 - Report and viva(50%)

CA3 involves preparing a written report on one of several selected scientific topics in biology, chemistry, or physics and a viva evaluation on student's understanding of course content and their report. Students will review relevant literature and critically evaluate the experimental techniques used to address the chosen problem. The goal is to develop a structured approach to designing NMR experiments for analyzing unknown substances. The report (30%) and the viva assessment (20%) will account for 50% of the final grade, a face-to-face discussion will be conducted during the tutorial sessions in the last two weeks of the semester as part of the overall assessment.

#### CA4 - In-class Participation (5%)

CA4 will consist of online questions given during lectures. Students are expected to respond in real time as part of this in-class activity.

#### Formative Feedback

For CA1, you will receive your grades.

For CA2, you will receive written feedback and grades.

For CA3, you will receive written grades about your reports and the viva assessment.

For CA4, you will receive your grades.

# NTU Graduate Attributes/Competency Mapping

This course intends to develop the following graduate attributes and competencies (maximum 5 most relevant)

Attributes/Competency	Level
Communication	Intermediate
Problem Solving	Advanced
Sense Making	Advanced
Transdisciplinarity	Advanced

## **Course Policy**

#### Policy (Academic Integrity)

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values. As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. On the use of technological tools (such as Generative AI tools), different courses / assignments have different intended learning outcomes. Students should refer to the specific assignment instructions on their use and requirements and/or consult your instructors on how you can use these tools to help your learning. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

#### Policy (General)

You are expected to complete all assigned readings, activities, assignments, attend all classes punctually and complete all scheduled assignments by due dates. You are expected to take responsibility to follow up with assignments and course related announcements. You are expected to participate in all project critiques, class discussions and activities.

#### Policy (Absenteeism)

If you are sick and unable to attend your mid-term, you have to:

- 1. Send an E-mail to the instructor regarding the absence.
- 2. Submit the Medical Certificate\* or official letter of excuse to administrator (undergraduate office).

A student who is absent from mid-term test without valid Leave of Absence will be given zero mark. In case of valid reason for absence one make-up test will be arranged upon discussion with the tutor.

\* The Medical Certificate mentioned above should be issued in Singapore by a medical practitioner registered with the Singapore Medical Association. In this case, a make-up test will be arranged.

#### Policy (Others, if applicable)

Diversity and inclusion policy

Integrating a diverse set of experiences is important for a more comprehensive understanding of science.

It is our goal to create an inclusive and collaborative learning environment that supports a diversity of perspectives and learning experiences, and that honours your identities; including ethnicity, gender, socioeconomic status, sexual orientation, religion or ability.

#### To help accomplish this:

If you are neuroatypical or neurodiverse, have dyslexia or ADHD (for example), or have a social anxiety disorder or social phobia;

If you feel like your performance in the class is being impacted by your experiences outside of class; If something was said in class (by anyone, including the instructor) that made you feel uncomfortable;

Please speak to your teaching team, our school pastoral officer or a peer or senior (either in-person or via email) about how we can help facilitate your learning experience.

As a participant in course discussions, you should also strive to honour the diversity of your classmates. You can do this by: using preferred pronouns and names; being respectful of others opinions and actively making sure all voices are being heard; and refraining from the use of derogatory or demeaning speech or actions.

All members of the class are expected to adhere to the NTU anti-harassment policy. if you witness something that goes against this or have any other concerns, please speak to your instructors or a faculty member.

#### Appendix 1: Assessment Criteria for Midterm Tests

One midterm test planned to be 90 minutes, consisting of questions similar in rigor and style to tutorial questions, and the range of questions to appropriately reflect the content coverage of the lectures.

#### By mark range

Marks	Criteria
> 90%	A complete and impressive demonstration of the achievement of the learning
	outcomes.
	Successful and impressive attempts at solving all the questions, including
	bonus questions. Demonstrates mastery of the various conceptual and
	technical aspects of quantum field theory; be able to solve relevant questions
	reflecting understanding of the topic at the level of being able to apply to
	advanced problems in particle theory and condensed matter theory.
75% to 89%	A strong demonstration of the achievement of the learning outcomes
	Correct solutions to most of the questions in the assignments. Demonstrates
	ability to solve a variety of questions in quantum field theory and a sound
	awareness of the central principles of QFT.
65% to 74%	A decent demonstration of the achievement of the learning outcomes.
	Able to solve most elementary questions with partially consistent and valid
	attempts in applying course content to unfamiliar questions.
50% to 64%	A superficial demonstration of the achievement of the learning outcomes
	Able to solve only the most basic questions relevant to the course content. Has
	difficulty in applying ideas to new contexts. Lack of clarity in physical
	interpretations.
< 50%	An insufficient demonstration of the achievement of the learning outcomes
	Unable to solve most basic questions relevant to the course content, and lack
	of basic mathematical techniques to apply concepts presented in lectures to new contexts and problems.

#### Appendix 2: Assessment Criteria for the two point-based Assignments (CA2)

Assignments will consist of questions similar in rigor and style to tutorial questions, and the range of questions to appropriately reflect the content coverage of the lectures.

#### By mark range

Marks
-------

> 90%	A complete and impressive demonstration of the achievement of the learning outcomes.
	Successful and impressive attempts at solving all the questions, including bonus questions. Demonstrates mastery of the various conceptual and technical aspects of quantum field theory; be able to solve relevant questions reflecting understanding of the topic at the level of being able to apply to advanced problems in particle theory and condensed matter theory.
75% to 89%	A strong demonstration of the achievement of the learning outcomes
	Correct solutions to most of the questions in the assignments. Demonstrates ability to solve a variety of questions in quantum field theory and a sound awareness of the central principles of QFT.
65% to 74%	A decent demonstration of the achievement of the learning outcomes.
	Able to solve most elementary questions with partially consistent and valid attempts in applying course content to unfamiliar questions.
50% to 64%	A superficial demonstration of the achievement of the learning outcomes
	Able to solve only the most basic questions relevant to the course content. Has difficulty in applying ideas to new contexts. Lack of clarity in physical interpretations.
< 50%	An insufficient demonstration of the achievement of the learning outcomes
	Unable to solve most basic questions relevant to the course content, and lack of basic mathematical techniques to apply concepts presented in lectures to new contexts and problems.

## Appendix 3: Assessment Criteria for Report (CA3)

The report will be graded based on the depth and breadth of analysis manifest in the literature review.

### By mark range

Marks	Criteria
> 90%	A complete and impressive demonstration of the achievement of the learning outcomes.
	Report indicates excellent understanding of the scientific article(s); demonstrates not only an overall solid understanding of the broad ideas in the literature review but also some of the important concrete details to the extent of being able to reproduce equations and conclusions in the scientific articles; demonstrate ability to critically evaluate articles; demonstrates some form of original work built upon the known results in the literature review.
70% to 89%	A strong demonstration of the achievement of the learning outcomes

	Report demonstrates that the student read and understood most of the concepts presented in the scientific articles. There is some fair attempt in critically responding to the conclusions of the articles and not just a mere summary of facts.
60% to 69%	A valiant effort to achieve the learning outcomes  Report demonstrates a devoted attempt in covering the ideas presented in the scientific articles, but review lacks in depth and clarity. There is some modest and reasonable attempt in responding to conclusions of various articles more than a cursory summary of the facts presented in the papers, demonstrating some form of original thoughts.
50% to 59%	A weak attempt at achieving the learning outcomes  Report shows a minimal summary of the results of various papers, put together without a strong sense of organization. Very little original response to the content of the articles in the form of critical evaluation.
< 50%	An insufficient demonstration of the achievement of the learning outcomes  Report is very poorly written with a depth that is far less than what is expected if basic concepts covered in this course have been properly assimilated. Very little or complete lack of critical evaluations of the papers.

#### Appendix 4: Assessment Criteria for viva (CA3)

A face-to-face discussion will be conducted as part of the student's overall assessment. This session aims to evaluate both the student's grasp of the concepts covered throughout the course and their depth of understanding of the submitted report. The discussion will be at least 20 minutes long and will be guided by two sets of questions. The first set will focus on testing the student's comprehension of the theoretical knowledge, methodologies, and principles taught during the course (50%). The second set will consist of specific questions related to the report, assessing the student's ability to justify their research design, interpret results, and critically analyze the literature reviewed (50%). In addition to content knowledge, the discussion will also provide an opportunity to evaluate the student's ability to communicate scientific ideas clearly and respond thoughtfully to questions.

#### By mark range

Marks	Criteria
> 90%	A complete and impressive demonstration of the achievement of the learning outcomes.
	Oral presentation demonstrates clear and strong ability to communicate various concepts in the literature review with high amount of clarity in presentation, a sound understanding of physical ideas and conclusions of

	various scientific articles. Student is able to comment constructively on the importance of various results. Able to respond coherently to questions.
70% to 89%	A strong demonstration of the achievement of the learning outcomes
	Oral presentation shows excellent ability in communicating various concepts at various levels, and genuine understanding of the scientific articles. Able to respond fairly and soundly to most questions.
60% to 69%	A valiant effort to achieve the learning outcomes
	Oral presentation shows effort in presenting a summary of results in the various scientific articles; unable to respond to some (basic) questions showing possible lack of rigorous grasp of key ideas in the literature review.
50% to 59%	A weak attempt at achieving the learning outcomes
	Oral presentation lacks strong structural coherence and inability to convey clearly the results of various articles. But there is a decent attempt to furnish a summary containing basic ideas; unable to respond to most basic questions.
< 50%	An insufficient demonstration of the achievement of the learning outcomes
	Oral presentation is very weak, with signs of confusion indicating a weak grasp of the basic physical ideas in the literature review; unable to respond to basic questions.

### Appendix 5: Learning Analytic Questions

This is an in-class activity; evaluation will not be based on the level of student participation or feedback. Marks will be awarded based on the percentage of questions answered by each student.