

## 2025 年度シラバス

科目分類/Subject Categories			
学部等/Faculty	/大学院工学科学研究科（博士前期課程）： /Graduate School of Science and Technology (Master's Programs)	今年度開講/Availability	/有：/Available
学域等/Field	/物質・材料科学域：/Academic Field of Materials Science	年次/Year	/1～2年次：/1st through 2nd Year
課程等/Program	/機能物質化学専攻：/Master's Program of Functional Chemistry	学期/Semester	/春学期：/Spring term
分類/Category	/授業科目：/Courses	曜日時限/Day & Period	/：/

科目情報/Course Information				
時間割番号 /Timetable Number				
科目番号 /Course Number	61960021			
単位数/Credits	2			
授業形態 /Course Type	講義：Lecture			
クラス/Class				
授業科目名 /Course Title	Fundamentals of Spectroscopy : Fundamentals of Spectroscopy			
担当教員名 / Instructor(s)	/機能物質化学専攻関係教員：Related teacher of the Master's Program of Functional Chemistry			
その他/Other	インターンシップ実施科目 Internship	国際科学技術コース提供科目 IGP	PBL 実施科目 Project Based Learning	DX 活用科目 ICT Usage in Learning
	実務経験のある教員による科目 Practical Teacher			
科目ナンバリング /Numbering Code				

授業の目的・概要 Objectives and Outline of the Course	
日	
英	<p>The course is among the core activities of Master's Degree Programme in Science and Technology of Bio and Nanomaterials, having the aim of providing graduates with a solid multidisciplinary education in physics, chemistry and biology, and the ability to hold positions of high responsibility in complex process management such as planning, synthesis and characterization of materials, of a biological nature too.</p> <p>Within this framework, the course will provide a rigorous treatment of the spectroscopic phenomenon, covering the theoretical grounds as well as the corresponding formalism. The course will introduce also some relevant techniques employed for the spectroscopic characterization of biological molecules and macro-molecules, and for the studies on functionalized surfaces.</p> <p>At the end of the course students should:</p> <ul style="list-style-type: none"> <li>- have acquired a deep knowledge and understanding of both the theoretical concepts the different formalisms used in spectroscopy;</li> <li>- have acquired the knowledge of some relevant spectroscopic techniques for characterizing biological macromolecules and studying functionalized surfaces;</li> <li>- be able to apply the different formalisms for rationalizing the outcomes coming from the different spectroscopic characterization techniques discussed during the course.</li> </ul>

学習の到達目標 Learning Objectives
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英	have a deep knowledge and understanding of both the theoretical concepts the different formalisms used in spectroscopy know relevant spectroscopic techniques for characterizing biological macromolecules and studying functionalized surfaces know the formalisms for rationalizing the outcomes coming from the different spectroscopic characterization techniques

## 学習目標の達成度の評価基準 / Fulfillment of Course Goals (JABEE 関連科目のみ)

日	
英	

授業計画項目 Course Plan			
No.		項目 Topics	内容 Content
1	日 英	BASIC CONCEPTS OF QUANTUM MECHANICS (1)	Hilbertian vector space, Hermitian operators and their properties. Schrödinger wave equation: time-dependent and time-independent equation. The generalized uncertainty principle; the quantum mechanical virial theorem. Approximate solutions to the Schrödinger
2	日 英	BASIC CONCEPTS OF QUANTUM MECHANICS (2)	Processes of induced absorption, induced and spontaneous emission, and their corresponding Einstein transition-probability coefficients. Transition moment. Electric and magnetic interactions. Selection rules. Classification of spectroscopies. The harmonic
3	日 英	BASIC CONCEPTS OF QUANTUM MECHANICS (3)	Extension to polyatomic system: normal modes of vibration. The rigid rotator, its eigenvalues and eigenfunctions. The centrifugal distortion effect and its treatment within the framework of perturbation theory.
4	日 英	ROTATIONAL SPECTROSCOPY (1)	The tensor of inertia. Principal axes of inertia and principal moments of inertia. Classification of molecules according to their principal moments of inertia: linear molecules, symmetric tops, asymmetric and spherical tops. Selection rules.
5	日 英	ROTATIONAL SPECTROSCOPY (2)	ROTATIONAL SPECTROSCOPY (2)
6	日 英	INFRARED (IR) SPECTROSCOPY AND SOME EXPERIMENTAL TECHNIQUES (1)	The vibrating diatomic molecule and the anharmonic corrections. The diatomic vibrating-rotator and its selection rules. Polyatomic molecules: selection rules and ro-vibrational spectra. Examples of infrared spectra.
7	日 英	INFRARED (IR) SPECTROSCOPY AND SOME EXPERIMENTAL TECHNIQUES (2)	Discussion of some relevant modern experimental techniques: Attenuated Total Reflection (ATR) IR spectroscopy, Surface Enhanced InfraRed Absorption Spectroscopy (SEIRAS), Reflection-Absorption IR Spectroscopy (RAIRS), and Diffuse Reflectance Infrared Spec
8	日 英	RAMAN SPECTROSCOPY	basic concepts and experimental apparatus; SERS and TERS techniques.
9	日 英	NUCLEAR MAGNETIC RESONANCE (NMR) SPECTROSCOPY (1)	Review of spin angular momentum operators and their properties. Spin rotation and spin projection operators. Spin precession and Larmor frequency. The density matrix formalism and its application in NMR. Radio frequency pulse. Bloch equations and their so
10	日 英	NUCLEAR MAGNETIC RESONANCE (NMR) SPECTROSCOPY (2)	Relaxation processes: longitudinal (spin-lattice) and transversal (spin-spin) processes. Description of the NMR instrument. The phase correction. Hard and Soft pulses: their effects and uses.

11	日 英	NUCLEAR MAGNETIC RESONANCE (NMR) SPECTROSCOPY (3)	Descriptions of the main Hamiltonians employed for describing NMR spectroscopy. Direct product spaces. Product operator formalism. In-phase and anti-phase magnetization and their interconversion. Coherence quantum transfer.
12	日 英	NUCLEAR MAGNETIC RESONANCE (NMR) SPECTROSCOPY (4)	Description and analysis of some pulse sequences within the product operator formalism. The INEPT experiment (Insensitive Nuclei Enhanced by Polarization Transfer).
13	日 英	NUCLEAR MAGNETIC RESONANCE (NMR) SPECTROSCOPY (5)	Bi-dimensional (2D-) NMR. Homo-nuclear and hetero-nuclear 2D-NMR spectroscopy. Description of some 2D-NMR experiments within the product operator formalism: homo-nuclear CORrelation Spectroscopy (COSY); Double Quantum-Filtered COSY (DQF-COSY); HETERO-nucl
14	日 英	NUCLEAR MAGNETIC RESONANCE (NMR) SPECTROSCOPY (6)	Examples and applications. Solvent suppression techniques: pre-saturation and pulse sequences WET, WATERGATE and WASTED. Basic concepts of solid-state NMR.
15	日 英	Oral examination	It consists in a series of questions about the different topics covered in the course.

## 履修条件 Prerequisite(s)

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英	

## 授業時間外学習（予習・復習等）

Required study time, Preparation and review

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英	Basic knowledge in calculus (vectors, matrices, differential and integral calculus).

## 教科書／参考書 Textbooks/Reference Books

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英	For the quantum mechanics part the textbook mainly used in the course is D. J. Griffiths, "Introduction to Quantum Mechanics", Cambridge University Press, 2nd edition, 2016. For the optical spectroscopies, the textbook mainly used in the course is J. M

## 成績評価の方法及び基準 Grading Policy

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英	Oral examination (about 30'). It consists in a series of questions about the different topics covered in the course; the students will be asked also to apply the different formalisms for describing a given spectroscopic experiment, and to discuss the cor

## 留意事項等 Point to consider

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