

**COURSE CONTENT FOR PH7014 for Undergraduates**

|                           |   |                 |   |
|---------------------------|---|-----------------|---|
| <b>Academic Year</b>      | 2022-23   | <b>Semester</b> | 1 |
| <b>Course Coordinator</b> | A/P Cesare Soci   |                 |   |
| <b>Course Code</b>        | PH7014 (previously listed as PAP731)  |                 |   |
| <b>Course Title</b>       | Optical Spectroscopic Techniques  |                 |   |
| <b>Pre-requisites</b>     | PH3602 Photonics and PHY (PPHY) or PHY (APHY) programme and CGPA 4.0 or higher. |                 |   |
| <b>No of AUs</b>          | 4   |                 |   |
| <b>Contact Hours</b>      | Lecture: 52<br>(4 hrs of lecture each week)                                     |                 |   |
| <b>Proposal Date</b>      | 14 February 2022  |                 |   |

**Course Aims**

This course aims to teach students state-of-the-art optical spectroscopic and imaging techniques for non-destructive materials characterization, with widespread use in the study of conventional bulk and thin films as well as nanoparticles, nano-devices and bio-molecular systems.

The course should be taken by students interested in the fundamentals of light-matter interaction, optical spectroscopic techniques and instrumentation, as well as applications of optical spectroscopic techniques in real-life research situations.

The course will provide basic knowledge of optical spectroscopic techniques which may be useful to both, theoreticians and experimentalists pursuing a research career in physics, materials science, electronic engineering, chemistry and biology, or to those seeking employment in research & development sectors of related industries.

**Intended Learning Outcomes (ILO)**

In this course, you will understand both practical and physical principles behind common and advanced optical spectroscopic techniques, which are used in the study of a variety of material systems, from atoms and (bio)molecules to solids and extended systems. You will also practice self-learning and presentation skills by researching relevant topics of your choice and discussing them in front of the class.

By the end of this course, you should be able to:

1. formulate and examine interactions between photons with acoustic and optical phonons, and with electronic states in different material systems;
2. use the interactions to probe various properties of the samples non-destructively;
3. illustrate the working and design principles of related instrumentation;
4. analyse and interpret the results of these techniques to study actual samples.

**Course Content**

Topics of the course include reflection and transmission spectroscopy, Fourier transform infrared spectroscopy, Raman scattering, photoluminescence and ultrafast spectroscopy. A brief introduction to nonlinear optics and the basics of lasers will also be given.

The module deals with theoretical treatment, instrumentation, as well as examples from original research publications, illustrating how these techniques can be applied to various fields of research.

You will choose additional presentation topics based on your interest. Possible topics include, but are not limited to: ellipsometry, circular dichroism, fluorescence anisotropy, magneto-optic Kerr effect, atomic spectroscopy, photoinduced absorption detected magnetic resonance, photoacoustic spectroscopy, surface enhanced Raman scattering, hyperspectral/multidimensional imaging, near-field/confocal spectroscopy, fluorescence up-conversion, multi-dimensional femtosecond spectroscopy, femtosecond coherence spectroscopy, Terahertz time-domain spectroscopy, attosecond spectroscopy.

**Assessment (includes both continuous and summative assessment)**

| Component                            | ILO Tested | Related Programme LO or Graduate Attributes   | Weighting   | Team/ Individual | Assessment Rubrics |
|--------------------------------------|------------|---|-------------|------------------|--------------------|
| 1. Presentation and group discussion | 1-4        | *Communication (1-3), Character (1-3), Creativity (1-2), Competence (1-5, 7), Civic-mindedness (1). | 45%         | Individual       | See below          |
| 2. Mid-term test                     | 1-4        | *Communication (1-2), Character (1-2), Creativity (1-2), Competence (1-5, 7).                       | 35%         | Individual       | See below          |
| 3. CA1: Quiz/homework                | 2,3        | *Creativity (1-2), Character (1-3), Competence (1-5, 7)   | 10%         | Individual       | See below          |
| 4. CA2: Participation                | 2,4        | *Character (1-3), Civic-mindedness (1), Competence (1-5, 7)   | 10%         | Individual       | See below          |
| <b>Total</b>                         |            |   | <b>100%</b> |                  |                    |

\* The course intended learning outcomes (ILOs) are aligned with the 5Cs of NTU graduates, that is: 1. Communication, 2. Character, 3. Civic-mindedness, 4. Creativity & 5. Competence.

**Description of Assessment Components:**

**Presentation and Group Discussion:** You will give a presentation on an optical spectroscopic technique of your interest. The instructor will guide you to choose relevant readings and preparing the seminar. The presentation and the following Q&A session will be evaluated by both, your peers and the instructor based on rigour and accuracy of the technical content, background knowledge, examples and references provided, understanding of the topics, clarity of organization and timing of the presentation, as well as audience engagement.

**Mid-term Test:** An open-book examination on actual or plausible research problems that will test your overall understanding of the topics and your problem-solving skills.

**Continuous Assessment 1 (CA1):** You will be given some quizzes and homework that will test your understanding of specific topics and your problem-solving skills.

**Continuous Assessment 2 (CA2):** You are expected to actively and respectfully participate in class discussions and seminar peer-evaluation.

**Formative feedback**

Feedback is central to this course. You will receive both written and verbal feedback from the course instructor about your mid-term test and presentation. You will also receive peer-evaluations and comments about your presentation in consolidated (anonymized) form at the end of the module.

### Learning and Teaching approach

| Approach                                 | How does this approach support you in achieving the learning outcomes?  |
|--|---|
| Teacher-centred + inquiry-based learning | The course adopts a teacher-centred approach to introduce fundamental concepts and working principles of the most common optical spectroscopic techniques and their instrumentation, combined with an inquiry-based learning approach to develop critical thinking and problem-solving skills through preparation and delivery of individual presentations and solution of practical exercises. |

### Reading and References

- Optical Spectroscopy, Methods and Instrumentations, Nikolai V. Tkachenko, Elsevier Science, DOI: 10.1016/B978-0-444-52126-2.50048-4
- The photophysics behind photovoltaics and photonics, Guglielmo Lanzani, Wiley-VCH, DOI: 10.1002/9783527645138
- Principles of Fluorescence Spectroscopy, Joseph R. Lakowicz, ISBN 978-0-387-46312-4
- Molecular Fluorescence: Principles and Applications, Bernard Valeur, DOI: 10.1002/3527600248
- Modern Molecular Photochemistry of Organic Molecules, Nicholas J. Turro, V. Ramamurthy and Juan C. Scaiano, ISBN: 978-1891389252
- Laser Spectroscopy 1 (Basic Principles), Wolfgang Demtröder, Springer, Online ISBN: 978-3-540-73418-5
- Laser Spectroscopy 2 (Experimental Techniques), Wolfgang Demtröder, Springer, Online ISBN: 978-3-540-74954-7
- Physics of Nonlinear Optics, G. S. He and S. H. Liu, World Scientific, ISBN: 978-9-810-23319-8
- Handbook of Nonlinear Optical Crystals, V.G. Dmitriev, G.G. Gurzadyan, D.N. Nikogosyan, Springer, ISBN: 3-540-65394-5

Several original research articles will also be provided for reference during the module.

### Course Policies and Student Responsibilities

(1) General: You are expected to complete all assigned readings and activities, attend all seminar classes punctually and take all scheduled assignments and tests by due dates. You are expected to participate in all seminar discussions and peer-evaluation activities.

(2) Absenteeism: Absence from class without a valid reason will affect your overall course grade. Valid reasons include falling sick supported by a medical certificate and participation in NTU's approved activities supported by an excuse letter from the relevant bodies.

### 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. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

**Course Instructors**

| Instructor      | Office Location | Phone     | Email            |
|-----------------|-----------------|-----------|------------------|
| A/P Cesare Soci | SPMS-PAP-03-03  | 6514 1045 | csoci@ntu.edu.sg |

**Planned Weekly Schedule**

| Week   | Topic  | ILO | Readings / Activities                  |
|--------|--|-----|--|
| Week 1 | COURSE PRESENTATION AND INTRODUCTION: Optics, spectroscopy, photonics. Light, radiation. Photophysics, photochemistry.   | 1,2 | Suggested books and journal references |
| Week 2 | LIGHT ABSORPTION. Absorption parameters: transmittance, Beer-Lambert law and absorption coefficient, absorptance, absorption cross-section, absorbance, molar absorption coefficient. Composite samples. Dispersive absorption spectroscopy (UV-Vis): types of spectrophotometers, sources, monochromators, detectors.   | 1-4 | Suggested books and journal references |
| Week 3 | RADIATION-MATTER INTERACTION. Absorption in atoms and molecules: polarization, susceptibility and absorption coefficient. Two-level system: Einstein coefficients, rate equations, absorption cross-section.   | 1,2 | Suggested books and journal references |
| Week 4 | INFRARED ABSORPTION SPECTROSCOPY. Fourier transform infrared (FTIR) spectroscopy: principles of multiplexing spectroscopy; FTIR spectrometers: spectral range and resolution, advantages over dispersive spectroscopy, IR sources, detectors and beam splitters. Vibrational spectroscopy: IR active molecular transitions, transition strength; examples.   | 1-4 | Suggested books and journal references |
| Week 5 | OPTICAL PROPERTIES OF SOLIDS. Macroscopic fields and Maxwell's equation: general wave equation and complex dielectric functions, Kramers-Kronig relations and sum rules. Lorentz oscillator model: single and multiple resonances, anomalous dispersion. Drude model: plasmas. Optical properties of semiconductors: intraband and interband transitions, excitonic and defect absorption.   | 1,2 | Suggested books and journal references |
| Week 6 | EMISSION SPECTROSCOPY: Principles of photoluminescence: excitation selection rules, intersystem crossing, Franck-Condon principle; non-radiative relaxation: internal conversion, delayed fluorescence; emission: Stokes shift, Kasha's rule, mirror-image rule, Jablonski diagram. Photoluminescence instrumentation and measurements: spectrofluorometer, calibration, quantum yield, emission and excitation spectra, excitation-emission matrix. | 1-4 | Suggested books and journal references |
| Week 7 | LIGHT SCATTERING. Electromagnetic scattering: elastic and inelastic scattering. Elastic scattering: Rayleigh scattering, Mie scattering, diffuse reflectance and transmittance. Inelastic scattering:  | 1-4 | Suggested books and journal references |

|         |   |        |  |
|---------|---|--------|--|
|         | Raman scattering: induced dipole moment, selection rules, group frequencies, anisotropy, intensity, instrumentation. Brillouin scattering.  |        |  |
| Week 8  | MID-TERM test and discussion of results.  | 1-4    | Notes and suggested books/readings     |
| Week 9  | INTRODUCTION TO LASERS. General properties, TEM mode, Gaussian beam, examples of lasers, types of lasers. Working principles of lasers: three and four levels systems, Fabry – Perot resonator, rate equation and threshold, Q-switching, mode-locking, chirp pulse amplification.  | 3      | Suggested books and journal references |
| Week 10 | TIME-RESOLVED SPECTROSCOPY: Population dynamics: thermalization, internal conversion, energy migration. Transient fluorescence: lifetime and quantum yield. Stroboscopic methods: flash-photolysis, TCSPC, streak camera. Transient absorption: ground state bleaching, photoinduced absorption, stimulated emission, IRAV modes. Quasi-static PIA: continuous-scanning differential absorption, lock-in techniques. Ultrafast spectroscopy: transient absorption spectroscopy, fluorescence up-conversion, characterization of short pulses.                                       | 1-4    | Suggested books and journal references |
| Week 11 | NONLINEAR OPTICS: Second-order nonlinear effects. Three wave interaction. Nonlinear susceptibilities. Optics of uniaxial and biaxial crystals. Phase-matching. Formulas for the calculation of phase-matching angles. Third order nonlinear optical effects: four wave interactions, two-photon absorption, self-focusing, Stimulated Raman scattering, self-phase modulation, self-trapping, Kerr and Pockels effects, photon echo, coherent anti-Stokes Raman scattering (CARS).  | 1-4    | Suggested books and journal references |
| Week 12 | NONLINEAR LASER SPECTROSCOPY: Second order autocorrelation, instrument response function, two-photon fluorescence, pump-probe technique, fluorescence up-conversion. Examples: singlet fission, quasiparticle dynamics in graphene, surface enhanced metal organic frameworks. inhomogeneous and homogeneous broadening, saturation of absorption, hole burning, two-photon laser spectroscopy. TWO-QUANTUM PROCESSES: quantum yield, definition; singlet-singlet and triplet-triplet excitation. Rate equations. Nonlinear transmission/propagation.                               | 1-4    | Suggested books and journal references |
| Week 13 | ENERGY TRANSFER: Radiative energy transfer. Non-radiative energy transfer: Dexter ET, triplet-triplet annihilation; Förster ET, rate and efficiency. Application examples: determination of distance, molecular conformation, association reactions, orientation effects; molecular beacons; energy upconversion. CHARGE TRANSFER: Marcus theory: solvent reorganization, transition and reorganization energy, electron transfer rate, inverted region. Application examples: verification of the inverted region; ultrafast electron transfer in bulk heterojunction solar cells. | 1-2, 4 | Suggested books and journal references |

**Graduate Attributes**

**What we want our graduates from Physics and Applied Physics to be able to do:**

Upon the successful completion of the PHY, APHY, PHME and PHMS programs, graduates should be able to:

|                   |   |  |
|-------------------|---|--|
| <b>Competency</b> | 1 | demonstrate a rigorous understanding of the core theories and principles of physics involving (but not limited to) areas such as classical mechanics, electromagnetism, thermal physics and quantum mechanics<br><br>[PHMS only] demonstrate a rigorous understanding of the core theories and principles of mathematical sciences involving (but not limited to) areas such as analysis, algebra and statistical analysis |
|                   | 2 | read and understand undergraduate level physics content independently;   |
|                   | 3 | make educated guesses / estimations of physical quantities in general;   |
|                   | 4 | apply fundamental physics knowledge, logical reasoning, mathematical and computational skills to analyse, model and solve problems;  |
|                   | 5 | develop theoretical descriptions of physical phenomena with an understanding of the underlying assumptions and limitations;  |
|                   | 6 | critically evaluate and distinguish sources of scientific/non-scientific information and to recommend appropriate decisions and choices when needed;   |
|                   | 7 | demonstrate the ability to design and conduct experiments in a Physics laboratory, to make measurements, analyse and interpret data to draw valid conclusions.   |

|                   |   |  |
|-------------------|---|--|
| <b>Creativity</b> | 1 | propose valid approaches to tackle open-ended problems in unexplored domains;    |
|                   | 2 | offer valid alternative perspectives/approaches to a given situation or problem. |

|                      |   |   |
|----------------------|---|---|
| <b>Communication</b> | 1 | describe physical phenomena with scientifically sound principles;   |
|                      | 2 | communicate (in writing and speaking) scientific and non-scientific ideas effectively to professional scientists and to the general public; |
|                      | 3 | communicate effectively with team members when working in a group.  |

|                  |   |   |
|------------------|---|---|
| <b>Character</b> | 1 | uphold absolute integrity when conducting scientific experiments, reporting and using the scientific results; |
|                  | 2 | readily pick up new skills, particularly technology related ones, to tackle new problems;                     |
|                  | 3 | contribute as a valued team member when working in a group.   |

|                         |   |  |
|-------------------------|---|--|
| <b>Civic Mindedness</b> | 1 | put together the skills and knowledge into their work in an effective, responsible and ethical manner for the benefits of society. |
|-------------------------|---|--|