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## A COURSE SYLLABUS – DOCTORAL SCHOOL

REGARDING THE QUALIFICATION CYCLE FROM 2025/2026 TO 2028/2029

| GENERAL INFORMATION ABOUT COURSE                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                                                                                                                                                                                                                                                                                                                                                       |
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| Course title                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | <b>WORKSHOPS WITH AN EXPERT</b><br>Scientific focus: Beyond the Born–Oppenheimer approximation: effective Hamiltonians and isotope spectra                                                                                                                                                                                                            |
| Name of the unit running the course                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | Doctoral School at University of Rzeszów                                                                                                                                                                                                                                                                                                              |
| Type of course ( <i>obligatory, optional</i> )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | <b><i>obligatory</i></b>                                                                                                                                                                                                                                                                                                                              |
| Year and semester of studies                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | <b>Year II / semester III</b>                                                                                                                                                                                                                                                                                                                         |
| Discipline                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | PHYSICS                                                                                                                                                                                                                                                                                                                                               |
| Language of Course                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | English                                                                                                                                                                                                                                                                                                                                               |
| Name of Course coordinator                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | Prof Roman Pasechnik                                                                                                                                                                                                                                                                                                                                  |
| Name of Course lecturer                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | Prof Roman Pasechnik                                                                                                                                                                                                                                                                                                                                  |
| Prerequisites                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | Basic quantum mechanics: the Schrödinger equation, complex amplitudes, elementary matrix algebra, derivatives, and the harmonic oscillator. Familiarity with molecular spectroscopic notation is helpful. Perturbation theory and effective-Hamiltonian methods are introduced within the workshop; no prior quantum field theory course is required. |
| BRIEF DESCRIPTION OF COURSE<br>(100-200 words)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                       |
| <p>What is lost when electronic motion is replaced by a potential for the nuclei, and how can isotope spectra reveal the missing effects? The workshop connects this question to the <math>B^2\Sigma^+-X^2\Sigma^+</math> spectroscopy of <math>CO^+</math>. Starting from the molecular Schrödinger equation, the student develops the electronic-channel expansion, derivative couplings and the diagonal Born–Oppenheimer correction. An exactly solvable coupled-oscillator model shows why virtual fast excitations also modify nuclear inertia, providing a concrete introduction to effective Hamiltonians and matching. The calculation then leads to isotope mass scaling, common-upper-level differences and uncertainty-aware spectral diagnostics. The distinction between an analytic benchmark and a quantitative molecular prediction is maintained throughout. The outcome is an account of what fitted isotope corrections can establish and which microscopic interpretations require additional molecular information.</p> |                                                                                                                                                                                                                                                                                                                                                       |

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| COURSE LEARNING OUTCOMES AND METHODS OF EVALUATING LEARNING OUTCOMES |                                                                                                                                                                                                                                                                                                                                                                                                           |                                                    |                                         |                                                                                             |
|----------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------|-----------------------------------------|---------------------------------------------------------------------------------------------|
| Learning outcome                                                     | The description of the learning outcome defined for the course                                                                                                                                                                                                                                                                                                                                            | Relation to the degree programme outcomes (symbol) | Learning Format (Lectures, classes,...) | Method of assessment of learning outcomes (e.g. test, oral exam, written exam, project,...) |
| Knowledge (no.)                                                      | (Knows and understands)                                                                                                                                                                                                                                                                                                                                                                                   |                                                    |                                         |                                                                                             |
| P8S_WG2                                                              | Possesses knowledge of research directions and current achievements, including international work, in Born–Oppenheimer separation, nonadiabatic corrections, effective Hamiltonians and isotope-dependent molecular spectra, and understands their connection to the doctoral student’s research interests.                                                                                               | P8S_WG                                             | Individual workshop and discussion      | Written report and scientific discussion                                                    |
| P8S_WK1                                                              | Knows and understands how technological development influences scientific and societal progress in high-resolution molecular spectroscopy and isotope analysis. Can discuss the resulting consequences for the wider world, including the capabilities and limitations of the methods considered.                                                                                                         | P8S_WK                                             | Individual workshop and discussion      | Discussion of technological context and wider implications                                  |
| Skills (no.)                                                         | (Able to)                                                                                                                                                                                                                                                                                                                                                                                                 |                                                    |                                         |                                                                                             |
| P8S_UW1                                                              | Based on interdisciplinary knowledge, the doctoral student is able to identify and solve research problems related to the topic of scientific research conducted in the discipline of physical sciences, define research goals, formulate hypotheses and the subject of scientific research, develop research methods, techniques and tools, and draw constructive conclusions based on research results. | P8S_UW                                             | Individual workshop and discussion      | Report derivations and interpretation                                                       |

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| <b>COURSE LEARNING OUTCOMES AND METHODS OF EVALUATING LEARNING OUTCOMES</b> |                                                                                                                                                                                                                                                                                                                         |                                                    |                                         |                                                                                             |
|-----------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------|-----------------------------------------|---------------------------------------------------------------------------------------------|
| Learning outcome                                                            | The description of the learning outcome defined for the course                                                                                                                                                                                                                                                          | Relation to the degree programme outcomes (symbol) | Learning Format (Lectures, classes,...) | Method of assessment of learning outcomes (e.g. test, oral exam, written exam, project,...) |
| <b>P8S_UK6</b>                                                              | Using a foreign language at least at the B2 level of the Common European Framework of Reference for Languages, a doctoral student is able to present research results, take part in discussions and actively participate in scientific and professional debates both at the national and international level.           | P8S_UK                                             | Individual workshop and discussion      | Scientific discussion and report in English                                                 |
| <b>P8S_UU1</b>                                                              | A doctoral student is able to independently acquire and update knowledge, develop analytical skills based on current interdisciplinary scientific achievements, and inspire others to conduct research and development activities.                                                                                      | P8S_UU                                             | Individual workshop and discussion      | Report sources and independent reconstruction                                               |
| <b>P8S_UU2</b>                                                              | A doctoral student is able to share his or her knowledge, thanks to his or her extensive interdisciplinary knowledge, he or she is able to plan and implement interesting classes, and is also able to inspire others by supporting the learning process and by using modern and innovative teaching methods and tools. | P8S_UU                                             | Individual workshop and discussion      | Structured explanation of a derivation in the report and discussion                         |
| <b>P8S_UU3</b>                                                              | Thanks to the continuous learning process, the doctoral student updates his/her interdisciplinary knowledge, improves his/her scientific competences and plans his/her own development and the development of others.                                                                                                   | P8S_UU                                             | Individual workshop and discussion      | Discussion of limitations and further study                                                 |

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| COURSE LEARNING OUTCOMES AND METHODS OF EVALUATING LEARNING OUTCOMES |                                                                                                                                                                                                                                                             |                                                    |                                         |                                                                                             |
|----------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------|-----------------------------------------|---------------------------------------------------------------------------------------------|
| Learning outcome                                                     | The description of the learning outcome defined for the course                                                                                                                                                                                              | Relation to the degree programme outcomes (symbol) | Learning Format (Lectures, classes,...) | Method of assessment of learning outcomes (e.g. test, oral exam, written exam, project,...) |
| <b>Social competence (no.)</b>                                       | <b>(Ready to)</b>                                                                                                                                                                                                                                           |                                                    |                                         |                                                                                             |
| <b>P8S_KK1</b>                                                       | The doctoral student is ready to critically evaluate scientific achievements in the chosen scientific discipline of physical sciences, taking into account current research trends and quality standards of scientific research in the field of physics     | P8S_KK                                             | Individual workshop and discussion      | Critical evaluation of sources in the report                                                |
| <b>P8S_KK2</b>                                                       | Is ready to critically evaluate his/her own research contribution to scientific achievements in the chosen scientific discipline of physics, in the area of his/her interests and research.                                                                 | P8S_KK                                             | Individual workshop and discussion      | Attribution of reproduced results and appraisal of the student's own reasoning              |
| <b>P8S_KK3</b>                                                       | Is ready to solve theoretical and practical problems using his/her knowledge of exact and natural sciences within the discipline of physical sciences and related disciplines, in particular those relating to the doctoral student's scientific interests. | P8S_KK                                             | Individual workshop and discussion      | Report reasoning and scientific discussion                                                  |

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| LEARNING FORMAT – NUMBER OF HOURS |          |          |             |             |                  |        |
|-----------------------------------|----------|----------|-------------|-------------|------------------|--------|
| Semester<br>(no.)                 | Lectures | Seminars | Lab classes | Internships | others           | ECTS   |
| III                               | -        | -        | -           | -           | 5 academic hours | 1 ECTS |

**METHODS OF INSTRUCTION**

Individual, expert-led workshop combining blackboard derivations with guided scientific discussion. Definitions and intermediate steps are developed from quantum mechanics; the student checks limiting cases, assumptions and physical interpretations. Selected literature and the supplied notes support independent study and preparation of a written report. The student explains selected reasoning during discussion; the report presents the calculation in a form understandable to another doctoral student.

**COURSE CONTENT**

Programme allocation in academic hours; discussion is integrated into each block.

1. Separating electronic and nuclear motion (1 academic hour): molecular Hamiltonian; electronic-channel expansion; derivative couplings; phase-independent diagonal correction; electronic gaps and the validity of a single-channel approximation.
2. Testing the approximation in an exactly solvable model (1 academic hour): coupled oscillators; normal modes and quantum spectrum; Born–Oppenheimer limit; controlled slow-frequency expansion; the limitations of a potential-only correction.
3. Eliminating virtual excitations (1 academic hour): projected Schrödinger equations; energy-dependent effective Hamiltonian; induced nuclear inertia; comparison with the exact response; matching and its connection to effective field theory.
4. Connecting molecular energies to isotope spectra (1 academic hour): reduced mass; vibrational, anharmonic and rotational scaling; Dunham coefficients; spin-resolved CO<sup>+</sup> assignments; common-upper-level differences and extraction of rotational constants.
5. Interpreting an isotope test (1 academic hour): equilibrium mass-scaled residuals; covariance and uncertainty propagation; identifiability of carbon and oxygen correction terms; limits of microscopic inference; synthesis and report discussion. Discuss the role of experimental and computational advances and the wider implications of the methods.

**COURSE ASSESSMENT CRITERIA**

Assessment: pass/fail, based on a written report related to the workshop, supported by the scientific discussion. A written report addressing the six questions in the final student notes: electronic-channel projection and the diagonal correction; the exact coupled-oscillator model; induced inertia and matching; isotope mass scaling; a spectral residual with correlated uncertainties; and identifiability of microscopic corrections.

A pass requires a coherent account of the central problem; substantially correct, traceable calculations; explicit conventions, approximations and applicable limits; critical physical interpretation; and appropriate citation of sources. Numerical results, where requested in the notes, must include a convergence or consistency check. The report should distinguish reproduced literature results from the student’s own analysis and explain at least one derivation clearly for a doctoral peer.

A fail applies if no report is submitted or the work does not demonstrate these essential outcomes. The submission date is communicated by the lecturer.

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| <b>TOTAL PhD STUDENT WORKLOAD REQUIRED TO ACHIEVE THE INTENDED LEARNING OUTCOMES – NUMBER OF HOURS AND ECTS CREDITS</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|-------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Activity                                                                                                                | Number of hours                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| Scheduled course contact hours                                                                                          | <b>5 hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| Other contact hours involving the teacher (consultation hours, examinations)                                            | <b>1 hour</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| Non-contact hours – student's own work (preparation for classes or examinations, project, etc.)                         | <b>24 hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| <b>Total number of hours</b>                                                                                            | <b>30 hours</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| <b>Total number of ECTS credits</b>                                                                                     | <b>1 ECTS</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| <b>INSTRUCTIONAL MATERIALS</b>                                                                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| Compulsory literature:                                                                                                  | <p>1. J. K. G. Watson, The isotope dependence of diatomic Dunham coefficients, <i>Journal of Molecular Spectroscopy</i> 80, 411–421 (1980). DOI: 10.1016/0022-2852(80)90152-6. Selected sections on isotope scaling and parameter conventions.</p> <p>2. C. Puzzarini and J. Gauss, Quantum-chemical determination of Born–Oppenheimer breakdown parameters for rotational constants: the open-shell species CN, CO<sup>+</sup> and BO, <i>Molecular Physics</i> 111, 2204–2210 (2013). DOI: 10.1080/00268976.2013.797614. Selected sections on microscopic contributions and fitted constants.</p>                                                                                                                                                           |
| Complementary literature:                                                                                               | <p>1. M. Born and K. Huang, <i>Dynamical Theory of Crystal Lattices</i>, Oxford University Press (1954). Electronic-channel expansion and separation of nuclear and electronic motion.</p> <p>2. N. Brambilla, G. Krein, J. Tarrús Castellà and A. Vairo, The Born–Oppenheimer approximation in an effective field theory language, <i>Physical Review D</i> 97, 016016 (2018). DOI: 10.1103/PhysRevD.97.016016; arXiv:1707.09647.</p> <p>3. S. Spezzano et al., Accurate High-N Rest Frequencies for CO<sup>+</sup>, an Ideal Tracer of Photon-Dominated Regions, <i>Journal of Physical Chemistry A</i> 117, 9814–9818 (2013). DOI: 10.1021/jp312616u. Isotopically invariant CO<sup>+</sup> analysis including Born–Oppenheimer-breakdown corrections.</p> |

ONE ECTS CREDIT CORRESPONDS TO 25–30 HOURS OF TOTAL DOCTORAL-STUDENT WORKLOAD.

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Date and signature of the Course lecturer

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Approved by the Head of the Department or an authorised person