

DOCTORAL STUDIES COURSE UNIT DESCRIPTION

Name of subject	Scientific Field	Faculty	Center/Institute/ Department
Molecular and molecular compounds theory (8 ECTS credits)	Physics N 002	Faculty of Physics	Institute of Chemical Physics
Student's workload	Hours	Student's workload	Hours
Lectures	4	Consultations	16
Individual study	170	Seminars	10

Course annotation			
Quantum molecular theory. Adiabatic approximation. State functions of many electronic systems. Methods of investigation of many electronic systems. One electronic approximation. Huckel method. Hartree-Fock method. Koopmans, Brillouin theorems. Atomic basis functions. Multicenter integrals in molecular theory. Methods accounting electronic correlation: multiconfigurational self consistent field method, configuration interaction, coupled cluster, perturbation theory and valence bond methods. Density functional theory, Kohn-Sham equations. Time dependent density functional theory. Semiempirical methods. QM/MM, ONIOM methods. Molecular reactions. Molecular collisions, dynamics of many atomic molecules. Reaction rates. Energy transfer in molecules. Dynamics in condensed phase, near the surfaces. Account of solvents. Quantum molecular dynamics. Group theory and it's application in molecular quantum mechanics. The description of the group. Subgroup. Conjugated elements and classes. Isomorphic and homomorphic groups. Direct product groups. Group presentations. Reducible and irreducible presentations. Schur's lemmas. Presentation characters. Projection operators. Symmetry of wave functions. Classification of eigenfunctions according to the symmetry. Space symmetry of molecules. Point symmetry groups. Classification of vibrational spectra. Vanishing integrals. Applications of quantum molecular theory. Determination of molecular equilibrium geometry parameters, dipole moments, molecular electronic potential energy surfaces, atomization energies, reaction enthalpies, conformational barriers, electronic and vibrational spectra.			
List of literature			
1. Helgaker T., Jorgensen P., Olsen J. Molecular Electronic Structure Theory. John Wiley & sons, Ltd, 2004. 908 p. 2. David S. Sholl, Janice A. Steckel. Density Functional Theory. A JohnWiley & Sons, inc., 2009, 238 p. 3. Levine R.D. Molecular Reaction Dynamics. Cambridge University Press, 2004. 554 p. 4. John Zeng Hui Zhang. Theory and Application of Quantum Molecular Dynamics. World Scientific, 1999, 366 p. 5. David M. Bishop. Group Theory and Chemistry. Dover Publications, Inc., 1993, 300 p. 6. Atkins P., Friedman R. Molecular Quantum Mechanins. Oxford University Press, 2007, 573 p. 7. Martin R.M. Electronics structure. Basic theory and practical methods. Cambridge University Press, 2007. 624 p.			
Consulting teachers	Scientific degree	Pedagogical name	Main scientific works published in a scientific field in last 5 year period
Mindaugas Mačernis	Dr.	Doc.	1. Macernis, M., Component-wise AO basis reduction: norm loss, negative contribution

			normalization, and functional implications. Physical Chemistry Chemical Physics, 2025. 27(27): p. 14555-14564. 2. Diska, L., et al., Interactions of lycopene with β-cyclodextrins: Raman spectroscopy and theoretical investigation. Physical Chemistry Chemical Physics, 2025. 27(15): p. 7874-7881. 3. Halimski, I., et al., -Stilbene aggregates and crystallites in polystyrene films: microscopy and spectroscopy studies. Physical Chemistry Chemical Physics, 2024. 26(36): p. 23692-23702. 4. Karpicz, R., et al., Two phases of -stilbene in a polystyrene matrix. Physical Chemistry Chemical Physics, 2023. 25(32): p. 21183-21190. 5. Macernis, M., et al., Electronic and Vibrational Properties of Allene Carotenoids. Journal of Physical Chemistry A, 2022. 126(6): p. 813-824. 6. Macernis, M., et al., Mechanism of Proton Transfer in Bacteriorhodopsin. Lithuanian Journal of Physics, 2022. 62(3): p. 179-193. 7. Macernis, M., et al., Raman study for β-ring positioning in β-Carotene complexes with Cyclodextrins and Chitooligosaccharides. Journal of Molecular Structure, 2021. 1226. 8. Karpicz, R., et al., Unusual temperature dependence of the fluorescence decay in heterostructured stilbene. Physical Chemistry Chemical Physics, 2021. 23(5): p. 3447-3454.
Certified during the Doctoral Committee session on 29/09/2026, protocol No. 5.2.2 E-15600-KT-3702			
Committee Chairman prof. Jūras Banys			