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 consistend 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 ofmolecules. 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 JohnWilley & 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
Juozas Šulskus	Dr.	Prof.	1. Mačernis M., Galzerano D., Šulskus J., Kish E. , Kim Y. , Koo S. Valkūnas L. ,

			Robert B. Resonance Raman spectra of carotenoid molecules: influence of methyl substitutions. Journal of physical chemistry. A. Vol. 119, iss. 1 (2015) p. 56-66. 2. Redeckas K.,Toliautas S., Steponaviciute R., Sackus A., Sulskus J., Vengris M. A femtosecond stimulated Raman spectroscopic study on the oxazine ring opening dynamics of structurally-modified indolobenzoxazines. Chem. Phys. Lett. Vol. 653 (2016) p. 67-72. 3. Toliautas S., Dodonova J, Zvirblis A, Ciplys I, Polita A, Devizis A, Tumkevicius S Sulskus J. Vysniauskas A. Enhancing the Viscosity-Sensitive Range of a BODIPY Molecular Rotor by Two Orders of Magnitude. Chemistry-A European Journal. Vol. 25, iss. 44, (2019) p. 10342-10349. 4. Jasiūnas R., Zhang H., Yuan J., Zhou X., Qian D., Zou Y., Devižis A., Šulskus J., Gao F., and Gulbinas V. From Generation to Extraction: A Time-Resolved Investigation of Photophysical Processes in Non-fullerene Organic Solar Cells. J. Phys. Chem. C 2020, 124, 21283−21292.
Certified during Doctoral Committee session 02/02/2022, protocol No. (7.17 E) 15600-KT-32			
Committee Chairman prof. S. Juršėnas			