DOCTORAL STUDIES COURSE UNIT DESCRIPTION

Name of subject	Scientific Field	Center	Department
Optical Spectroscopy (10 ECTS credits)	Physics N 002	Center for Physical Sciences and Technology	Optoelectronics Molecular Compound Physics Organic Chemistry
Student's workload	Hours	Student's workload	Hours
Lectures	20	Consultations	30
Individual study	200	Seminars	

Course annotation

Electronic spectrosopy of molecular materials.

Theoretical background. Electronic transitions in atoms and molecules. Intensities of electronic transitions, selection rules. Line broadening. Energies of electronic transitions. Absorption and luminescence of molecules. Fluorescence and phosphorescence. Einstein relations. Fluorescence and phosphorescence. Absorption and luminescence spectra of large molecules, their interrelations. Influence of environment on absorption and luminescence spectra. Wannier-Mott, charge transfer and Frenkel excitons, Exciton delocalization in aggregates and molecular solids. Exciton locaization. Energy transfer. Fluorescence quenching. Charge transfer, Marcus theory.

Experimental investigation methods. Steady state absorption and luminescence spectroscopy. Time-resolved luminescence and ultrafast transient absorption. Dynamic gratings for time-resolved spectroscopy. Two-dimensional coherent electronic and vibrational spectroscopy. Electroabsorption and electroluminescence spectroscopy. Single molecule spectroscopy.

Vibrational spectroscopy.

Theoretical background. Origin of infrared (IR) absorption and Raman spectra. Vibrations of diatomic molecules. Vibrations of polyatomic molecules. Normal modes of vibrations. Symmetry of molecules and vibrations. Fermi resonance. Selection rules for infrared and Raman spectroscopy. Resonance Raman and Coherent Anti-Stokes Raman spectroscopy (CARS). Surface-enhanced Raman spectroscopy (SERS), enhancement mechanisms, surface plasmons. Vibrations of isotopic molecules. Depolarization ratios of Raman bands. Inverse polarization of Raman bands. Characteristic vibrations and interpretation of vibrational spectra. Fundamentals of sum frequency generation (SFG) vibrational spectroscopy.

Experimental investigation methods. FTIR spectroscopy. Attenuated total reflection (ATR), reflection absorption (RAIRS) and polarization modulation reflection absorption infrared spectroscopy (PA-RAIRS). Selection rules for molecules adsorbed at metal surfaces. Preparation of samples for FTIR measurements. Calibration of Raman spectrometer. Surfaces and nanoparticles employed in SERS. Lasers for Raman spectroscopy. Comparison of UV-RR, Vis-Raman, and FT-Raman methods. Raman microscopy. Peculiarities of SFG experiment.

Application. Probing of chemical bonding, intramolecular and intermolecular interactions, hydrogen bonding, and formation of complexes. Vibrational spectroscopy of biomolecules. Resonance Raman spectroscopy of active centers in proteins. Probing of orientation and interactions of adsorbed molecules, and molecular structure of self-assembled monolayers. Vibrational spectroscopic study of conducting polymers. Single molecule SERS.

Spectroscopy of semiconductor nanostructures.

Quantum solid state nanostructures. Quantum structures: quantum wells, superlattices, quantum wires, quantum dots. Excitons. Plasmons. Magnons. Two level system. Bloch equations. Dephasing processes. Principles of phase relaxation measurements. Carrier relaxation in nanostructures. Quantum beats. Bloch oscillations. Dynamics of phonons. Exciton dynamics. Non-Markovian processes. Tunelling phenomena in semiconductor nanostructures.

Experimental technique:

Photoluminescence and photoluminescence excitation spectroscopy, optical modulation spectroscopy, transmission spectroscopy, reflection spectroscopy, time-resolved spectroscopy, single-photon counting technique. Principles of ultrafast spectroscopy. Pump-probe technique. Four-wave mixing method.

Terahertz spectroscopy. Coherent spectroscopy and its applications to study transport phenomena in nanostructures. Terahertz spectroscopy of semiconductor compounds.

Principles of nonlinear spectroscopy in solid state and quantum structures. High-intensity induced effects in solid state. Mott density. Optical bistability.

List of literature

1. W. Demtroder, Laser spectroscopy: basic concepts and instrumentation, Springer-Verlag, Berlin 1996.
2. V. Gulbinas. Šviesos sukelti molekuliniai vyksmai ir jų lazerinė spektroskopija, Vilnius, leidykla TEV, 2008
3. B. Valeur, M. N. Berberan-Santos „Molecular fluorescence : principles and applications“, Wiley-VCH, 2001.
4. R. Ferraro, K. Nakamoto, Introductory Raman spectroscopy, Academic Press, 2003.
5. F. Siebert, P. Hildebrandt, Vibrational spectroscopy in life science, Wiley-VCH, 2008.
6. E. C. Le Ru, P. G. Etchegoin, Principles of surface-enhanced Raman spectroscopy and related plasmonic effects, Elsevier, Amsterdam, 2009.
7. V. Vaičikauskas, G.-J. Babonas, Z. Kuprionis, G. Niaura, V. Šablinskas, Paviršiaus optinė spektroskopija, TEV, 2008.
8. C. F. Klingshirn, Semiconductor optics, Springer-Verlag, Berlin-Heidelberg, 1997.
9. Jagdeep Shah, Ultrafast Spectroscopy of Semiconductors and Semiconductor Nanostructures, Springer-New York, 1999.

List of additional literature

1. S. Mukamel, Principles of Nonlinear Spectroscopy, Oxford Univ. Press, 1999.
2. P. Atkins, J. De Paula, Physical Chemistry, W. H. Freeman and Company, 2006.
3. J. R. Lakowicz. Principles of Fluorescence Spectroscopy, Springer, 2006.
4. S. Juršėnas. Organiniai puslaidininkiai. Vilniaus universitetas, 2008.
5. B. Stuart, Infrared spectroscopy: fundamentals and applications, John Wiley & Sons, 2004.
6. K. Nakamoto, Infrared and Raman spectra of inorganic and coordination compounds, Parts A and B, John Wiley and Sons, 1997.

Consulting teachers	Scientific degree	Pedagogical name	Main scientific works published in a scientific field in last 5 year period
Vidmantas Gulbinas	habil. Dr.	Prof.	1. R Jasiūnas, R Gegevičius, M Franckevičius, N Phung, A Abate, V. Gulbinas, Suppression of Electron Trapping in MAPbI3 Perovskite by Sr2+ Doping, Physica status solidi (RRL)–Rapid Research Letters 14 (11), 2000307. 2020. 2. R Jasiūnas, H Zhang, J Yuan, X Zhou, D Qian, Y Zou, A Devižis, J. Sulskus, F. Gao, V.

			Gulbinas, From Generation to Extraction: A Time-Resolved Investigation of Photophysical Processes in Non-fullerene Organic Solar Cells, The Journal of Physical Chemistry C 124 (39), 21283-21292, 2020. 3. R Jasiūnas, R Gegevičius, M Franckevičius, V Jašinskas, V Gulbinas, Energy Barriers Restrict Charge Carrier Motion in MAPI Perovskite Films, Advanced Optical Materials 8 (16), 2000036, 2, 2020. 4. K.M.M. Salim, E. Hassanabadi, S. Masi, A.F. Gualdrón-Reyes, M. Franckevicius, A. Devižis, V. Gulbinas, A. Fakharuddin, I. Mora-Sero, Optimizing Performance and Operational Stability of CsPbI3 Quantum-Dot-Based Light-Emitting Diodes by Interface Engineering, ACS Applied Electronic Materials 2 (8), 2525-2534, 2020. 5. V Jašinskas, F Oberndorfer, T Hertel, V Gulbinas, Electronic and Ionic Electric Field Screening and Persistent Built-In Electric Field in Carbon Nanotube/PCBM Films, Physica status solidi (a) 217 (6), 1900673, 2020.
Gediminas Niaura	habil. Dr.		1. A. Zdaniauskiene, T. Charkova, I. Ignatjev, V. Melvydas, R. Garjonyte, I. Matulaitiene, M. Talaikis, G. Niaura, Shell-isolated nanoparticle-enhanced Raman spectroscopy for characterization of living yeast cells, Spectrochimica Acta Part A – Molecular and Biomolecular Spectroscopy 240 (2020) 118560. 2. M. Talaikis, S. Strazdaite, M. Ziaunys, G. Niaura, Far of resonance: multiwavelength Raman spectroscopy probing amide bands of amyloid-beta-(37-42) peptide, Molecules 25 (2020) 3556. 3. S. Strazdaite, E. Navakauskas, J. Kirschner, T. Sneideris, G. Niaura, Structure determination of hen egg-white lysozyme aggregates adsorbed to lipid/water and air/water interfaces, Langmuir 36 (2020) 4766-4775. 4. M. Talaikis, G. Valincius, G. Niaura, Potential-induced structural alterations in the tethered bilayer lipid membrane-anchoring monolayers revealed by electrochemical surface-enhanced Raman spectroscopy,

			Journal of Physical Chemistry C 124 (2020) 19033-19045. 5. R. Trusovas, K. Ratautas, G. Raciukaitis, G. Niaura, Graphene layer formation in pinewood by nanosecond and picosecond laser irradiation, Applied Surface Science 471 (2019) 154-161.
Gintaras Valušis	habil. Dr.	Prof.	1. Siemion, L. Minkevičius, L. Qi, G. Valušis, Spatial filtering based terahertz imaging of low absorbing objects, Optics and Lasers in Engineering 139, 106476, 2021. 2. D. Seliuta, J. Vyšniauskas, K. Ikamas, A. Lisauskas, I. Kašalynas, A. Reklaitis, G. Valušis..., Symmetric bow-tie diode for terahertz detection based on transverse hot-carrier transport, Journal of Physics D: Applied Physics 53 (27), 275106, 2020. 3. L. Minkevičius, L. Qi, A Siemion, D. Jokubauskis, A. Sešek, A. Švigelj, J. Trontelj, D. Seliuta, I. Kašalynas, G. Valušis,Titanium-Based Microbolometers: Control of Spatial Profile of Terahertz Emission in Weak Power Sources, Applied Sciences 10 (10), 3400, 2020. 4. L. Minkevičius, D. Jokubauskis, I. Kašalynas, S. Orlov, A. Urbas, G. Valušis, Bessel terahertz imaging with enhanced contrast realized by silicon multi-phase diffractive optics, Optics express 27 (25), 36358-36367, 2019. 5. R. Ivaškevičiūtė-Povilauskienė, L. Minkevičius, D. Jokubauskis, I. Kašalynas, S. Orlov, A. Urbas, G. Valušis, Flexible materials for terahertz optics: advantages of graphite-based structures, Optical Materials Express 9 (11), 4438-4446, 2019.
Certified during Doctoral Committee session 02/02/2022, protocol No. (7.17 E) 15600-KT-32			
Committee Chairman prof. S. Juršėnas			