

DOCTORAL STUDIES COURSE UNIT DESCRIPTION

Name of subject	Scientific Field	Center	Department
Chemistry and Physics of Organic Materials (7,5 ECTS credits)	Materials Engineering N 002	Center for Physical Sciences and Technology	Molecular Compounds Physics
Student's workload	Number of credits ECTS	Student's workload	Number of credits ECTS
Lectures		Consultations	1
Individual study	6,5	Seminars	

Course annotation

Organic materials. Structure: bonds, conjugation, aromaticity and heteroaromaticity. Fundamentals of reactivity of organic compounds, synthesis of new structures. Influence of functional groups on photophysical and chemical properties of materials, polarity and intermolecular interactions. Influence of a medium on material properties: solvatochromic effect, influence of pH, concentration effects. Systems of increased regularity. Purity of materials: methods of determination, methods of purification and influence on the photophysical and chemical properties of materials.

Electronic structure of molecules. Electronic structure of organic compounds, variety of energy levels. Atomic and molecular orbitals. Hybridization of orbitals. Electron delocalization. Electronic jumps in organic molecules. The intensity of the jumps. Selection rules. Singlet and triplet excitations of molecules. Optical absorption and luminescence. Excited electronic-vibrational states and their evolution channels. Frank-Condon principle.

Excitation energy transfer. Förster and Dexter energy transfer mechanisms. Energy migration. Damping of excitations. Excitonic interactions between molecules. Molecular dimers and aggregates. Electronic states, absorption and luminescence of dimers. Molecular aggregates. J- and h-aggregates. Excitons.

Electron transfer between organic molecules. Marcus theory. Charge transfer complexes, excimers, exciplexes. Mulliken theory. Intramolecular charge transfer. TICT states.

Electronic events in molecular solids. Excitons in molecular materials. Excitonic states. Exciton motion and relaxation. Charge carriers in molecular materials. Ionized states. Generation and injection of charge carriers. Carrier recombination.

Fundamentals of fluorescence. Basic terminology. Classes of fluorophores: natural and artificial fluorophores, fluorescent proteins. Fluorescence kinetics. Fluorescence anisotropy.

Environmental influence on fluorescence. Solvent effect on fluorescence properties, spectral relaxation influenced by the solvent. Fluorescence quenching.

Fluorescence microscopy. Multiphoton microscopy. Fluorescence lifetime microscopy. Suitable fluorescent markers.

List of literature

1. Pope M., Svenberg C.E. Electronic processes in organic crystals. N.Y.: Oxford Uni. Press, 1999, 1328 p.
2. Foundations of spectroscopy / Simon Duckett, Bruce Gilbert, Oxford : Oxford Univ. Press, 2001. 90 p.
3. Molecular spectroscopy / Jeanne L. McHale, CRC Press, 2017
4. J. R. Lakovicz, Principles of Fluorescence spectroscopy, Springer, 2006
5. Donatas Mickevičius. Cheminės Analizės metodai. Žiburio leidykla, Vilnius.
6. V. Gulbinas. Molekulinių vyksmų fizika: lazerinė spektroskopija. Vilniaus universitetas, 2007, 167 psl.

Subject submission and evaluation			
<p>Doctoral students prepare individually. There are two or three mandatory individual consultations. Oral examination will take place. The final evaluation also depends on the knowledge demonstrated by the doctoral student during consultations.</p>			
Consulting teachers	Scientific degree	Pedagogical name	Main scientific works published in a scientific field in last 5 year period
<p>Viktoras Masevičius (viktoras.masevicius@chf.vu.lt)</p>	<p>Dr.</p>	<p>Prof.</p>	<ol style="list-style-type: none"> 1. Stankevičius V, Gibas P, Masiulionytė B, Gasiulė L, Masevičius V, Klimašauskas S, and Vilkaitis G (2022). Selective chemical tracking of Dnmt1 catalytic activity in live cells. <i>Molecular Cell</i>, 82(5): 1053-1065. doi:10.1016/j.molcel.2022.02.008. Impact Factor: 19.3; Q1. 2. Ličytė J, Kvederavičiūtė K, Rukšėnaitė A, Godliauskaitė E, Gibas P, Tomkutė V, Petraitytė G, Masevičius V, Klimašauskas S, Kriūkienė E (2022). Distribution and regulatory roles of oxidized 5-methylcytosines in DNA and RNA of the basidiomycete fungi <i>Laccaria bicolor</i> and <i>Coprinopsis cinerea</i>. <i>Open Biology</i>, 12(3):210302. doi:10.1098/rsob.210302. Impact Factor: 7.1; Q1. 3. Rakauskaitė R, Urbanavičiūtė G, Simanavičius M, Lasickienė R, Vaitiekaitė A, Petraitytė G, Masevičius V, Žvirblienė A, Klimašauskas S (2020). Photocage-Selective Capture and Light-Controlled Release of Target Proteins. <i>ISCIENCE</i>, 23(12): 101833. doi:10.1016/j.isci.2020.101833. Impact Factor: 6.1; Q1. 4. Petraitytė G, Vaitkevičius V, Özer B, Masevičius V (2019). Synthesis of 5-substituted and 5,6-disubstituted furo[2,3-d]pyrimidines from 2-methylthio-4,6-pyrimidindione and bifunctional electrophiles. <i>Tetrahedron Letters</i>, 60(15): 1019-1021. doi:10.1016/j.tetlet.2019.03.017. Impact Factor: 2.4; Q2. 5. Mickutė M, Nainytė M, Vasiliauskaitė L, Plotnikova A, Masevičius V, Klimašauskas S, and Vilkaitis G (2018). Animal Hen1 2'-O-methyltransferases as tools for 3'-terminal functionalization and labelling of single-stranded RNAs. <i>Nucleic Acids Research</i>, 46(17): e104. doi: 10.1093/nar/gky514. Impact Factor: 19.2; Q1.

<p>Vidmantas Gulbinas, (vidmantas.gulbinas@ftmc.lt)</p>	<p>habil. Dr.</p>	<p>Prof.</p>	<ol style="list-style-type: none"> 1. R. Jasiūnas, H. Zhang, A. Devižis, M. Franckevičius, F. Gao, V. Gulbinas, Thermally Activated Reverse Electron Transfer Limits Carrier Generation Efficiency in PM6:Y6 Non-Fullerene Organic Solar Cells, SOLAR RRL,. 2. L Abdelrazik, V Jašinskas, Ž Podlipskas, R Aleksiejūnas, G Tamulaitis, V. Gulbinas, A. Vyšniauskas, Exciton Transfer Dynamics and Annihilation in Rubidium–Cesium-Alloyed, Quasi-Two-Dimensional Perovskite, Photonics 9 (8), 578, 2022. 3. R Jasiūnas, H Zhang, A Gelžinis, J Chmeliov, M Franckevičius, F Gao, V. Gulbinas, Interplay between charge separation and hole back transfer determines the efficiency of non-fullerene organic solar cells with low energy level offset, Organic Electronics 108, 1066011, 2022 4. A. Fakharuddin, M. Franckevičius, A. Devižis, A. Gelžinis, J. Chmeliov, P. Heremans, V. Gulbinas, Double charge transfer dominates in carrier localization in low bandgap sites of heterogeneous lead halide perovskites, Advanced Functional Materials 31 (15), 2010076, 2021. 5. J. Chmeliov, K. Elkhoully, R. Gegevičius, L. Jonušis, A. Devižis, A. Gelžinis, M. Franckevičius, I. Goldberg, J. Hofkens, P. Heremans, W. Qiu, V. Gulbinas, Ion Motion Determines Multiphase Performance Dynamics of Perovskite LEDs, Advanced Optical Materials 9 (24), 2101560, 2021.
<p>Certified by the Doctoral Committee of Material Engineering (T 008) on 09/02/2023, protocol No. (7.17 E) 15600-KT-39</p>			<p>Committee Chairman prof. habil. dr. Valdas Sirutkaitis</p>