MASTER OF SCIENCES

"ADVANCED SPECTROSCOPY IN CHEMISTRY"

Master Thesis - 30 ECTS credits
Spring 2018 (Semester 4)

Title: *Spectroscopic signatures of dysfunctional endothelium in liver steatosis - a study towards organ-specific mechanisms*

University 1: Jagiellonian University in Krakow
Main Laboratory: Faculty of Chemistry
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University 2 (if any): **Jagiellonian University in Krakow**
Laboratory 2: **Jagiellonian Centre for Experimental Therapeutics**
*Tutor(s) :***Prof. Stefan Chlopicki**
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Topic

Impairment of endothelial function (endothelium - a single layer of cells covering each artery) is a primary cause or a result of many human diseases. Although the mechanisms causing the primary endothelial dysfunction are known (i.e. those leading to the development and progression of atherosclerotic plaque), still there are many diseases in which the secondary endothelial dysfunction occurs, but underlying mechanisms remains unknown. Particularly a dysfunction of liver sinusoidal endothelial cells (LSEC) mediated by alterations in hepatocyte-derived paracrine signals is essential for the development of liver steatosis.

In the presented project we aim to examine the progression of changes of various aspects of endothelial phenotype (structure, function, biochemical profile) in LSECs in the course of the development of liver steatosis in mice model induced with high-fat diet.

Analysis of spectroscopic signatures of biochemical state of the endothelium will be done with the use of vibrational spectroscopy including Raman imaging technique and chemometric analysis.

keywords: Raman spectroscopy, chemometrics, biomedical analysis, liver, cells,

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"ADVANCED SPECTROSCOPY IN CHEMISTRY"

Master Thesis - 30 ECTS credits
Spring 2018 (Semester 4)

Title: *Spectroscopic signatures of dysfunctional endothelium in heart failure - in vitro study*

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Topic

In the project a unique, interdisciplinary panel of methods will be employed to investigate endothelial dysfunction (endothelium - a single layer of cells covering each artery).

Impairment of endothelial function is a primary cause or a result of many human diseases. Although the mechanisms causing the primary endothelial dysfunction are known (i.e. those leading to the development and progression of atherosclerotic plaque), still there are many diseases in which the secondary endothelial dysfunction occurs, but underlying mechanisms remains unknown. E.g. a dysfunction of cardiac microvascular endothelial cells (CMEC) mediated by changes in cardiomyocyte-derived paracrine signals is an important determinant of the development of heart failure.

In the presented project we aim to examine the progression of changes of various aspects of endothelial phenotype in CMECs in the course of the development of heart failure in the genetic mice model Tg¤g*44.

Analysis of spectroscopic signatures of biochemical state of the endothelium will be done with the use of Raman spectroscopy and Raman imaging technique, in the relation to the comprehensive description of the development of these pathologies (fluorescence and various biochemical tests).

keywords: Raman spectroscopy, chemometrics, biomedical analysis, heard tissue, single cells,

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"ADVANCED SPECTROSCOPY IN CHEMISTRY"

Master Thesis - 30 ECTS credits
Spring 2018 (Semester 4)

Title: *Raman Optical Spectroscopy to study self-organisation of biological molecules*

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Topic

Self-organization, including the creation of aggregates and other spatial systems, with a view of the configuration will be studied using the chiraloptical methods such as VCD (vibrational circular dichroism) and complementary method - ROA (Raman optical activity). Self-organization can also change the properties of the electron system in relation to individual units, so the ECD (electronic circular dichroism) measurements are also planned.

Experimental part of the project will be supported by quantum-chemical calculations.

keywords: ROA, VCD, ECD, proteins, DFT, aggregates,

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"ADVANCED SPECTROSCOPY IN CHEMISTRY"

Master Thesis - 30 ECTS credits
Spring 2018 (Semester 4)

Title: Synthesis and photophysical and photochemical characterization of polypyridyl ruthenium complexes for application in photochemotherapy.

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Topic

Student will be involved in synthesis of the selected polypyridyl ruthenium complexes (the general synthetic procedure is known however the purifying process has to be optimized). The purity of the obtained Ru complexes will be confirmed using the following techniques: elementary analysis, MS, HPLC, IR. Student will perform photophysical characterization of these compounds (absorption and emission properties) using steady-state and time-resolved spectroscopic techniques. The photochemical characterization will include determination of reactive oxygen species (ROS) production upon irradiation at various experimental conditions, in particular those resemble physiological environment. One of the important issues will be optimization of experimental procedures for ROS detection using various commercially available dyes.

keywords:ruthenium complexes, photochemistry, synthesis, reactive oxygen spiecies

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"ADVANCED SPECTROSCOPY IN CHEMISTRY"

Master Thesis - 30 ECTS credits
Spring 2018 (Semester 4)

Title: Spectroscopic evaluation of active sites for small molecule transformations

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Topic

The detailed characterization of micro- or mesoporous materials had to provide information not only on their chemical composition, structure and morphology, the main efforts are concentrated on the evaluation of sorption properties and facility to chemically convert molecules to desired products.
It has been recognized that the particular active centers can be differentiated in catalytic reactivity toward substrate molecules thus only one path of the molecule transformation is determined. Comprehensive characterization of the active species, both in qualitative and quantitative aspects, as well as the accessibility studies offer the possibility to modify the structure and properties of catalysts by the generation of the sites of known properties and in required quantity. Information on the catalytic speciation of active centres are believed to be useful in the new catalysts development and in tuning their properties with the regard to the introduction of sites active in the particular process. As the main effort is concentrated for designing of catalysts with clearly defined parameters, such as speciation of the active centres which states the type (qualitative aspect) and quantity (qualitative aspect) of desired active sites the development of the methodology of IR investigations is one of the most demanding tasks for current scientific community. Nevertheless, the IR quantitative studies are still open problem, especially with respect to catalysts (i) hosting transition metal cations of more than one type/nature as well as (ii) of the different level of pore hierarchy. The employment of new probes molecules together with the optimization of the experimental procedure seems to be the most demanding tasks for forthcoming improvements.
Elaboration of the experimental conditions allows for overcoming the main difficulty of IR quantitative studies in which the probe molecule has to react selectively with active species according to perfectly known stoichiometry. The reactive valence and coordination states of controlled dispersion of the TMIs (Co, Cu, Ni, Ag) are attained from IR studies. With the use of IR spectroscopy we have offered fully quantitative tool for discrimination between active TMI sites of various nature. Comparison of the respective forms concentrations with the amounts of TMI derived from chemical analysis becomes useful to obtain information on the dispersion degree of those species. Furthermore, the quantification of TMI sites in zeolites usually is performed with the use of carbon monoxide and nitrogen monoxide molecules, the representative reagents in environmental catalysis. It meets the expectation of using the probes that are molecules of similar chemical properties as the reactants or the reactants themselves. Adaption of the probes of a comparable kinetic diameter, basicity and polarizability as the reactant ones is the critical issue. It ensures full recognition of the interaction between the reactant molecules and the active site as well as further prediction of catalyst performance. Nevertheless, such molecules are rather reactive, the extent of their transformations on the surface of catalysts is problematical to estimate and their use is still one of unresolved problems in IR spectroscopy studies. In many literature reports the reactivity in processes involving hydrocarbons has been used to describe acidic/redox picture. Hydrocarbons cracking reactions are in direct and indisputable relation to Brønsted acidity. The comprehensive studies with the implementation of reagents in quantitative manner are planned to be realized to advance the understanding of the issues involved in the quantitative measurement of molecules transformations.

keywords: IR spectroscopy, probe molecules, material characterization

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"ADVANCED SPECTROSCOPY IN CHEMISTRY"

Master Thesis - 30 ECTS credits
Spring 2018 (Semester 4)

Title: Microscopic and spectroscopic characterizations of conjugated surface-grafted polymer brushes

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Topic

The proposed studies aim at detailed characterizations of novel surface-grafted polymer brushes with conjugated chains such as poly(thiophene), poly(pyrrole). Surface-grafted chains in the brushes due to high grafting density adopt elongated conformations that are crucial for e.g. directional and efficient transport of electrons along the chains. Such newly developed structures may find applications in e.g., ordered organic photovoltaic systems or fabrication of nanosensors.
The molecular structures of the brushes (composition, orientation of the chains, conjugation length, etc.) will be studied using surface spectroscopic techniques including reflection-absorption FTIR and UV/Vis spectroscopies, spectroscopic ellipsometry, and XPS. In addition, such brushes will be investigated using atomic force microscopy working also in spectroscopic current-voltage mode for characterization of conductive properties of the chains on nanoscale.

Information about the research group: http://www2.chemia.uj.edu.pl/nfpm/

keywords: polymer brushes, surface-sensitive spectroscopies, conjugated polymers

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"ADVANCED SPECTROSCOPY IN CHEMISTRY"

Master Thesis - 30 ECTS credits
Spring 2018 (Semester 4)

Title: Crystal engineering of new hybrid polyoxomolybdates - materials for new technologies and catalysis

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Topic

In the study, we plan synthesis and comprehensive study of the new hybrids polyoxomolybdates. The resulting compounds will consist of large inorganic polyoxomolybdate cores to which organic groups will be attached, changing physical and chemical properties of the obtained materials. Using multifunctional organic linkers we hope to obtain a number of new hybrid materials creating: isolated clusters (0-d), polymeric (1-d), layered (2-d) or 3-dimention structures. Dimensionality of polyoxomolybdate cores, and used organic linkers, will in our opinion, determine the crystallite morphology, physical, optical and catalytic properties.
The main research methods include chemical synthesis, powder diffraction, X-ray crystallography, spectroscopic studies. If necessary, also catalytic and computing studies will be performed in collaboration with other scientific groups.

Information about the research group: http://www2.chemia.uj.edu.pl/~lasocha/EN/

keywords: powder diffraction, hybrid organic-inorganic materials