List of doctoral projects available for the academic year 2024/2025

INTiBS PAN
WROCŁAW

Wrocław 29.05.2024

Chemistry/Physics

Supervisor: Dariusz Kaczorowski, prof. (d.kaczorowski@intibs.pl)
Auxiliary Supervisor: Grzegorz Chajewski, dr.

Subject: ***Unconventional superconductivity and magnetic ordering in Ce-Pd-In and Ce-Pt-In dense Kondo systems.***

Discipline: Physical sciences

Description: Since the spectacular discovery of the phenomenon in 1979, advanced experimental and theoretical studies on heavy-fermion superconductivity have continued to be at the very forefront of modern condensed matter physics. This is due to the special character of the superconducting state, which cannot be described in terms of the conventional theory of superconductivity, as well as due to a variety of unusual physical behavior observed in the normal state. The microscopic nature of all these anomalous phenomena originates from strong electronic correlations in metallic systems bearing localized magnetic moments. In recent years, significant progress has been made in understanding the fundamental mechanisms responsible for the simultaneous presence of magnetism and superconductivity (by a number of decades considered as entirely antagonistic). In consequence, the scenarios of competition, coexistence or sometimes even interplay of the two cooperative phenomena have been recognized. Nevertheless, a consistent universal theory of the heavy-fermion superconductivity that might account for all its intriguing aspects is still lacking. Furthermore, new experimental discoveries in the field often result in identification of novel scientific challenges.

The ternary Ce-Pd-In and Ce-Pt-In systems comprise several phases crystallizing with diverse crystal structures, including a few prototype ones. Some of them have been found to exhibit the coexistence of superconductivity and magnetic ordering. Amidst those materials, especially interesting are dense Kondo compounds with multiple Ce atoms sites in their crystallographic unit cells.

In this doctoral work, we intend to investigate comprehensively a few representatives of this unique family of Ce-based heavy-fermion superconductors. The research will be carried out on high-quality single-crystalline specimens in wide ranges of temperature, magnetic field and hydrostatic pressure, employing a variety of modern bulk and local-probe research techniques. We expect that successful accomplishment of this PhD project will significantly contribute to the general understanding of the emergence of magnetism and superconductivity in strongly correlated electron systems.

Supervisor: Jan Janczak, prof. (j.janczak@intibs.pl)

Subject: ***Stereochemistry and properties of metallophthalocyanine derivatives.***

Discipline: Chemical sciences

Description: Metal (II) phthalocyanines (for example MgPc, ZnPc, MnPc, FePc, CoPc), although they have been known for several decades, are still of great interest due to their various applications. The properties of metallophthalocyanines of the transition metals, as representatives of the metallophthalocyanine family with the metal at +2 oxidation state, differ significantly from magnesium and zinc phthalocyanine (Mg, d^0, Zn, d^{10}) due to the electronic structure of the central ion (Mn^{2+} (Ar)$3d^5$; Fe^{2+}, (Ar)$3d^6$, Co^{2+}, (Ar)$3d^7$). Therefore, the aim of the work will be to obtain and characterize new complexes of metal phthalocyanines with additional axially coordinating N and O-donor ligands in the crystalline form as well as perform their structural analysis. In addition, the physicochemical characterization of the obtained metallophthalocyanines especially in the therapeutic window should be performed. Moreover, DFT calculations of the geometry of the obtained derivatives and TD-DFT calculations as well as correlation with the experimental UV-Vis spectra should be performed.

Supervisor: Mirosław Mączka, prof. (m.maczka@intibs.pl)

Subject: ***Synthesis, lattice dynamics and tunable ferroelectric and optical properties of multilayered hybrid perovskites.***

Discipline: Chemical sciences

Description: Organic-inorganic hybrids have been the subject of intense studies in recent years due to their functional properties. One of the most important group of hybrid perovskites constitute lead halides since these compounds are attractive photovoltaic materials. These compounds are also promising materials for optical applications (for instance light-emitting diodes, LEDs). In recent years there is growing interest in synthesis of perovskite structures built up from two- or trilayered slabs separated by sheets composed of organic cations. These compounds have advantages of both three-dimensional (for instance good photovoltaic performance) and two-dimensional perovskites (efficient emission and good chemical stability, especially to moisture). The aim of PhD student will be synthesis and single-crystal growth of novel multilayered hybrid perovskites exhibiting linear (efficient photoluminescence) and nonlinear optical properties (second harmonic generation, efficient two-photon absorption) as well as ferroelectric and switchable dielectric properties. These obtained compounds will be studied using infrared, Raman and optical spectroscopes. Additional x-ray diffraction, dielectric, and nonlinear optical studies will be performed in cooperation with other research groups from our Institute as well as from Wrocław University of Technology.

Additional information: The doctorate will be implemented as part of a project led by prof. Mirosław Mączka: " Synthesis, lattice dynamics and tunable ferroelectric and optical properties of multilayered hybrid perovskites ", NCN OPUS 25 grant no. 2023/49/B/ST5/00119) at the Division of Optical Spectroscopy (INTiBS PAN) in Wrocław.

Supervisor: Łukasz Marciniak, prof. (l.marciniak@intibs.pl)

Subject: ***Optical manometry based on the luminescence kinetics of Mn^{4+} ions.***

Discipline: Chemical sciences

Description: The aim of the work will be to create a library of luminescent materials that can be used in lifetime-based thermometry and to build a semi-empirical model enabling predefined design of thermometers with precisely defined sensory properties, taking into account relative sensitivity, operating temperature range and absolute sensitivity. As part of this PhD thesis, work will be carried out to determine the impact of the crystal field strength on the thermal depopulation of the 2E level of Mn^{4+} ions. The electronic configuration of these ions ($3d^3$) is the reason for the extraordinary sensitivity of their spectroscopic properties to changes in the crystal field intensity caused by changes in the stoichiometry of the material. Such modifications enable to change the spin-orbit coupling between levels 2E and 4T2, influencing the depopulation kinetics of level 2E. Hence thermometric performance of this kind of sensors can be very smoothly modify by optimizing the composition of the host material. The PhD student will be responsible for both the synthesis of luminescent materials and the characterization of their luminescent properties. Based on the results obtained, the thermometric parameters of the analyzed systems will be determined via the machine learning module.

Additional information: The doctorate will be implemented as part of a project (NCN OPUS) led by prof. Łukasz Marciniak at the Division of Biomedical Physico-Chemistry (INTiBS PAN) in Wrocław.

Supervisor: Łukasz Marciniak, prof. (l.marciniak@intibs.pl)
Auxiliary Supervisor: Karolina Elżbieciak-Piecka, dr.

Subject: ***Novel materials based on lignin from biomass with enhanced luminescent activity.***

Discipline: Chemical sciences

Description: Nowadays, phosphors are ubiquitous in our daily lives from the lighting industry to remote temperature sensors and biological markers. Therefore, the possibility of producing low-cost, biocompatible, environmentally friendly phosphors from biomass is particularly important from an economic and environmental perspective. The goal of this project is to develop a method for producing high-intensity carbon luminescent dots from lignin. The proposed solution will enable the development of efficient and low-cost luminophores with controlled emission properties. The application potential of the produced materials will be verified for their use in the production of remote temperature and pressure sensors.

Additional information: The doctorate will be implemented as part of a project (NCN OPUS) led by prof. Łukasz Marciniak at the Division of Biomedical Physico-Chemistry (INTiBS PAN) in Wrocław.

Supervisor: Leszek Kępiński, prof. (l.kepinski@intibs.pl)
Auxiliary Supervisor: Karolina Ledwa, dr.

Subject: ***Nanostructured catalysts for CO_2 thermochemical valorization.***

Discipline: Chemical sciences

Description: Global warming due to anthropogenic greenhouse gas emissions is our generation's greatest challenge. Carbon dioxide, which is by far the most significant contributor to global warming, is currently considered a promising prospective for potential applications as a raw material for the production of fine chemicals, like hydrocarbons, alcohols, ethers, etc.
The proposed thesis aims to develop well-defined, highly active nanostructured heterogeneous catalysts dedicated to CO_2 hydrogenation into more valuable chemicals. The catalysts will be composed of a high surface area support with well-defined 3D geometry (e.g., amorphous mesoporous support with uniform ordered pores, various types of 3D hierarchical flower-like supports, etc.) as well as optimized chemical composition and structure, and nanosized active phase with uniform particle size distribution (cheap transition metals in mono- or bimetallic configurations). Obtained systems will be characterized using a wide range of experimental methods (electron microscopy, X-ray diffraction, NMR, FTIR, Raman spectroscopy, XPS, gas adsorption, etc.) to find how the catalyst structure, chemical architecture, and geometry influence their chemical properties. Then, the catalytic activity and selectivity of the catalysts will be checked in the appropriate CO_2 hydrogenation process, depending on the chosen active phase activity. An essential step to elucidate the catalysts' behavior at reaction conditions will be in situ investigations (e.g., in situ TEM and in situ DRIFTS), which are planned to be performed in collaboration with other institutions.

Supervisor: Leszek Kępiński, prof. (l.kepinski@intibs.pl)
Auxiliary Supervisor: Rafael de Lima Oliveira, dr.

Subject: ***Metal nanoparticles confined in doped porous carbonaceous materials and their application in catalysis.***

Discipline: Chemical sciences

Description: Hydrogenation and oxidation of organic compounds are essential reactions in the chemical industry. Traditionally, these reactions are conducted by stoichiometric amounts (or excess) of toxic reagents such as sodium borohydride as a reduction agent or potassium permanganate as an oxidizing agent, resulting in processes with low selectivity and the generation of much waste. Thus, these traditional processes are environmentally and economically unsuitable. Supported catalysts emerged as an alternative for producing valuable chemicals more sustainably. The project's primary goal is to develop a new class of doped porous carbonaceous materials synthesized using diverse techniques, such as the hard template method or the post-activation of carbons. Waste materials such as glycerol (a by-product of biodiesel synthesis) will be used as a carbon precursor. Metal nanoparticles (NPS) will be deposited in the structure of the carbon materials, aiming for a strong interaction between the metal NPS and the carbon materials, creating a synergy between them. The materials will be characterized using various techniques such as electron microscopy (TEM and SEM), N_2 physisorption, XRD, XPS, and XAS. The prepared metal/carbon materials will be tested as catalysts for the oxidation reactions (such as selective oxidation of alcohols and alkenes), hydrogenation reactions (CO_2 or biomass compounds), and hydrogen transfer reactions.

Supervisor: Adam Pikul, prof. (a.pikul@intibs.pl)
Auxiliary Supervisor: Grzegorz Chajewski, dr. or Orest Pavlosiuk, dr.

Subject: ***Unconventional Superconductivity, Complex Magnetism and Nontrivial Topology in van der Waals U-Te systems.***

Discipline: Physical/Chemical sciences

Description: The objective of this dissertation is to identify and elucidate the distinctive physical properties of several uranium tellurides. These compounds are derivatives of uranium telluride, a recently discovered unconventional superconductor. In contrast, they possess a layered structure and are van der Waals materials, which have also been the subject of condensed matter physics due to the potential for exotic magnetic states, superconductivity, and the formation of so-called topologically nontrivial states. The discovery of the latter was awarded the 2016 Nobel Prize in Physics, which has made van der Waals materials an attractive object of research due to their potential applications in electronics, particularly in quantum computers.

The research methodology will entail the synthesis and characterization of high-quality uranium telluride monocrystals, their exfoliation (similar to that used to obtain graphene), and a comprehensive study of their physical properties under extreme conditions (i.e., low temperatures, strong magnetic fields, and high pressure). The dissertation will be carried out in collaboration between two leading research centers in Poland (in Wroclaw and Krakow) and two analogous centers in the Czech Republic (in Prague and Ostrava). Each country will have one experimental and theoretical group.

Additional information: No medical contraindications to work with radioactive isotopes.

Supervisor: Adam Pikul, prof. (a.pikul@intibs.pl)
Auxiliary Supervisor: Grzegorz Chajewski, dr. or Orest Pavlosiuk, dr. or Maria Szlawska, dr.

Subject: ***Thermal expansion and magnetostriction of uranium intermetallic compounds a potential advanced next-generation nuclear fuel.***

Discipline: Physical/Chemical sciences

Description: Construction of nuclear reactors based on advanced nuclear fuels is one of the conditions for effective decarbonization of the world energy industry. The most commonly used fuel in modern nuclear power plants is semi-conducting uranium dioxide, which (although relatively cheap and easy to produce) is not free from defects and limitations in its use. Problems include swelling and cracking of fuel rods and their low thermal conductivity which is a consequence not only of the burning of uranium dioxide but also of its physical and chemical properties. Therefore, a new generation of nuclear fuels referred to as ATF (accident tolerant fuel) is being searched for i.a. among uranium intermetallic compounds. The proposed PhD thesis will support this search at the level of basic research. Its aim will be to synthesize and study physical properties of selected uranium intermetallic compounds and to attempt to relate these properties to magnetism of the 5f electrons of uranium. The research will consist of growing monocrystals of several carefully selected compounds and their physical characterization mainly through thermal expansion and magnetostriction measurements. Part of the experiments will be carried out in France and the USA (as part of an ongoing collaboration of the supervisor), and the results obtained will be published in specialized journals and presented at international scientific conferences.

Additional information: The condition of admission to work with radioactive isotopes is positive qualification by a doctor of occupational medicine (medical examinations will be conducted at the expense of INTiBS PAN).

Supervisor: Jacek Ćwik, D.Sc. (dr. hab.) (j.cwik@intibs.pl)

Subject ***The influence of modifying composition on the structural, magnetic and magnetocaloric properties of $Dy(Ni_{1-x}Al_x)_2$ and $Tb(Ni_{1-x}Al_x)_2$ solid solutions.***

Discipline: Physical sciences

Description: Hydrogen is rapidly becoming a preferred type of fuel, however, its liquefaction using today's vapor-compression technology is energy consuming and expensive. Magnetic cooling based on the magnetocaloric effect (MCE) is an energy-efficient and environmentally friendly alternative, but improvements in refrigerants are crucial for its success. This method can be implemented across a broad temperature range, from ultra-low to a few hundred Kelvin temperatures. The ideal magnetic refrigerant exhibits consistent magnetocaloric properties across system's operating temperature range. The proposed dissertation will include medium- and high-magnetic field studies, intermetallic lanthanide compounds with Laves phase structure, i.e. $R(Ni_{1-x}Al_x)_2$ (where R - selected lanthanides and $0.0 \leq x \leq 1.0$) aimed at proposing a multilayer magnetocaloric material for cryogenic applications. The selected starting compounds that are the basis for the proposed solid solutions exhibit second-order magnetic phase transitions and are characterized by large reversible magnetocaloric effect values in the cryogenic temperature range due to special properties associated with high localized magnetic moments originating from the incompletely filled 4f-electron shell of rare earth atoms, while selected Ni and Al atoms in these compounds remain in a non-magnetic state. A magnetic material in multilayer form, which will include individual solid solutions, will allow to obtain a material with unchanged high enough MCE values over a wide temperature range.

Supervisor: Artur Bednarkiewicz, prof. (a.bednarkiewicz@intibs.pl)
Auxiliary Supervisor: Aleksandra Pilch-Wróbel, dr.

Subject: ***Investigation of the influence of composition, size, and chemical architecture of Tb- and Eu-doped nanoluminophores on the efficiency of energy transfer to an organic acceptor.***

Discipline: Physical sciences

Description: Due to the long excited-state lifetimes, Tb^{3+} and Eu^{3+} ions have been investigated in the form of chelates and complexes for use in time-resolved, sensitive biodetection and bioimaging. The goal of this work is to develop, model, and characterize the spectral and time-resolved properties of new luminescent inorganic colloidal nanocrystals doped with Tb^{3+}, Eu^{3+}, or both Tb^{3+} and Eu^{3+}. The impact of concentration and chemical architecture on energy transfer efficiency (such as Förster resonance energy transfer, FRET) to organic acceptors on the surface will be verified. Additionally, a time-resolved measurement method using a sensitive camera and microscope will be developed.

Supervisor: Rafał Wiglusz, prof. (r.wiglusz@intibs.pl)

Subject: ***Design, preparation, and investigation of hydrogel materials intended for tissue engineering.***

Discipline: Chemical sciences

Description: The main aim of the PhD thesis is to design and develop an intelligent biocomposite based on three-dimensional (3D) hydrogels (e.g. poly(ethylene glycol) (PEG or PEO), poly(propylene oxide) (PPO) and aliphatic polyesters, such as poly(glycolide) (PGA), as well as polysaccharides – e.g. cellulose derivatives) and their biocomposites as a specific scaffold for nanosized phosphates doped with metal ions (e.g. lithium (I) ions) dispersed inside it.
The obtained biocomposites will be used in further stages of the PhD thesis to evaluate regenerative and proliferative properties of nerve cells such as olfactory cells. In addition, the work will undertake the task of reconstructing the damaged neuronal pathway. The work will focus on obtaining nanosized phosphates doped with various ions, e.g., lithium(I), dispersed in a hydrogel carrier and evaluating its effect on olfactory cells to stimulate limited nerve regenerative properties and neuronal growth and consequently restore the sense of smell.

Supervisor: Rafał Wiglusz, prof. (r.wiglusz@intibs.pl)

Subject: ***Nanosized mixed fluorite-structured optically active compounds as potential materials for thermal imaging and pressure sensors.***

Discipline: Physical/Chemical sciences

Description: The main aim of the PhD thesis is to synthesize fluoride nanosized compounds mixed systems with the chemical formula $X_{1-x}Z_xF_2$ (where X, Z = Ca^{2+}, Sr^{2+} ions) doped and co-doped with lanthanide ions in the form of nanosized materials and ceramics. The structural and luminescence properties of the obtained materials will be compared to each other depending on the desired application. Potential applications of nanomaterials as thermal agents and nanosized ceramics for pressure sensing will be studied.

The most crucial aspect of the PhD thesis is to investigate how the composition and synthesis method of $X_{1-x}Z_xF_2$ mixed systems doped and co-doped with rare earth ions influence the clustering phenomenon. It is well known that clusters of rare earth ions are created in fluorite-type materials and greatly impact their physicochemical properties.

For the evaluation of the crystal structure and morphology of obtained materials, the X-ray powder diffraction and electron microscopy, both SEM (Scanning Electron Microscopy) and TEM (Transmission Electron Microscopy) techniques will be used. Additionally, an EDX (Energy-Dispersive X-ray spectroscopy) measurement will be performed to get the exact data on phase composition. Detailed structural properties will be obtained by FT-IR (Fourier-Transform Infra-Red) and Raman spectroscopy. Both techniques will give information about the type and energy of vibrations in obtained materials.

The spectroscopic characterization will involve such measurements as absorption spectra in the UV-VIS-NIR region, emission and excitation spectra in the UV-VIS-NIR region measured at 77 and 300 K, the kinetics of luminescence measured with different excitation and at 77 and 300 K.

Fabrication of nanoceramics will be performed using the low-temperature, high-pressure (LTHP) sintering technique. Before sintering, pellets will be formed from the powder and coldly pressed in a cylindrical cell under a pressure of 0.8 GPa. Pellets of a diameter of 4 mm and height of about 2 mm will be prepared in this way.

Supervisor: Włodzimierz Miśta, D.Sc. (dr. hab.) (w.mista@intibs.pl)

Subject: ***Synthesis, characterization and catalytic activity of graphitic carbon nitride (g-C_3N_4) - based hybrid nanomaterials doped with metals.***

Discipline: Chemical Sciences

Description: The work will concern methods of preparation of hybrid materials based on g-C_3N_4/nanocarbon components (GR, CNT) doped with metals. The synthesis of carbon nitride involves the thermal condensation of organic precursors, such as melamine, urea, dicyanodiamide. For high surface area materials hard (silica: SBA-15) and soft templates (P-123, Triton X-100) will be used. Due to its physical properties, it is a suitable carrier for active phases (e.g. metals). Due to the fact that it is a semiconductor with a small bandgap (2.7 eV), it can catalyze several environmentally important photodegradation reactions of organic pollutants, as well as to produce hydrogen in the photoreduction reaction of water splitting with the participation of sunlight.
The obtained materials will be characterized using the following methods: XRD, SEM-EDX, HRTEM, thermal analysis (TG), nitrogen adsorption (77 K), thermoprogrammed methods (TPR-H2, TPO-MS, TPD-MS), Raman spectroscopy, IR, UV-VIS, luminescence and testing of catalytic activity (CO oxidation, photocatalytic water decomposition).

Supervisor: Włodzimierz Miśta, D.Sc. (dr. hab.) (w.mista@intibs.pl)

Subject: ***Synthesis, characterization and catalytic activity of metal-organic framework HKUST-1 with encapsulated selected noble metals.***

Discipline: Chemical sciences

Description: This thesis focuses on developing a hydro/solvothermal method and/or microwave-assisted synthesis for the rapid synthesis of good quality copper benzene-1,3,5-tricarboxylate (Cu-BTC also referred to as HKUST-1) with high yield under mild preparation conditions. Different synthesis conditions and activation methods were studied to understand their influence on the properties of HKUST-1. An additional attempt will be made to in situ synthesis/ immobilization of HKUST-1 in macro-/mesoporous silica/nickel monoliths for continuous flow catalysis with low-pressure drop.
As synthesized MOF will be activated by encapsulation of selected noble metals (Au, Pt, Pd, …). Interactions between metal nanoparticles (NPs) and metal–organic frameworks (MOFs) in their composite forms have proven to exhibit beneficial properties, such as enhanced catalytic performance through synergistic effects. As prepared hybrid MOF materials will be characterized by: XRD , SEM–EDS, HRTEM, thermal analysis (TG), N_2 (77 K) physisorption analysis, CO_2 and H_2 volumetric adsorption, termoprogrammed reaction (TPR-H2, TPD-MS, TPO), Raman, IR spectroscopy and by catalytic activity (CO oxidation).

Supervisor: Edyta Piskorska-Hommel D.Sc. (dr. hab.) (e.piskorska@intibs.pl)
Auxiliary Supervisor: Dominika Majchrzak, dr., Sieć Badawcza Łukasiewicz – PORT Polski Ośrodek Rozwoju Technologii

Subject: ***Chemical surface modification of group-III nitrides for sensitivity improvement of open gate sensors.***

Discipline: Physical/Chemical sciences

Description: Nitrides are polar materials with large internal piezoelectric fields, making them ideal for open-gate sensors. These sensors are poised to play a crucial role in various applications, from environmental monitoring to medical diagnostics. For example, AlGaN/GaN HEMT-based biosensors and pH sensors have been employed in food analysis, medical diagnosis, and chemical research laboratories. The use of HEMT as a biosensor has also been demonstrated for detecting c-erbB-2 protein, as well as glucose, MIG, C-erbB-2, KIM-1, and PSA, and in the development of ion sensors.
Chemical surface modification of GaN is a powerful technique for enhancing the functionality of open-gate sensors. By tailoring the surface properties, sensors can achieve higher sensitivity, selectivity, and stability. The choice of modification method and functionalization agents depends on the specific application and the target analytes to be detected.
The aim of the PhD work is to prepare group-III nitride compounds using epitaxial methods such as Metal Organic Vapour Phase (MOVPE) and Molecular Beam Epitaxy (MBE), choose an appropriate chemical surface modification method, surface chemical and electronic analysis using X-ray Photoemission Spectroscopy (XPS), surface morphology analysis using Atomic Force (AFM) and Scanning Electron Microscopy (SEM), and structural study using X-ray Diffraction (XRD) and synchrotron radiation -based technique X-ray absorption Spectroscopy.

Supervisor: Małgorzata Małecka, D.Sc. (dr. hab.) (m.malecka@intibs.pl)

Subject: ***Self-regeneration in highly dispersed $Ce_{1-x}M_xO_{2-y}$ (M - transition metal) nanoparticles anchored in porous oxide materials.***

Discipline: Chemical sciences

Description: The main research goal of the project is to design active oxidation catalyst with a hierarchical 3D structure based on modified CeO_2. Porous oxide materials, including mesoporous silica (MCM-41, SBA-15 and others), are extremely interesting carriers of a highly dispersed active phase. However, active particles such as pure and doped cerium oxides have excellent reversible reduction-oxidation capabilities of cerium ions and oxygen transport in the ceria lattice. The combination of these advantages may lead to the development of highly active catalysts. The possibility of self-regeneration of the active phase gives hope for the creation of a so-called "intelligent catalyst" with the desired properties.
Work in the laboratory will be carried out on the basis of wet chemistry methods. The samples prepared in this way will be characterized by the following techniques: TEM, SEM, EDX, XRD, IR, RAMAN, N_2 adsorption-desorption, TG, catalytic oxidation tests. The candidate is expected to be involved in laboratory work and to expand his knowledge.

Supervisor: Piotr Solarz, D.Sc (dr. hab.) (p.solarz@intibs.pl)

Subject: ***Synthesis and explanation of energy transfer in Pr-Ce systems.***

Discipline: Physical/Chemical sciences

Description: The aim of this work is to explain the energy transfer processes in Pr-Ce systems. Knowledge of these phenomena was initially documented in the 1970s. However, it is not clear to this day.
What is known is that in the presence of cerium ions, praseodymium ions do not show emission from 3P0 levels. All emissions come from the 1D2 level of praseodymium.
This is not a trivial problem and a PhD student is expected to have basic mathematical analysis skills. It is expected that the doctorate will result in the publication of about 7 works, which will open up his further career. In the first period, the doctoral student will be able to choose about 3 inorganic compounds on which he will be able to conduct his research. The works are expected to be published in the best journals.

Supervisor: Marek Drozd, prof. (m.drozd@intibs.pl)
Auxiliary Supervisor: Vasyl Kinzhybalo, dr.

Subject: ***Investigation of the Spectroscopic Properties of Guanidine Complexes as Functional Hybrid Materials.***

Discipline: Chemical sciences

Description: Hybrid organic-inorganic guanidine compounds are studied and obtained mainly as new molecular complexes with strictly defined properties. Among this group of compounds, ferroic materials exhibiting phase transitions and being generators of the second harmonic are being searched for. The first stage of the work will be the synthesis of completely new molecular complexes containing the guanidine cation, in which the main interactions are hydrogen bonds of different strengths and geometry. For the newly obtained complexes, the structure will be determined using diffraction methods (X-ray). The main method used for property measurements will be vibrational spectroscopy with particular emphasis on infrared spectroscopy and Raman spectroscopy. The combination of the results of X-ray methods and vibrational spectroscopy will allow to select potential second harmonic generators (complexes without a macroscopic center of symmetry) from the group of studied compounds. These materials are widely used in laser technology as well as optoelectronics in the broadest sense. For all obtained materials, tests will be carried out using differential scanning calorimetry. These studies will determine the occurrence of possible phase transitions. On their basis, it will be possible to initially select materials with ferroic properties, i.e. ferroelectrics or ferroelastics. Experimental research will be supplemented by quantum-mechanical calculations concerning equilibrium structures, theoretical vibrational spectra as well as first- and second-order hyperpolarizability.