WROCŁAW DOCTORAL SCHOOL OF INSTITUTES
OF POLISH ACADEMY OF SCIENCES

List of doctoral projects available for the academic year 2021/2022

INTiBS PAN
WROCŁAW

Wrocław 2021

Chemistry/Physics

Supervisor: Przemysław Dereń, prof. (p.deren@intibs.pl)
Auxiliary Supervisor: Natalia Miniajluk-Gaweł, dr

Subject: ***Study of the spectroscopic properties of solid solutions of double perovskites Ba2MgWO6 and La2MgTiO6 doped with selected lanthanide ions.***
Discipline: Chemistry

Description: The objective of the thesis is to obtain phosphors based on solid solutions of Ba2MgWO6 and La2MgTiO6 with a regular structure of a double perovskite doped with selected lanthanide ions and to study their spectroscopic properties.
Materials whose optical properties are not known until now will be studied. The regular structure of such a matrix can make it possible to obtain transparent or translucent ceramics and therefore new photonic materials.
The samples will be synthesized using a mechanochemical method supported by high-temperature annealing. After their receipt and verification of phase purity, electronic spectroscopy, IR, and Raman measurements will be performed.
We are expecting skilled chemists, experience in synthesizing polycrystalline materials applying different methods will be an advantage. A Ph.D. student should have a basic knowledge and skills to perform structural and spectroscopic measurements and to analyze the obtained research results.

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

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

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, d0, Zn, d10) due to the electronic structure of the central ion (Mn2+ (Ar)3d5; Fe2+, (Ar)3d6, Co2+, (Ar)3d7). 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 metallophthalocyanine derivatives 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: 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: Chemistry

Description: This thesis focuses on the development of a hydro/solvothermal method and or microwave-assisted synthesis for the rapid synthesis of good quality copper benzene-1,3,5-tricarboxylate (Cu-BTC referred also 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. Additional attempt will be made to in situ synthesis/immobilization of HKUST-1 in macro-/mesoporous silica/nikel 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), N2 (77K) physisorption analysis, CO2 and H2 volumetric adsorption, termoprogrammed reaction (TPR-H2, TPD-MS, TPO), Raman, IR spectroscopy and by catalytic activity (CO oxidation).

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

Subject: ***Synthesis, characterization and catalytic activity of selected perovskites ($LaMO_3$; M= Mn,Co, Fe…) doped with noble metals.***
Discipline: Chemistry

Description: This thesis focuses on the preparation, characterization of perovskite materials ($LaMO_3$; M=Mn, Co, Fe…). The following preparation methods will be use:
sol-gel citrate methods, solvothermal methods / microvawe assisted, nanocasting technique using mesoporous SBA-15 silica materials as a template. The perovskite structures ABO_3 can incorporate ions of various size and charge showing great flexibility of composition. Moreover, substitutions of ions into the A- and/or B-sites forming $A_{1-x}A'_xB_{1-y}B'_yO_3$ or deviation from ideal stoichiometry resulted in altering the electronic properties and also catalytic activity of the perovskites. Therefore the effect of substitution of additional different metal cations (Ce^{+4}, Ca^{+2}, …) in A and/or B sites of perovskite cell on catalytic activity will be investigated. Therefore the incorporation of selected noble metals into perovskite lattice will be studied. Exposing the catalyst to oxidizing and reducing atmosphere resulted in the recovery of the high dispersion state of noble metal dispersion state of incorporated metal and the excellent stability of the perovskite structure.
As prepared perovskite samples will be characterized by: XRD, SEM–EDS, HRTEM, thermal analysis (TG), N_2 (77K) physisorption analysis, termoprogrammed reaction (TPR-H_2, O_2-TPD-MS, TPO), Raman and FTIR spectroscopy and catalytic activity for CO, VOC, and soot oxidation.

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

Subject: ***Investigation of luminescence and non-radiative energy transfer between lanthanides in double-doped systems.***
Discipline: Chemistry/Physics

Description: The aim of the project is to synthesize and determine the efficiency of energy transfer between sensitizer ions and donor ions in new phosphors.
It is postulated that selected pairs of lanthanides may, by synergy effect, constitute a new type of phosphors with properties distinct from singly doped systems. Particular attention will be given to systems emitting in the red spectrum. The red range is especially important for indoor lighting. Its deficit in the currently used LED sources contributes to a number of diseases such as: cardiological problems, sleep problems, depression, endocrine disorders.
After synthesizing a selected fluoride or oxide system, doped with lanthanide ions, e.g. with Ce + Pr or Tb + Eu pairs, the research will focus on determining the areas of optical pumping and its efficiency depending on the concentration of impurities. The energy transfer rates, luminescence efficiency, its spectral area and mechanisms of interaction will be determined. The obtained material will be subjected to structural and morphological analysis. Spectroscopic measurements will consist in determining the areas of optical pumping (absorption and excitation spectra), determining the lifetime of impurities (activator and acceptor) and detailed luminescence analysis. Time resolving femtosecond spectroscopy using a streak camera will play a special role.

Supervisor: Wiesław Stręk, prof. (w.strek@intibs.pl)
Auxiliary Supervisor: Paweł Głuchowski, dr.

Subject: ***Synthesis of the graphene structures for the photocatalytic conversion of CO2 into methanol in an aquatic environment.***
Discipline: Chemistry

Description: The work will be focused on the technology that allow to storage CO2 by dissolving it in the subcritical water and then thanks to graphene catalyst converting the gas into methanol that could be reused in the CO2 generating unit. The first step will be to increase efficiency of the photocatalysis, what is possible by using graphene structure as a catalyst. Graphene have high surface area and under UV or IR radiation may generate free electrons on the surface that accelerate photocatalysis process. New type of the pure and intercalated with metal particles graphene structures will be developed. Then it will be developed technology where gas dissolution and its processing will operate in one continuous technological process. The biggest challenge of this work will be the increase of CO2 solubility in water, and effective methanol recovery during the photocatalysis process. The preliminary results has shown that it is possible to increase the solubility of CO2 in water due to its earlier interaction with the plasma. Increasing CO2 solubility in water and acceleration conversion process using graphene structures will increase efficiency of the process what thanks to which the process will become profitable also for industry and will allow effective removal of harmful gases in industrial processes. The work allow to possess the knowledge and practical experience in large-scale CO2 storage and processing.

Supervisor: Wiesław Stręk, prof. (w.strek@intibs.pl)
Auxiliary Supervisor: Paweł Głuchowski, dr.

Subject: ***Synthesis of oxide materials stabilized with alkali ions with high ionic conductivity for use as solid electrolytes.***
Discipline: Chemistry

Description: The aim of the work is to develop new oxide materials stabilized with alkali ions (Li, Na) showing high ionic conductivity (σ≥ 10-3 S / cm) and low electronic conductivity (<10-9 S / cm). During the work synthesis methods of the materials with the structure of spinels, perovskites and fluorites will be developed. The syntheses will be carried out using wet chemistry, sol-gel, precipitation and combustion methods. The stoichiometry of the compounds will be optimized so that they show high chemical, temperature and electrical stability. The powders made by various techniques will be sintered into ceramics using high pressure and low temperature technology. This method allows to keep the small size of the crystallites during the whole sintering process and the high density of ceramics also at low sintering temperatures (below 800 °C). The physical properties of the ceramics will be controlled through experimental selection of pressure, time and sintering temperature. Ceramics will be characterized structurally, morphologically and by impedance spectroscopy. For materials showing the best physical properties, electrochemical tests will be carried out in cooperation with foreign partners to determine the application potential of the developed materials.

Supervisor: Tomasz Cichorek, prof. (t.cichorek@intibs.pl)

Subject: ***Determining the gap symmetry of chiral superconductors: A lower critical field study using Hall micromagnetometry.***
Discipline: Physics

Description: Chiral superconductivity is a striking quantum phenomenon in which an unconventional superconductor spontaneously brakes time reversal symmetry and lowers its free energy by eliminating nodes in the gap. Chiral superconductivity is a type of topological state. The odd-parity chiral state provides a natural platform for realizing Majorana edge modes, which are central to several proposals for topological quantum computation. However, despite intensive theoretical study and huge experimental efforts, no material has been proven definitively to be a chiral superconductor.
The main task of a Ph.D. thesis is intended to find experimental evidence for the emergence of the spin-triplet pair state with odd-parity energy gap in candidate chiral superconductors via a detailed investigation of the temperature dependence of the lower critical field Hc1(T) - one of the basic properties of a superconductor. We plan to measure a local magnetization of various unconventional superconductors using a Hall micromagnetomery down to temperatures as low as 10 mK. We expect to observe unusual Hc1(T) characteristics, including an unsaturated behaviour in the limit T = 0. Such experimental findings supported by a numerical analysis should narrow down the possible descriptions of the electron-pair wave function. So far, triplet pairing is rare in nature and has not been unambiguously identified in any bulk compound.
Investigations of an emergence of chiral superconductivity will be conducted in collaboration with École Polytechnique, France and performed among others on newly discovered superconductors UTe2 and 4Hb-TaS2 as well as on long-studied but still unsolved systems like Sr2RuO4, UPt3, and PrOs4Sb12.

Supervisor: Adam Pikul, D.Sc.(dr hab.) (a.pikul@intibs.pl)

Subject: ***Thermal expansion and magnetostriction of uranium intermetallic compounds as potential advanced next-generation nuclear fuel***
Discipline: Physics/Chemistry

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 (as potential nuclear fuel) 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), 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: Małgorzata Samsel-Czekała, D.Sc. (dr hab.) (m.samsel@intibs.pl)

Subject: ***Theoretical investigations of two-dimensional magnetic topological materials.***
Discipline: Physics

Description: Three-dimensional Dirac/Weyl semimetals are extensively studied due to the variety of their exotic physical properties. However, the corresponding semimetallic states in two-dimensional magnetic materials, which may be the most promising for quantum information technology, have been not well recognized. The PhD studies will be based on first-principles and model calculations of crystal stability, electronic and magnetic structures and related quantities of candidates for topological semimetals among realistic two-dimensional magnetic materials.

Supervisor: Piotr Stachowiak, D.Sc. (dr hab.) (p.stachowiak@intibs.pl)
Auxiliary Supervisor: Daria Szewczyk, dr

Subject: ***Thermal properties of bi-component porous materials***
Discipline: Physics

Description: In the frame of the current research project experimental investigations of thermal conductivity and heat capacity of synthetic opals with fully or partially saturated pores will be carried out in the temperature range 1 – 300K. It is planned to utilize the opals of various, carefully chosen globule dimensions to cover the region from microporous to nanoporous structure. The investigations will be mostly focused on the microstructure size region where the thermal wave length becomes comparable to the linear dimensions of the porous structure, i.e. where start phenomena which have no counterpart in the macro-size region. As it was shown theoretically, in this region substantial changes of thermal vibrations of the porous structure such as change of the phonon density of sates, appearance of non-propagating, diffusive modes or reduction of group velocity of the propagating modes take place. All these changes may influence thermal properties of the material and will be significant part of the investigations carried out in the project.

Supervisor: Vinh Hung Tran, prof. (V.H.Tran@intibs.pl)

Subject: ***Research on hyperfine interactions near the quantum critical point.***
Discipline: Physics

Description: Quantum phase transitions (QPTs) and their related phenomena generally referred to as Quantum criticality have been studied for many years but these issues currently are still ones of hot topics in the modern condensed matter physics. Very frequently, such QPTs have been observed in an unstable regime of magnetic-nonmagnetic phases, being driven by non-thermal control parameters like pressure (hydrostatic, chemical), magnetic/electric fields or electron/hole doping. Up to now, useful methods for investigating various quantum critical materials were these based on the measurements of bulk-properties (specific heat, electrical resistivity, magnetic susceptibility). Obviously, there are few studies using
Mossbauer spectroscopy, which may provide valuable information about local electronic environment of magnetic atoms and further encouragement to identify the influences atomic disorder and magnetic quantum critical fluctuations.
The main aim of this PhD thesis proposal is to locally investigate the development of magnetic/nonmagnetic orders and the related hyperfine parameters at the doped 57Fe site in several solid solutions of uranium intermetallic compounds.
The starting point for the research is proposed the solid solution systems formed between the uranium ferromagnetic superconductors UCoGe, URhGe and nonmagnetic UFeGe. The data obtained so far by bulk property measurements reveal that the Fe substitution in the ferromagnetic superconductors lowers Curie temperature and finally destroys the magnetic order at a critical concentration xcr ≈ 0.22. Simultaneously, the Fe substitution suppresses superconductivity and the Non-Fermi-liquid behavior emerges. It is remarkable that in contrast to the first-order QPT in numerous materials, the QPT in UCo1-xFexGe and URh1-xFexGe is presumably of the second-order.
The 57Fe nucleus served as probe of Mossbauer spectroscopy will be most suitable for establishing the role of short-range interaction, atomic disorder, and fluctuations nearby the QPT.

Supervisor: Maciej Winiarski, D. Sc. (dr hab.) (m.winiarski@intibs.pl)

Subject: ***Studies of electronic structures of 2D materials with ab initio calculations.***
Discipline: Physics

Description: Exceptional electronic properties of two-dimensional materials draw great interest in the scientific community due to potential applications in spintronics and catalysis. Monolayers of such systems, e.g., transition metal dichalcogenides and hexagonal boron nitride may also form some heterostructures. In this study, the structural properties and electronic structures of selected 2D systems are investigated with calculations based on the density functional theory (DFT). The full potential and pseudopotential approaches are employed. A particular emphasis is placed on influence of stress/strain on band gaps of monolayer and multilayer systems as well as functionalization of these materials via adsorption of transition metal ions.