List of doctoral projects available for the academic year 2020/2021

INTiBS PAN
WROCŁAW

Wrocław 2020

Chemistry/Physics

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 metallo-phthalocyanine derivatives should be performed.

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

Subject: ***Synthesis and studies of novel organic-inorganic hybrid materials for optoelectronic applications.***
Discipline: Chemistry

Description: Organic-inorganic hybrids have been the subject of intense studies in recent years due to their functional properties. One of the most famous group are those crystallizing in a perovskite type structure of general formula ABX3. Important group constitute also layered perovskites. These materials are of interest due to their photovoltaic and light emitting properties but some of them show also ferroelectric and NLO properties. The aim of PhD student will be search for novel hybrids exhibiting linear (efficient photoluminescence) and nonlinear optical properties, ferroelectric and switchable dielectric properties. These compounds will be studied using IR, Raman and optical spectroscopes as well as other experimental methods.

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: Zbigniew Bukowski, D.Sc. (dr hab.) (z.bukowski@intibs.pl)
Ancillary promoter: Michał Babij, dr

Subject: ***Magnetism and superconductivity in single crystals of selected Remeika phases R3T4X13***
Discipline: Physics/Chemistry

Description: Intermetallic compounds of the chemical formula R3T4X13 (R = Ca, Sr, Eu; T = transition element; X = Sn, Ge) called Remeika phases show a very broad spectrum of interesting physical properties from superconductivity to magnetic ordering and are therefore intensively studied for many years . The aim of the work will be to learn the method of obtaining single crystals of selected compounds from this family and their characterization in terms of chemical composition and crystal structure. In the next stage, the basic physical properties of the obtained single crystals will be comprehensively investigated by means of magnetization, ac magnetic susceptibility, electrical resistivity measurements etc. in applied magnetic fields in the temperature range of 300-1.9 K.

Supervisor: Dariusz Kaczorowski, prof. (d.kaczorowski@intibs.pl)

Subject: ***Unconventional superconductivity and magnetic ordering in Ce-Pd-In and Ce-Pt-In dense Kondo systems***
Discipline: Physics/Chemistry

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: Dariusz Kaczorowski, prof. (d.kaczorowski@intibs.pl)

Subject. ***Electronic transport and thermodynamic properties of magnetic topological semimetals***
Discipline: Physics/Chemistry

Description: Topological Dirac semimetals with accidental band touching between conduction and valence bands protected by time reversal and inversion symmetry are at the frontier of modern condensed matter research. A majority of discovered topological semimetals are nonmagnetic and thus conserve time reversal symmetry. However, it has been theoretically predicted that combination of magnetic order and nontrivial topology can generate exotic quantum phenomena, such as quantum anomalous Hall effect, axion insulator states, chiral Majorana modes, etc., which are utmost alluring for fundamental science studies, yet also highly attractive for a number of revolutionary technological applications. Therefore, experimental search for topological materials with long-range magnetism has recently become a major subject in comprehensive investigations on topological states of matter, intensively conducted worldwide.
In this doctoral work, we intend to investigate a series of Eu-based pnictides with the overall composition EuM2X2, where M = Zn, Cd, Ga, In, Sn, Pb, and X = P, As, Sb. Recently, the arsenide EuIn2As2, an antiferromagnetic member of the family, has been recognized as an axion topological insulator candidate that additionally harbors tunable higher-order topological insulating states. Most remarkably, preliminary results of our experimental investigations by means of bulk and spectroscopic techniques, combined with ab-initio electronic band structure calculations, seem to corroborate these exciting theoretical findings.
At the first stage of his/her PhD work, the doctoral student will join our ongoing research on EuIn2As2. Deep hands-on involvement in our experimental activities should provide him/her with a quick and effective training in the growth of single crystals, their crystal-chemical characterization and various physical properties measurements, carried out using state-of-the-art equipment. Then, he/she will focus on other EuM2X2 compounds, aiming to determine their temperature-, magnetic field-, and pressure-driven magnetic states, and understand their interplay with topological nature of the particular phases.

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

Subject: ***Influence of magnetocrystalline anisotropy and on physical properties of selected intermetallic uranium compounds*.**
Discipline: Physics/Chemistry

Description: One of the most important modern trends in the study of solid magnetism is the search for new physical phenomena resulting directly or indirectly from magnetic interactions. It usually starts with the synthesis and investigation of new or poorly known chemical compounds containing elements with partially filled electron shell f (i.e. lanthanides and actinides) and having anomalous or rare physical properties. Among them an exceptional place occupy compounds with uranium, which – in addition to the well-known weak radioactivity – has unique magnetic properties. The PhD thesis of mainly experimental character will be devoted to the search for dependencies between unconventional physical properties of such systems (e.g. proximity of quantum critical point or exotic superconductivity) and their strong magnetocrystalline anisotropy and effective dimensionality

Supervisor: Tomasz Cichorek, prof. (t.cichorek@intibs.pl) **Subject:** ***Multi-band effects in heavy-fermion superconductors. Lower critical field studies.*** **Discipline:** Physics **Description:** Recent experimental and theoretical research shows that multiband superconductivity is a complex phenomenon, often leading to new physical effects not found in classical superconductors. It is believed that experimental observation of multi-band effects in heavy-fermion superconductors may change our current understanding of both the structures of their energy gaps and the symmetry of their order parameters.
Supervisor: Detlef Hommel, prof. (d.hommel@intibs.pl) **Ancillary promoter: Edyta Piskorska-Hommel, dr** **Subject:** ***Growth of low-dimensional structures using epitaxial methods*** **Discipline:** Physics **Description:** The scope of the work considers the molecular beam (MBE) and the gas phase (MOCVD) epitaxy methods. The selected applicant will be familiar with the physical base of the molecular beam epitaxy, the principles of operation of molecular beam epitaxy and MOCVD devices, modeling of the semiconductor structures growth, and their characterization. As a result, the PhD applicant has to prepare and characterize selected semiconductor structures based on II-VI or III-V elements.
Supervisor: Tadeusz Kopeć, prof. (t.kopec@intibs.pl) **Ancillary promoter: Vardan Apinian, dr** **Subject:** ***Excitonic effects and correllations in graphene-based nanostructures and heterostructures*** **Discipline:** Physics **Description:** The proposed thematics for the PhD studies covers a very large area in condensed matter physics. The principal subject of the PhD proposal is related to the study of the excitonic effects and general correlation mechanisms in the low-dimensional graphene-based nanostructures and heterostructures. The graphene has been proved as a purposeful material for its mechanical and electrical properties and high-performance thermoelectric efficiency. The principal advantage of this material is related to its extraordinary electronic band structure. The study of the excitons in the structures based on the graphene could have an unprecedented impact on the modern solid states physics and quantum technologies. Extraordinary properties of the excitonic quasiparticles have been proved already in the semiconductors and materials with the large band gaps in the electronic spectrum. In the graphene-based technologies, the excitons could be the effective quasiparticles which will have the dominant character under certain conditions and coherence regimes. During the PhD study, the candidate will be integrated into our theoretical research group and will conduct the studies on the theoretical aspects of the excitons in proposed nano- and heterostructures. The candidate should have a solid background in solid states physics (at least at the level of the book of Kittel "Introduction to Solid State Physics") and should have a strong motivation to learn the new Theoretical methods related to strongly correlated electron systems. The knowledge in the methods of numerical computation techniques is very welcome.

Supervisor: Piotr Stachowiak D.Sc. (dr hab.) (p.stachowiak@intibs.pl)
Ancillary promoter: 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 pass smoothly from microporous to mesoporous 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 influence thermal properties of the material and will be investigated in the project.

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

Subject: ***Investigation of hyperfine interactions and electron-phonon coupling in Fe-based superconductors***
Discipline: Physics

Description: Several families of FeAs-based high-temperature superconductors are being intensively studied, e.g. AFeAs (A = Li, Na), AFe2As2 (A = Sr, Ba, Eu), RFeAsF (R - rare earth elements), A2MFeAsO3 (A = Sr, Ba, Ca, and M = Sc, Ti, V, Cr, Co), Sr3Sc2Fe2As2O5, Ca10PtnAs8 (Fe2As2) 5 ...
This fact is due to, at least, two reasons: 1) superconductivity is associated not only with the presence of Fe ions, but also with other magnetic ions, e.g. V or Cr. All these magnetic ions are responsible for the coexistence of superconductivity and magnetism. 2) Fe-based superconductors have a layered structure, and the FeAs layers are separated from each other by non-conductive layers, in particular, by blocks of perovskite structure. The presence of a perovskite block in a unit cell certainly modifies the electron-phonon coupling, which has an impact distinct from those in the CuO-based or other FeAs-based superconductors without perovskite units. Therefore, it is clear that the mechanism responsible for superconductivity in this superconductor family is interesting and presumably unconventional.
The subject of the proposed doctoral dissertation includes studies of hyperfine interactions and electron-phonon coupling, magnetic and thermodynamic properties in selected iron superconductors. The main research tools are Mössbauer spectroscopy (57Fe) and theoretical calculations of the electronic structure using the DFT method.

Supervisor: Piotr Wiśniewski, D.Sc. (dr hab.) (p.wisniewski@intibs.pl) **Ancillary promoter: Orest Pavlosiuk, dr** **Subject:** ***Topological properties of electronic states in dichalcogenides of transition metals and lanthanides.*** **Discipline:** Physics **Description:** PhD student will synthesize single crystals of selected dichalcogenides (selenides or tellurides) of transition metals and lanathanides, and study their electronic properties by means of magnetotransport and thermodynamic measurements, and when possible photoemission spectroscopy.
Supervisor: Piotr Wiśniewski, D.Sc. (dr hab.) (p.wisniewski@intibs.pl) **Ancillary promoter: Orest Pavlosiuk, dr** **Subject:** ***Multifunctional half-Heusler phases, antimonides of transition metals and lanthanides - single crystals and their physical properties.*** **Discipline:** Physics **Description:** PhD student will synthesize single crystals of selected half-Heusler phases, antimonides of transition metals and lanathanides, and study their electronic and functional properties by means of magnetotransport and thermodynamic measurements, and when possible photoemission spectroscopy.