

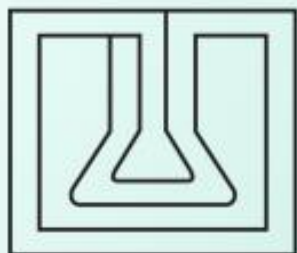


Augmenting Chemistry

14-16 APRIL 2024

International Young Chemists Conference

Book Of Abstracts



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Augmenting Chemistry – International Young Chemist Conference

April 14-16, 2024

Augustów, Poland



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Dear Participants, Honorable Guests

It is my great pleasure to welcome you to the International Young Chemists Conference Augmenting Chemistry in Augustów. I am very glad to see that we have managed to attract such a great number of young scientists from so many different countries.

Augmenting chemistry is an excellent place to share the experience of young researchers of diverse backgrounds, exchange ideas and to integrate the forthcoming generation of chemists. The participants will have a chance to enjoy lectures prepared by scientists from various fields of chemistry. The invited keynote speakers will present their recent research and share their enormous experience in our common passion - chemistry. I am truly honored and thankful that our guests, top-class researchers, want to share their time, knowledge, and experience with so many young scientists.

The Organizing Committee would also like to express their thanks to all the sponsors. It would not be possible to reach such a high organizational standard without their help. We also wish to thank the authorities of the Faculty of Chemistry at Warsaw University of Technology, for their trust and giving us freedom in every aspect of organizing Augmenting Chemistry. Last but not least, we thank all the participants of the Conference, for having come even from very distant places.

Personally, I would like to thank the members of the Chemical Scientific Society Flogiston, for their great effort in preparations. Thanks to their hard work throughout the last ten months, and the atmosphere of friendship that we all create, the Augmenting Chemistry Conference would not be possible.

We wish all the participants success in their presentations, exciting discussions, lots of new experience and knowledge, plentiful new contacts, and a lovely, unforgettable time in Poland.

Bruno Skoczeń

President of Organizing Committee



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Spis treści

A SERIES OF NOVEL ALKYLALUMINIUM CARBOXYLATES WITH UNPRECEDENTED PHOTOLUMINESCENCE PROPERTIES	6
SOLUBILITY STUDIES OF QUINOLONE DERIVATIVES	7
COMPARATIVE ANALYSIS OF SYNTHESIS ROUTES AND ALUMINUM DOPING EFFECTS ON NMC TYPE CATHODE MATERIAL	8
NOVEL GENERATION OF ANODES BASED ON HALIDE PEROVSKITES FOR LI-ION BATTERIES	9
EVALUATING CORROSION IN ELECTROCHEMICAL SETUPS – FROM WELL-KNOWN BATTERY TECHNOLOGIES TO NOVEL SYSTEMS.....	10
HÜCKEL ANION BASED CONCENTRATED ELECTROLYTES FOR LITHIUM-SULFUR BATTERIES	11
OPERANDO RAMAN MICROSCOPY STUDIES ON NEXT GENERATION POSITIVE ELECTRODE AND ELECTROLYTE MATERIALS	12
METALLIC ORGANIC FRAMEWORKS (MOF) APPLICATIONS IN NOVEL LITHIUM-SULFUR BATTERIES	13
INFLUENCE OF MATRIX STRUCTURE ON THE PROPERTIES OF SHEAR THICKENING ELECTROLYTES FOR LITHIUM-ION BATTERY	14
POLY(AN-CO-PEGMEA) ELECTROLYTES FOR 3D PRINTED LITHIUM-ION BATTERIES	15
INFLUENCE OF THE METAL CENTRE ON THE INCLUSION PROPERTIES OF GROUP-13 ORGANOMETALLIC CINCHONINE COMPLEXES.....	16
CIRCULAR FUELS – PRODUCING EUROPE’S SUSTAINABLE AVIATION FUELS	17
ACTIVITIES OF ORLEN S.A. RESEARCH AND DEVELOPMENT CENTER (CBR) IN PŁOCK – BITUMEN PRODUCTION TECHNOLOGIES DEVELOPMENT.....	18
ELECTROCHEMICAL INTERCALATION OF SELECTED ALKYLAMMONIUM IONS INTO THE STRUCTURE OF IRON SELENIDE.....	19
STUDY ON CORROSION PHENOMENA OF LEAD ALLOYS	20
BREAKING BARRIERS – DUAL DOPING FOR INCREASING ELECTRONIC CONDUCTIVITY IN LITHIUM GARNET ELECTROLYTE $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$	21
A NEW CONCEPT OF TERNARY AQUEOUS ELECTROLYTES BASED ON LITHIUM 4,5-DICYANOIMIDAZOLATE HYDRATES	22
STUDIES ON THE APTAMER RECEPTOR LAYER FORMATION – PROPERTIES AND ANALYTICAL APPLICATIONS	23
MECHANOCHEMICAL SYNTHESIS OF IRMOFS	24
ZWITTERIONIC-TYPE LIGAND-COATED ZINC OXIDE QUANTUM DOTS ENGINEERED BY THE ORGANOMETALLIC APPROACH	25
NOVEL SUMANENE BASED CAESIUM CATIONS SELECTIVE MOLECULAR RECEPTIONS	26
NOVEL TRANSMETALATION SYNTHETIC APPROACH AND ISOMERISM OF $\text{M}_4(\mu_4\text{-O})\text{L}_6$ METAL OXIDO CLUSTERS STABILISED WITH AMIDATE LIGAND.....	27

PLA STEREOCOMPLEX CRYSTALLIZATION IN COMPOSITES WITH GRAPHENE NANOPLATELETS: EFFECT ON THERMAL CONDUCTIVITY, ITS ANISOTROPY AND TEMPERATURE DEPENDANCE	28
UNIQUE Mn(II) ₄ (μ ₄ -O)-OXIDO CLUSTERS. VERSATILITY OF TRANSMETALATION/HYDROLYSIS APPROACH.	29
SYNTHESIS AND CHARACTERIZATION OF NEW BIS(β-DIKETIMINE)S	30
MECHANOCHEMICAL VS WET APPROACH FOR DIRECTING CO ₂ CAPTURE TOWARD VARIOUS CARBONATE AND BICARBONATE NETWORKS	32
UTILIZATION OF TWO PHOTON ABSORPTION PHENOMENON IN DEVELOPMENT OF EFFECTIVE REACTIVE OXYGEN SPECIES GENERATORS FOR APPLICATION IN PHOTODYNAMIC THERAPY	33
EFFECT OF DRY-MILLING COATING METHOD ON STRUCTURAL PROPERTIES OF LITHIUM IRON PHOSPHATE.....	34
BODIPY COMPLEXES DEMONSTRATING TWO PHOTON ABSORPTION AS EFFICIENT PHOTOSENSITIZERS	35
AGING PROCESSES OF SECONDARY ORGANIC AEROSOL IN THE ATMOSPHERICAL WATER USING KINETICS AND TANDEM MASS SPECTROMETRY.....	36
SYNTHESIS, POLYMORPHISM AND SHAPE COMPLEMENTARITY-INDUCED CO- CRYSTALLIZATION OF HEXANUCLEAR CO(II) CLUSTERS	38
THE STUDY OF NEWLY PROPOSED WORKING FLUIDS IN ABSORPTION REFRIGERATION TECHNOLOGY	40
TRIBLOCK COPOLYMERS PREPARED THROUGH RAFT, COMPRISING CYCLIC ANHYDRIDE MOIETIES, ACTING AS RECYCLING ENHANCERS FOR POLYAMIDES.....	42
SYNTHESIS OF AZO DERIVATIVES OF CHALCONES.....	43
STUDIES ON THE AIE EFFECT IN MECHANOCHEMICALLY SYNTHESIZED POLYAROMATIC AMIDES.....	44



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A SERIES OF NOVEL ALKYLALUMINIUM CARBOXYLATES WITH UNPRECEDENTED PHOTOLUMINESCENCE PROPERTIES

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Luminescent organic and organometallic compounds are of widespread interest due to their versatile application potential. With the earlier discovery of Alq₃ (q = 8-hydroxyquinolato) and its successful use as an emissive layer in OLEDs,¹ an intensive search for luminescence materials based on the aluminium metallic centre was initiated. Over the last few decades, numerous examples of high fluorescence Al-based could be found, including the most recent dinuclear dimethylaluminium β-diketiminato with unprecedented photoluminescence quantum yield in the solid state and in the solution.² Emitting solids are important in the context of their further application in optoelectronic devices. It is, therefore, crucial to manage competing aggregation-induced enhancement of emission (AIEE) and aggregation-caused quenching (ACQ) effects, where the first is highly desirable and the second should be minimised.³ In this context, it is important to constantly seek new efficient luminophores in order to gain a deeper understanding (i.a. through the insight into their molecular structure) of these effects in each specific case and achieve further milestones in the field.

In this work, we focused on the synthesis and structure characterisation of novel alkylaluminium complexes supported by an o-substituted benzoic acid framework. Reactions of R₃Al compounds with selected pro-ligands in the non-coordinating solvent lead to the formation of a number of oligonuclear alkylaluminium carboxylate complexes of different molecular structures. The resulting compounds were fully characterised using spectroscopic techniques and single-crystal X-ray diffraction studies. Remarkably, some of them possess an unprecedented photoluminescence quantum yield.

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SOLUBILITY STUDIES OF QUINOLONE DERIVATIVES

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Quinolones are chemotherapeutic agents with antimicrobial activity obtained entirely by chemical methods, having no equivalent in nature. There are three groups of chemotherapeutics that can be distinguished in terms of their activity: antibacterial, antiviral and antifungal with one common feature of causing inhibition of bacterial growth, microbial cell death or inhibition of replication, when used in low concentrations. Quinolones are characterized by strong bactericidal activity and a broad spectrum of action against many clinically relevant pathogens causing inter alia infections of the respiratory tract, urinary tract, gastrointestinal tract, skin. In addition, it also serves as therapy for infectious diseases that are resistant to penicillin [1]. The mechanism of action of quinolones is based on inhibition of DNA synthesis in bacterial cells. This is done by blocking type II topoisomerases and type IV topoisomerases, which are enzymes that separate DNA strands after the replication process is complete. Inhibition of enzyme activity results in DNA damage and blockage of cellular, resulting in the death of the bacterial cell [2].

The selection of these active pharmaceutical ingredients (API) was made due to the numerous possibilities of their use in medicine caused by their biological activity and the desire to solve the problems that prevent their implementation in future therapies such as low solubility in water [3]. One of the representatives of quinolones is nalidixic acid as one of the first pharmaceuticals synthesized from this group. It was used to treat urinary tract infections in humans. However, due to its limited therapeutic utility and the rapid development of microbial resistance, it ceased to be of interest. This prompted the development of research on structure modification and the search for relationships between structure and biological properties [4].

The studies carried out are aimed at determining the solubility of the substance in solvents relevant to the administration of the substance, namely water, ethanol and 1-octanol. They were presented in the form of phase equilibria in binary systems {solid (1) + liquid (2)} over a wide temperature range. The experimental data were described using thermodynamic equations based on the local concentration theory. Thermal analyses of pure substances were performed by differential scanning calorimetry and ionization constants were determined. This research is used to further explore the possibility of changing the formulation or modifying the API to improve unfavorable pharmacokinetic parameters including, in particular, water solubility.

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COMPARATIVE ANALYSIS OF SYNTHESIS ROUTES AND ALUMINUM DOPING EFFECTS ON NMC TYPE CATHODE MATERIAL

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This study presents a comprehensive analysis of the synthesis techniques and the impact of aluminum doping on Nickel Manganese Cobalt (NMC) 811 cathode materials. Our research focuses on comparing two distinct synthesis methods: hydroxide co-precipitation followed by solid-state calcination for polycrystalline (PC) cathodes and molten salt calcination for single-crystalline (SC) cathodes. Additionally, the study systematically integrates aluminum dopants at various stages of these processes.

The objective is to explore the influence of doping via various approaches on the structural, morphological, and electrochemical properties of NMC cathodes. Through extensive characterizations using methods like X-ray diffraction (XRD), scanning electron microscopy (SEM), and galvanostatic cycling tests, our results highlight the promise of aluminum doping in enhancing the performance of polycrystalline NMC cathodes.



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NOVEL GENERATION OF ANODES BASED ON HALIDE PEROVSKITES FOR LI-ION BATTERIES

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The escalating global energy demands require development of clean energy sources and efficient energy storage systems. In this pursuit, a range of energy storage devices, including batteries, fuel cells, and supercapacitors, have been subject to extensive investigation. At this point, lithium-ion cells have been the dominant choice for portable power storage devices for over 30 years. Despite their many advantages, continuous research is being carried out to improve the performance of the cells. There is a need to search for new battery components including electrodes and electrolytes, assuring higher battery capacity, better safety, and enhanced electrochemical stability range. Critical research area involves understanding and controlling the phenomena at the anode-electrolyte interface where energy storage occurs, and the initiation of degradation takes place. The formation of solid electrolyte interphase (SEI) is a crucial property responsible for ensuring cycling stability and extended thermodynamic stability of organic electrolytes in Li-ion batteries.

Metal halide perovskites (MHPs) represent a revolutionary class of compounds that can be used in lithium-ion batteries. While metal halide perovskites are predominantly recognized for their applications in energy conversion, their unique structure allowing fast lithium-ion diffusion has prompted exploration in energy storage. The typical preparation of halide perovskites relies on solution-based methods, yet this approach encounters challenges in both compositional engineering and long-term storage. In this context, solid-state chemical reactions induced by mechanical forces have emerged as an effective and straightforward method for solvent free compositional engineering within a relatively short timeframe.

In this work we present the development of a new generation of electrodes using all-inorganic and hybrid inorganic-organic halide perovskites. Different MHPs have been used as the main active material for high-performance electrodes. Beyond serving as anodes, MHPs have also found application as an electrode additive. In this case, the use of another well-known active material as the head component of the anode and MHPs as an additive involved in the formation of the SEI layer is likely to improve the cyclability, capacity and lifetime of the cell. Our study includes electrochemical characterization and cycling performance analysis of electrodes based on carbonous materials and tailor-made halide perovskites.

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EVALUATING CORROSION IN ELECTROCHEMICAL SETUPS – FROM WELL- KNOWN BATTERY TECHNOLOGIES TO NOVEL SYSTEMS

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Corrosion is often connected with macroscopic systems, such as pipes in multi-tonne factories. It can also affect microscopic systems like batteries and electrochemical cells. Few research teams focus on corrosive aspects of the media they use for electrochemical testing, thus changes in testing cells can become unnoticed and hinder obtained data. We have tested corrosion in different kinds of battery cells used in manufacturing and in laboratory conditions: lithium-ion (LIBs), lithium-sulphur and magnesium-ion (RMBs) batteries. We have taken into consideration different places corrosion can occur: steel case of coin cell type testing equipment, aluminum current collector and metal working electrode. In LIBs we have tested how storage time affects steel coin cell case. Using chronoamperometric techniques we have determined how current is distributed in freshly assembled cell and stored cell. Potentiodynamic tests allowed us to correlate cathodic current to post-mortem analysis of the case. With increasing storage time corrosion products accumulate on the surface of steel and hinder proper electric contact. In some cases it can lead to perforation of the case which causes electrolyte leakage and increases probability of thermal runaway. In Li-S batteries we have tested two commercially available salts: lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) and lithium 2-trifluoromethyl-4,5-dicyanoimidazole (LiTDI) in PEO liquid analogue (PEG DME 500). Different electrochemical tests including two and three electrode configurations were conducted. Additionally the in-situ Raman spectroscopy allowed us to follow the changes on Al electrode in potentiodynamic conditions. Polysulfides present in the electrolyte may prevent corrosion at 70 °C. Additionally LiTDI salt rise the corrosion potential much above Li-S operational potential, however the corrosion current is rising for LiTFSI electrolytes. In RMBs we have tested Mg(TFSI)₂ salt in diglyme as standard reference electrolyte for laboratory-scale experiments. Immersion tests and potentiodynamic experiments allowed us to evaluate corrosion potential of magnesium and explore stability of its oxide layer in the electrolyte. Additional photos from optical microscope showed structural changes of metal surface connected with passivation.

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HÜCKEL ANION BASED CONCENTRATED ELECTROLYTES FOR LITHIUM-SULFUR BATTERIES

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The electrolyte is a crucial component in lithium-sulfur (Li-S) batteries, governing essential aspects such as the problem of polysulfide (PS) dissolution and formation of the solid-electrolyte interphase (SEI) layer. Achieving long-term cycling stability of Li-S batteries necessitates to select anions exhibiting low mobility and weak interactions with PSs [1]. Electrolytes based on Li-salts with Hückel anions, widely employed in lithium-ion batteries, shows potential for enhanced performance in Li-S batteries owing to their reduced polysulfide solubility, as compared to for example the prevalent LiTFSI-based electrolytes [2].

We have here explored various Hückel anion based Li-salts, characterized by different alkyl chains attached: lithium 4,5-dicyano-2-(trifluoromethyl)imidazolide (LiTDI), lithium 4,5-dicyano-2-(pentafluoroethyl)imidazolide (LiPDI), and lithium 4,5-dicyano-2-(heptafluoropropyl)imidazolide (LiHDI). All were dissolved in DOL:DME (1:1, v/v) to create Li-S battery electrolytes. The local structure as function of salt concentration was elucidated using Raman and FTIR spectroscopy, and correlated with ion transport properties and electrochemical performance. Additionally, we have calculated the PS solubility in the electrolytes using a combined DFT and statistical mechanics approach; the conductor-like screening model for real solvents (COSMO-RS).

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OPERANDO RAMAN MICROSCOPY STUDIES ON NEXT GENERATION POSITIVE ELECTRODE AND ELECTROLYTE MATERIALS

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Li-ion batteries (LIBs) are a concern nowadays because they are widely used in grid-scale energy storage. The ever-increasing demand for their better performance has encouraged researchers to deeply understand the impact of ageing mechanisms on various battery components [1,2]. Nickel rich metal oxides are currently garnering attention as electrode materials due to their applicability in electric vehicles. However, they suffer from capacity loss and thermal instability in highly deintercalated states [3].

Raman microscopy can be used to probe structural evolution and chemical composition of battery elements during cycling. Despite the advantages of this technique, it presents some challenges related to limitations throughout Operando measurements [4]. The aim of this work was to monitor electrode and electrolyte materials using Raman spectroscopy under in situ commercially relevant conditions. The relationship between the spectra features and battery properties was established with the support of Jupyter-based application PRISMA [5]. Additionally, intrinsic characteristics and dynamics were identified for several electrode materials over 3 cycles. Overall, the capability of Operando Raman microscopy to reveal physical and electrochemical phenomena of battery constituents was demonstrated.

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METALLIC ORGANIC FRAMEWORKS (MOF) APPLICATIONS IN NOVEL LITHIUM-SULFUR BATTERIES

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Today lithium-ion batteries are the basis of portable energy source. Widely used in electronic devices and electric vehicles lithium-ion type of batteries became a standard. Despite good electrochemical performance and their universality, fast development of the market for efficient power sources makes them unable to meet this challenge. As a promising competitor or even a successor of lithium-ion batteries often named are lithium-sulfur batteries. It's mostly because of their high specific capacity (1675 mAh g⁻¹) and relatively big deposit of sulfur on Earth. The main reason, why this type of batteries is not commercialized yet is the problem with the application and stability of the sulfur electrode. The expansion of the sulfur when charging, its insulation and dissolution in organic solvents from the electrolyte, resulting the creation of polysulfides chains, are the remaining problems to solve before lithium-sulfur batteries could be spread in the commerce devices. To solve these issues many additives and compounds have been examined. One of the idea is to use metal-organic frameworks (MOFs) as a sulfur host on the electrode. Because of the porosity of the structure of these materials they are able to “hold” sulfur inside them. Not only it improves the electronic conductivity but also can be a solution to reduce the electrode expansion and sulfur reactions with electrolyte. This report presents a few methods of the possible ways of doping MOFs with sulfur and electrode slurry preparation. All the research was made in cooperation of Warsaw University of Technology from Poland and NTNU and SINTEF from Norway in M-ERA.NET 2 MOGLIS project.



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INFLUENCE OF MATRIX STRUCTURE ON THE PROPERTIES OF SHEAR THICKENING ELECTROLYTES FOR LITHIUM-ION BATTERY

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Shear thickening electrolytes (STEs) are becoming more popular because they could offer greater operating safety in extreme working conditions of lithium-ion batteries. During high-speed impacts, such as those occurring during a car accident, they create a barrier similar to solid electrolytes properties. This prevents the short-circuiting of the electrodes in the lithium-ion cell and the consequence of this issue. Currently, the literature presents shear thickening electrolytes as suspensions of inorganic nanoparticles in a solution of lithium salt in organic solvents with low molecular weight. However, such suspensions tend to sediment and contain volatile and flammable organic solvents, significantly restricting the safety of the cell. Typical carbonate solvents can be replaced by polymers. This solution enables the reduction of concentration gradient forms in the electrolyte volume. Additionally, polymer components should allow elimination of another serious problem, which is the high vapor pressure of organic solvents. This prevents an explosion and potential ignition of battery [1, 2].

We obtained shear thickening electrolytes containing silica nanoparticles and lithium salt (LiCF₃SO₃). We used star-shaped poly(ethylene glycol) and poly(propylene glycol) as the matrix, which were synthesized via anionic polymerization by us. Polyol was used as the core. To easily introduce the filler into the matrix and obtain a shear thickening fluid, it is necessary that the glycols are liquids at room temperature. However, ethylene glycols with higher molecular weight tend to crystallize. Therefore, average molecular weight polymer applied was 1000 g/mol. Changing the repeating units to oxypropylene units allows operation in a wider temperature range. Moreover, we found that the addition of nanosilica would slightly change the electrolyte conductivity values and the DSC curve of the material. The addition of lithium salt (LiCF₃SO₃) to star shaped poly(ethylene glycol) inhibits its crystallization. We also observed this effect in shear thickening electrolytes with the same matrix. As a result, we obtained a material that can be used in a wide temperature range. Moreover, the addition of lithium salt does not affect the rheological character of the fluid, and the conductivity of electrolytes in the case of oligomeric forms of ethylene oxide is approximately half an order of magnitude higher than of propylene oxide.

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POLY(AN-CO-PEGMEA) ELECTROLYTES FOR 3D PRINTED LITHIUM-ION BATTERIES

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The properties of lithium-ion batteries, such as high energy density, lack of memory effect, long lifespan, and low self-discharge rate, have made them the preferred electric power source for most portable devices. However, further device development and miniaturization are hindered by the limited availability of battery cells in shapes beyond cylinders and cuboids, stemming from current manufacturing methods. The ability to design custom-shaped devices is crucial for applications like microsensors, wearable electronics, and prototypes. Transitioning production lines to unconventional shapes is costly and impractical; thus, additive manufacturing methods like 3D printing present a promising solution. Developing techniques for manufacturing lithium-ion cells using these methods could streamline device design and accelerate prototyping. Moreover, it is proposed that such cells may exhibit enhanced efficiency due to the three-dimensional electrode and electrolyte architecture, allowing for more efficient lithium transfer [1].

Our study investigates the use of polymer materials in lithium-ion cells, with a focus on their application in additive manufacturing techniques, commonly known as 3D printing. One of the techniques we employ is Direct Ink Writing (DIW) with UV exposure capability, due to its potentially optimal use for printing both electrolytes and electrodes. As the polymer matrix for the electrolyte, we have synthesized a branched copolymer containing polar nitrile and oligoethylene groups through free radical copolymerization of acrylonitrile (AN) and poly(ethylene glycol) methyl ether acrylate (PEGMEA). By adjusting the ratio of comonomers within the PEGMEA:AN range from 1:1 to 10:1, we successfully reduced the glass transition temperature, thereby increasing the ionic conductivity. The DIW technique allows us to print both solid polymer electrolytes (SPEs) and gel polymer electrolytes (GPEs) through solvent evaporation or UV crosslinking. To create GPEs, copolymer mixtures were plasticized with blends of ethylene carbonate, propylene carbonate, and dimethyl carbonate. To facilitate printing, we introduced diacrylates with various molecular weights ranging from 250 to 1000 g/mol as crosslinkers. We successfully fabricated three-dimensional electrolytes incorporating lithium trifluoromethanesulfonate salt, achieving conductivities of nearly 10^{-5} S/cm for solid electrolytes and 10^{-4} S/cm for gel electrolytes, along with a lithium cation transference number of up to 0.5.

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INFLUENCE OF THE METAL CENTRE ON THE INCLUSION PROPERTIES OF GROUP-13 ORGANOMETALLIC CINCHONINE COMPLEXES

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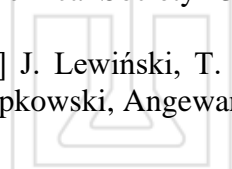
Nanoporous materials are a fertile field of study for modern chemists. Some of the types of such materials include Metal-Organic Frameworks (MOFs), Metal Organic Cages (MOCs) and Non-Covalent Porous Materials (NPMs). Such interest in those kinds of materials is thanks to their various applications, for example for small molecule separation, gas storage, selective catalysis or sensing. These functionalities are realized through the unique environment inside their pores and can be engineered to tailor the properties to specific needs. To manipulate the properties, however, it is of crucial importance to understand the factors that drive them.

This philosophy was applied to obtain several organoaluminium Non-covalent Porous Materials based on cinchonine – a commercially available chiral alkaloid. These materials proved effective in enantiospecific inclusion[1] and gas separation[2]. Therefore, we investigated the influence of the metal centre on the properties of the materials with aim of gaining insight on how the different steric and electronic factors of these atoms might help to tailor the final material.

Organoaluminium, organogallium and organoindium complexes of cinchonine were prepared and crystallized from THF. Al- and Ga- derived complexes crystallized as solvates, while In-derived was close packed. Obtained solvates were isostructural in regards to the cinchonine complex host matrix, however the Ga- complex intake of solvent was 50% higher. Exclusion of the solvent from these materials was performed and porosity of resulting materials was measured.

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CIRCULAR FUELS – PRODUCING EUROPE’S SUSTAINABLE AVIATION FUELS

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Adverse man-made climate change is forcing us to take action to reduce CO₂ emissions and bring us closer to a circular economy model.

To meet the challenges of air transport, the project 'Production of sustainable aviation fuels from waste biomass by coupling of fast pyrolysis with solar energy', abbreviated as 'Circular Fuels', was launched with the support of the European Union. The international consortium established to carry it out includes: Aalto University (Finland), Lund University (Sweden), Vienna University of Technology (Austria), VTT Research Institute (Finland), Orlen S.A. (Poland), CNRS (France), Bosmal (Poland), Ranido (Czech Republic) and Revolve (Belgium).

As part of the project, technology will be developed to produce pyrolytic bio-oil in a reactor heated by concentrated solar energy. The next step will be to stabilise and refine the bio-oil, using green hydrogen (also produced using solar energy), until a hydrocarbon fraction suitable for powering aircraft jet engines is obtained. The raw materials for pyrolysis will be waste from the wood industry, agricultural waste (straw) and demolition wood. Research will be carried out to maximise the yield of the jet fuel fraction. To this end, new catalysts will be developed, capable of working with renewable raw materials. The challenge is also to develop the technology in such a way that existing industrial installations in the refining and petrochemical sector can be used, without significant structural changes.

Meeting the project's objectives will significantly reduce the consumption of aviation fuels derived from non-renewable raw materials and contribute to environmental protection.



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ACTIVITIES OF ORLEN S.A. RESEARCH AND DEVELOPMENT CENTER (CBR) IN PŁOCK – BITUMEN PRODUCTION TECHNOLOGIES DEVELOPMENT

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ORLEN S.A. has a Research and Development Center in Płock, which is a space for the development of new refining and petrochemical technologies. One of the center's areas of activity is the development of bitumen technologies. For this purpose, a bitumen laboratory was created, the main equipment of which is a BITUROX pilot plant for bitumen oxidation, imitating the full-scale production process. Research infrastructure enables optimization and scaling of the bitumen oxidation and polymer modification process.

Research in the field of bitumen technologies focuses, among other things, on the development of new products. The products in the pre-implementation phase include: WMA bitumens, Bitumens for recycling and ECO bitumens. The proposed innovative products demonstrate significant environmental advantages, such as: energy reduction, circular economy, reduction of greenhouse gases and air pollution.

An example of optimization work using a bitumen pilot plant is assessment of the suitability of feedstocks from various crude oils for bitumen production. The aim of the work was to determine the possibility of producing all bitumen grades and to assess and compare the reactivity of feedstocks. Two distillation unit vacuum residues obtained from different types of crude oil were tested to the oxidation process in a pilot plant. Both tested feedstock are suitable for the production of all grades of bitumens. Based on the reaction rate constant, it was determined which vacuum residue was more reactive. Blowing time of a more reactive raw material can be lower. It helps reduce the required energy of the air blowing process to achieve a specific bitumen's penetration grade. The reductions in time have beneficial economic and environmental impacts.



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ELECTROCHEMICAL INTERCALATION OF SELECTED ALKYLAMMONIUM IONS INTO THE STRUCTURE OF IRON SELENIDE

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International Young Chemists Conference

Iron selenides is a big family of compounds with various properties and applications. Among them, the tetragonal iron selenide (β -FeSe $_{1-x}$) is a material with superconducting properties below critical temperature $T_c=8.5$ K[1]. Due to its layered structure and large van der Waals gaps between them (~ 3 Å)[2] it is possible to increase T_c to ~ 37 K by applying external hydrostatic pressure. Another method to further increase T_c is to intercalate various molecular spacers between layers of β -FeSe $_{1-x}$, thus increasing internal chemical pressure of the structure. For example, by intercalating alkali metal ions into the structure of β -FeSe $_{1-x}$ it is possible to achieve $T_c= \sim 47$ K[3]. Synthesis of pure phase β -FeSe $_{1-x}$ is difficult, because of narrow stoichiometric ratio in which iron selenide crystallizes in tetragonal form [1]. Due to strong reducing environment during the intercalation reaction, the material itself is decomposing, further decreasing the amount of superconducting phase. To avoid such state, a new method of electrochemical intercalation of β -FeSe $_{1-x}$ is proposed.

Using electrochemical intercalation method it is possible to obtain more stable material with bigger amount of β -FeSe $_{1-x}$ and with various types of intercalates such as cations of alkylammonium salts, which could yield higher T_c than the previous types of intercalates[4].

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STUDY ON CORROSION PHENOMENA OF LEAD ALLOYS

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In today's world, where every point of critical infrastructure is more or less electrified, there is a need to make them resistant to short- and long-term blackouts. While long-term back-up systems based on fuels, either generators, or fuel cells, they require start-up time, typically from seconds, to minutes. To ensure there's no power shortage during this period, battery based UPS (uninterruptible power supply) systems are used. They utilize mainly Lead-Acid and only rarely Li-Ion or NiMH cells. The former have not only developed an efficient recycle system, but as well, are highly reliable, cheap in production and work well in high or low ambient temperatures. Their main downside is low volume and mass energy density while compared to Li-Ion or NiMH technologies.

Every construction has its own problems to overcome while designing battery. In LABs (Lead-Acid Batteries) these are: sulphation (excessive growth of lead sulphate crystals) during discharge, and gassing (decomposition of water to hydrogen and oxygen) or corrosion of positive electrode grid (on which active material is suspended) during charging.

In this work corrosion resistance of three materials used in production of plate grids were studied. These were: 99,99% pure lead, lead-selenium alloy and lead-antimony alloy. Tests were conducted in three electrode cell, and consisted of PEIS (Potentiostatic Electrochemical Impedance Spectroscopy) and CV (Cyclic Voltammetry). The latter was, as well, used to simulate LAB working conditions, where lead structure becomes porous.

Best corrosion resistance was achieved in pure lead sample. As shown in Fig. 1., lead-antimony alloy is more resistant to corrosion than lead-selenium one. This is somewhat expected – alloy additions role is to enhance mechanical properties of the grid, castability of the material, or modifying the crystalline structure of lead, at the expense of weakening corrosion resistance.

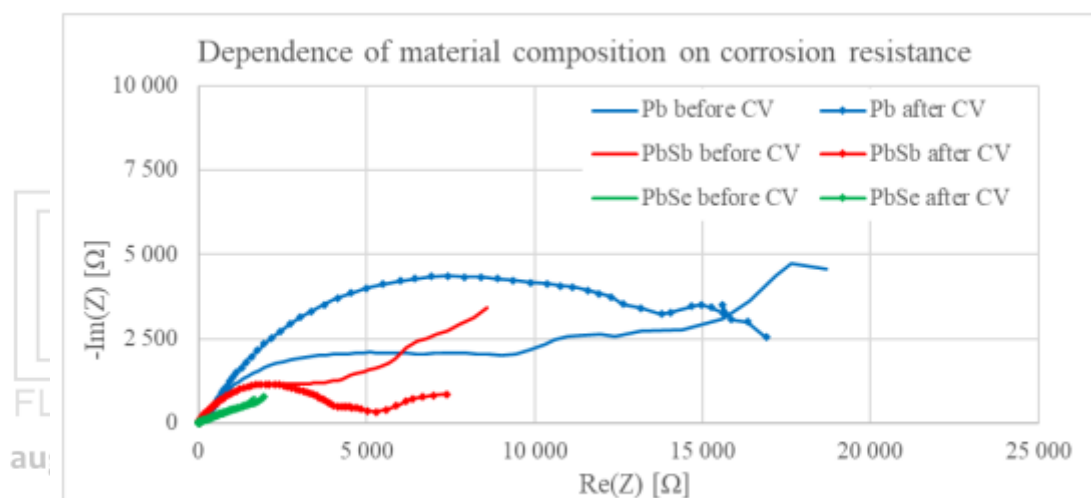


Figure 1. Dependence of material composition on corrosion resistance

BREAKING BARRIERS – DUAL DOPING FOR INCREASING ELECTRONIC CONDUCTIVITY IN LITHIUM GARNET ELECTROLYTE $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$

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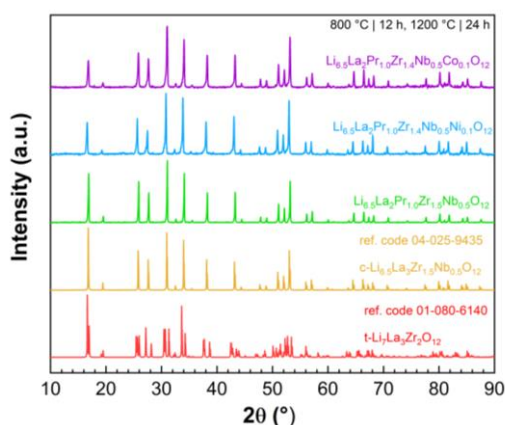
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Continual progress is underway in the field of all-solid-state lithium-ion battery technology. Presently, $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) stands out as a promising solid electrolyte due to its high ionic conductivity, reaching up to 10^{-3} S/cm at room temperature, and its wide stability window. This offers a potential solution to some ongoing challenges in the development of solid-state lithium-ion batteries. A desirable characteristic of a good electrolyte is as low an electron conductivity as possible. However, the evolution of next-generation composite electrodes challenges this norm by seeking both ionic and electronic conductivity. Intentional dual doping of LLZO's structure with metals capable of varying oxidation states (such as niobium and praseodymium) creates pathways for electron conduction within the electrolyte structure. This intentional dual doping aims to facilitate ion-electron conduction in emerging composite electrodes, which consist only of an active material and a modified solid electrolyte.



In this work, we investigate the impact of cobalt (Co) and nickel (Ni) dopants on co-doped niobium (Nb) and praseodymium (Pr) LLZO. Figure 1 displays diffractograms of the LLZO electrolyte in the tetragonal, regular structure, along with three samples: $\text{Li}_{6.5}\text{La}_{2.0}\text{Pr}_{1.0}\text{Zr}_{1.5-x}\text{Nb}_{0.5}\text{M}_x\text{O}_{12}$ where $\text{M} = \{\text{Co}, \text{Ni}\}$, and $x = \{0.0, 0.1\}$. These materials were synthesized using a solid-state reaction method. Calcination occurred at 800°C for 12 hours, followed by sintering at 1200°C for 24 hours. Diffractograms indicate that this synthesis method yielded single-phase materials with a well-formed regular structure.

Figure 1. XRD patterns for the LLZO electrolyte in the tetragonal and regular structure and the three samples $\text{Li}_{6.5}\text{La}_{2.0}\text{Pr}_{1.0}\text{Zr}_{1.5-x}\text{Nb}_{0.5}\text{M}_x\text{O}_{12}$ obtained, where $\text{M} = \{\text{Co}, \text{Ni}\}$ and $x = \{0.0, 0.1\}$.

This work was conducted under support of National Science Centre, grant No. UMO-2019/33/B/ST5/02134.

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A NEW CONCEPT OF TERNARY AQUEOUS ELECTROLYTES BASED ON LITHIUM 4,5-DICYANOIMIDAZOLATE HYDRATES.

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A new concept of aqueous electrolytes based on heterocyclic anions (hydrated anionic triplet electrolyte, HATE) has been presented. Structural studies showed that dimeric lithium 4,5-dicyanoimidazolate (LiTDI) dihydrate molecules, in the presence of acetonitrile, form an ionic system preserved in high concentrations and solid states. X-ray diffraction measurements show that electroneutral dihydrate units can coordinate additional lithium cations acting as charge carriers. The crystalline ionic phase was characterized using spectroscopic, thermal, and electrochemical methods and was used to prepare model electrolytes based on LiTDI hydrates. Linear sweep voltammetry and impedance spectroscopy measurements show, in this system, the depletion of water activity, high conductivity, and reversible cycling of full cells comprising examined electrolytes. We will prove that a concentrated triplet solution acts similarly to the anhydrous electrolyte; regardless of the concentration, it reaches high values of ionic conductivity (12-16 mS/cm at room temperature) and is electrochemically stable.

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STUDIES ON THE APTAMER RECEPTOR LAYER FORMATION – PROPERTIES AND ANALYTICAL APPLICATIONS

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Current expectations for biosensors largely focus on the use of inexpensive components and reagents, as well as the reduction of optimization steps in research. The establishment of a functional receptor layer is one of the most demanding stages in the construction of such devices, and the process of immobilizing receptors on the surface affects multiple parameters (e.g., layer density, molecule orientation, spherical hindrance) defining the analytical capabilities of the biosensor. Thus far, antibodies have been among the most commonly used molecules in receptor layers; however, in recent years, other type of receptor molecules are growing in popularity. Aptamers – single-stranded fragments of nucleic acids, usually DNA or RNA, with high affinity for specific analytes [1]. They are characterized by an exceptionally wide range of target compounds, ease of generating new families of analyte-selective aptamers, very good chemical and thermal stability, and significantly lower manufacturing costs. When designing an analytical method using aptamer-based receptor layers, one of many important factors is the distance between individual molecules; too small a distance limits the space for the analyte-aptamer bond formation, while too large may leave surface areas that non-specifically interact with the matrix of the tested solution [2].

As part of the conducted research, impact of these three parameters have been studied on:

1. Concentration of the aptamer solution used for immobilization,
2. Immobilization time of aptamers, density of the obtained layer on the analytical capabilities of SPR technique,
3. Distance of the aptamer binding site from the receptor layer for analytes of varying sizes

Based on the collected results, modifications to the protocols for preparing receptor layers used in the laboratory were proposed. The influence of the preparation method of the layers on their physicochemical properties was demonstrated. Further research will focus on expanding the investigated parameters and the potential for optimization for other analytical techniques utilizing aptamer-based receptor layers.

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MECHANOCHEMICAL SYNTHESIS OF IRMOFS

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Metal-Organic Frameworks are functional materials with wide variety of applications, which is why finding and optimizing better ways to synthesize those materials is of great importance. Mechanochemical synthesis emerged as environmentally-friendly, green and fast method of synthesis. It doesn't require excess use of bulk organic solvents, it saves energy spent on heating and it shortens reaction times. With minimal addition of solvents in Liquid Assisted Grinding (LAG), it's possible to obtain highly crystalline functional materials with high yields. Such synthesis is often based on relatively simple precursors. However, synthesizing $\{Zn^4O\}^{6+}$ cluster based MOFs via mechanochemistry required a different approach.

SBU-based Mechanochemical Approach for pRecursor Transformation (SMART) was developed to synthesize MOF-5 using preassembled oxo-zinc precursors. Main driving force behind this approach is acid-base reactivity between the ligands and oxo-zinc clusters.[1] This allowed for synthesis of MOFs previously unobtainable via mechanochemical methods and was expanded further upon for synthesis of family of IRMOFs bearing architectural similarity to MOF-5. In this case, combining $[Zn^4(\mu^4-O)(NHOCPh)_6]$ clusters with different organic ligands led to relatively simple and elegant synthesis of IRMOFs.[2]

Method of synthesis may also have an impact on functionality of any given material. MOFs, which can be used for catalysis, gas separation and drug delivery, may have their properties changed based on method they were obtained with. Differences in morphology can affect materials' performance and have impact on its potential applications.

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ZWITTERIONIC-TYPE LIGAND-COATED ZINC OXIDE QUANTUM DOTS ENGINEERED BY THE ORGANOMETALLIC APPROACH

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The nanocrystalline wurtzite core of zinc oxide quantum dots (ZnO QDs) is the essential element of this semiconductor nanomaterial. No less important is the outer organic stabilising shell. The nanoparticle morphology and structure/composition significantly impact the physiochemistry properties and allow further functionalisation.

The presented results continue research to obtain high-quality ZnO QDs by controlled hydrolysis and oxidation of organometallic precursors [1,2]. In the first crucial step, the synthetic procedure assumes the formation of an organozinc complex from a dialkylzinc compound and an appropriate organic ligand. In this case, the ligand is a zwitterionic compound classified as an amphoteric surfactant. Finally, luminescent ZnO QDs are obtained with a core diameter in the so-called "quantum-size regime" range by exposing the reaction mixture to air. The obtained nanoparticles form stable colloidal solutions in a wide range of organic solvents [3].

One of the materials was successfully tested as an electron transport layer in a perovskite photovoltaic cell, obtaining a record-breaking solar energy conversion factor for this type of construction [4]. Also, earlier ZnO QDs from our team were tested in the same role in perovskite photovoltaic cells, achieving high efficiency and stability during work [5].

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NOVEL SUMANENE BASED CAESIUM CATIONS SELECTIVE MOLECULAR RECEPTIONS

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Sumanene is a bowl-shaped C_3 symmetric fragment of fullerene C_{60} [1]. Due to its unique physicochemical properties resulting from presence of conjugated π - π bonds, sumanene attracts attention of researchers from many fields. The size of sumanene bowl is well matched to caesium cation what allows efficient and selective formation of cation- π complexes [2]. Despite large numbers of published papers on sumanene, only a few focus on the ability of these ligands to recognize caesium ions and on their use as selective molecular receptors in chemical sensors.

Direct application of unmodified sumanene in potentiometric sensors is not possible due to its limited solubility in ion-selective membranes based on PVC and 1-(2-nitro-phenoxy)octane (o-NPOE) as plasticizer. The solution of this problem was proposed in [3], where structural modification of sumanene molecule with functional group similar to plasticizer was described. This functionalization yielded sumanene derivative soluble in polymer membrane, leading to caesium selective and sensitive potentiometric sensors.

In this work, novel sumanene derivatives soluble in PVC/o-NPOE membranes were proposed [4]. The structure of sumanene molecule was modified at benzylic positions or at aromatic position. Ability of obtained sumanene derivatives to complex caesium ions was assessed using UV-Vis and fluorescence spectroscopies. Next, potentiometric sensors based on polymer membranes doped with as-synthesized sumanene derivatives were constructed. The selectivity and sensitivity of the ion-selective electrodes towards chosen cations were determined. The obtained results showed that simplified sumanene structure ensures satisfactory performance of the sensors, expanding spectrum of sumanene derivatives available for such purpose.

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NOVEL TRANSMETALATION SYNTHETIC APPROACH AND ISOMERISM OF $M_4(\mu_4-O)L_6$ METAL OXIDO CLUSTERS STABILISED WITH AMIDATE LIGAND

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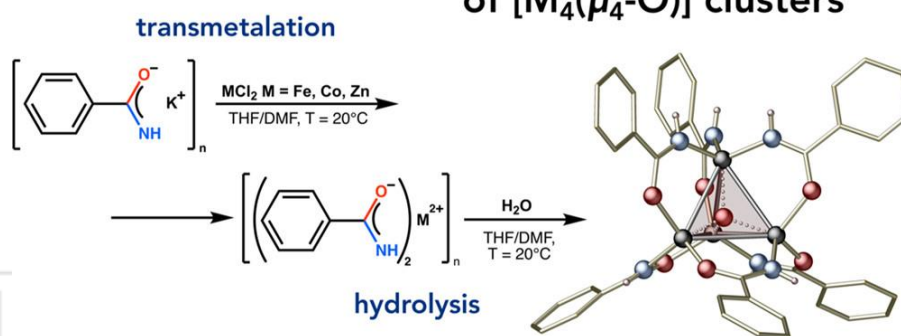
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Tetranuclear $M_4(\mu_4-O)L_6$ oxido clusters consists of tetrahedral core cage of four divalent metal cations with O_2^- oxygen anion inside, and shell of six bidentate organic $-O,O-$, $N,O-$, or $N,N-$ ligands. $M_4(\mu_4-O)L_6$ oxido clusters are prominent subset of metal-oxido compounds class containing also trinuclear $M_3(\mu_3-O)$ clusters and multinuclear polyoxometalates, which has found various applications in supramolecular chemistry, electrochemistry or catalysis [1]. Since the tetrahedral $Zn_4(\mu_4-O)$ structural motif is found in SBU of MOF-5, $M_4(\mu_4-O)L_6$ clusters are being used as precursors and model systems in MOF chemistry [2]. Unfortunately traditional metalloorganic and solvothermal methods do not allow to obtain systematically $M_4(\mu_4-O)L_6$ clusters with other transition metals than zinc, which significantly reduces their application potential [3].

Herein, is presented a novel approach for obtaining $M_4(\mu_4-O)L_6$ oxido clusters with other than zinc divalent transition metals [4]. Three step transmetalation/hydrolysis reaction is demonstrated on synthesis of two iron and cobalt novel μ_4 -oxido zinc analogues stabilized with benzamidate ligands. Also, an interesting coordination position isomerism is revealed and analyzed via 1H NMR spectroscopy.

One-pot three step synthesis

of $[M_4(\mu_4-O)]$ clusters



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PLA STEREOCOMPLEX CRYSTALLIZATION IN COMPOSITES WITH GRAPHENE NANOPATELETS: EFFECT ON THERMAL CONDUCTIVITY, ITS ANISOTROPY AND TEMPERATURE DEPENDANCE

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As the amount of waste from electrical and electronic equipment (WEEE) generated worldwide increases, and its recycling technologies focus on metal recovery, managing its plastics fraction becomes an increasingly pressing problem [1]. One of the suggested solutions is to replace traditional plastics with biodegradable alternatives, however, the properties of the latter, such as thermal conductivity and stability in elevated temperatures, are still insufficient for industrial application in electronic devices [2,3].

In this work we propose a strategy to enhance the thermal properties of graphene composites based on polylactide, a bio-derived and biodegradable polymer [4]. Its unusual ability to form stereocomplex, a crystalline phase containing two isotactic stereoisomers, was used to modify the filler distribution and, consequently, the effectiveness of the heat transfer within the composites. With the rise in ambient temperature the thermal conductivity further increased, which was described within the context of polymer matrix behavior in elevated temperatures. The morphological anisotropy, revealed by microscopic observations, resulted in the anisotropy of thermal conductivity, which was exposed by measurements using two different methods.

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UNIQUE Mn(II)₄(μ₄-O)-OXIDO CLUSTERS. VERSATILITY OF TRANSMETALATION/HYDROLYSIS APPROACH.

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Molecular metal-oxido clusters comprising a highly symmetrical tetrahedral [M₄(μ₄-O)]₆₊ core (M = divalent metal) are of particular interest due to their multifaceted chemistry arising from the presence of several spots of structural tailorability, including divalent metal centers in the tetrahedral core, the character of anchoring groups, and the organic backbone of ligands in the secondary coordination sphere.[1,2] Such diversity of structural features result in tunable optoelectronic and coordination properties, which turns μ₄-oxido compounds into suitable candidates for magnetic, luminescent and catalytic materials. Many of these properties are highly related to the character of the metal centers. Recently we developed an efficient systematic approach for the synthesis of homometallic [M₄(μ₄-O)L₆]-type clusters incorporating various divalent transition metal centers (Zn(II), Fe(II), and Co(II)) coated by bridging monoanionic benzamidate ligands.[3]

Herein, we present the versatility of this approach by extension of synthesis to the two unique clusters based on manganese (II) stabilized by amidinate and amidate monoanionic ligands (benzamidine and benzamide respectively). This makes our synthesis approach even more universal leading to higher diversity of compounds. Interestingly a complex stabilized by benzamidate ligands [Mn₈(μ₄-O)₂(NHCOPh)₁₂] compromise two [Mn₄(μ₄-O)]₆₊ cores connected into a dimer by six bridges made using oxygen atom from benzamidate ligand which is unusual the analogous based on other metals. It is also worth noting that tetrahedral μ₄-oxido clusters based on manganese (II) are extremely rare. There are only two reports of [Mn₄(μ₄-O)]L₆ type clusters both stabilized by amidinate monoanionic ligands (N,N-diphenylformamidine and N,N-dimethylformamidine).[4,5]

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SYNTHESIS AND CHARACTERIZATION OF NEW BIS(β -DIKETIMINE)S

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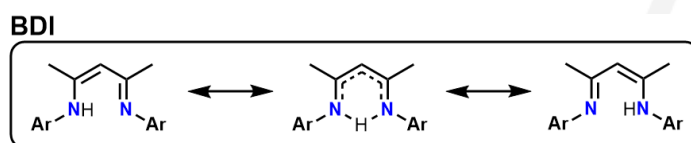
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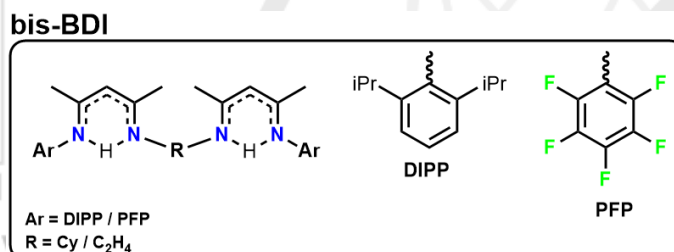
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One of the key aspects of modern coordination chemistry is the search for ligands capable of stabilizing systems with metallic cores whose atoms will remain properly coordinated in redox reactions regardless of their current oxidation state. Moreover, it is desirable that such ligands be non-innocent to the electron transfer processes and support redox-activity on metallic centers. In this context, β -diketimine (**BDI**) derivatives deserve special attention. BDI ligands are characterized by a unique universality. They can form complexes with different transition and main group metal cations, which paved the way for extensive research on coordination compounds with a huge range of potential applications and opens up new horizons for obtaining stable metal complexes on yet unknown or rare oxidation states.[1]



The combination of the universality of BDI ligands and the uncomplicated preparation of their bis-derivatives (**bis-BDI**) makes it possible to obtain compounds with unique properties, in which an important role is played by the possibility of cooperation of metallic cores, such as during complementary fixation and activation of small molecules and in polymerization processes.[2,3] Bis-BDIs have an organic linker in their structure that fuses coordination factions together. The linker, like other substituents at the N,N' -donor moiety, also has a significant effect on the electronic and steric properties of the resulting ligands.[4]

Herein I present the synthesis process and brief characterization of new homoditopic acyclic bis-BDIs differing in terminal aromatic groups and alkyl linkers. The analysis in addition to NMR spectroscopy is mainly based on DFT calculations.



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MECHANOCHEMICAL VS WET APPROACH FOR DIRECTING CO₂ CAPTURE TOWARD VARIOUS CARBONATE AND BICARBONATE NETWORKS

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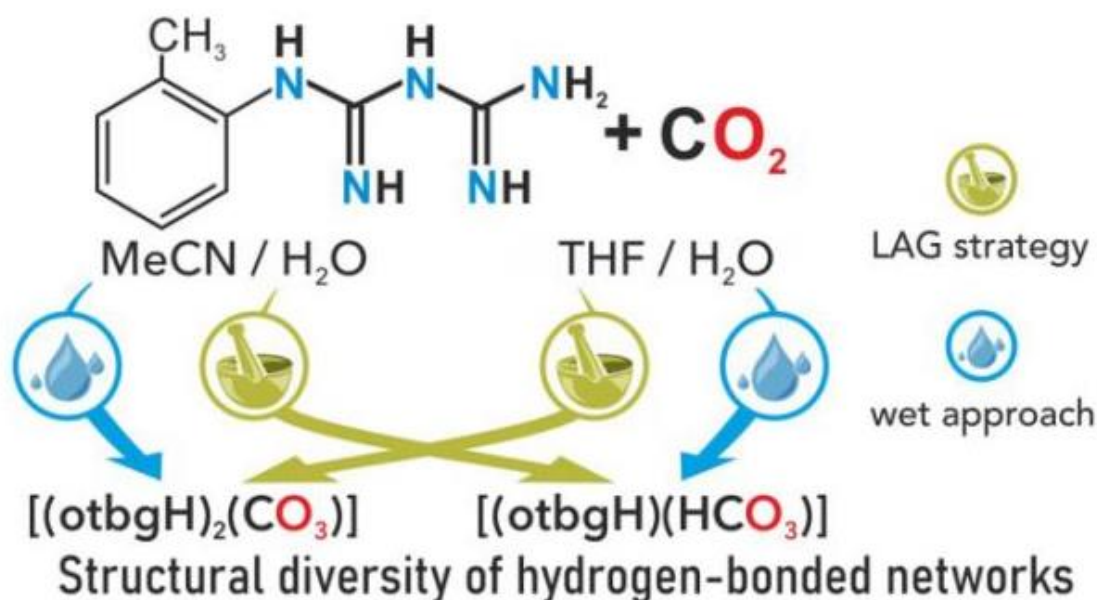
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The distinct research areas related to CO₂ capture and mechanochemistry are both highly attractive in the context of green chemistry. However, merger of these two areas, i.e. mechanochemical CO₂ capture, is still in an early stage of development. Here, the application of biguanidine as an active species for CO₂ capture is investigated using both solution-based and liquid-assisted mechanochemical approaches, which lead to a variety of biguanidinium carbonate and bicarbonate hydrogen-bonded networks. We demonstrate that in solution, the formation of the carbonate vs bicarbonate networks can be directed by the organic solvent, while, remarkably, in the liquid-assisted mechanochemical synthesis employing the same solvents as additives, the selectivity in network formation is inverted. In general, our findings support the view of mechanochemistry not only as a sustainable alternative but rather as a complementary strategy to solution-based synthesis. [1]



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UTILIZATION OF TWO PHOTON ABSORPTION PHENOMENON IN DEVELOPMENT OF EFFECTIVE REACTIVE OXYGEN SPECIES GENERATORS FOR APPLICATION IN PHOTODYNAMIC THERAPY

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Photodynamic therapy (PDT) is one of the most promising cancer treatments, posing as an alternative to chemo- and radiotherapy. Small amounts of photosensitizer given to the patient, are localized in the vicinity of cancerous cells. Treated tissues are irradiated to excite the photosensitizer capable of energy transfer to oxygen molecules present in cells. This leads to the formation of singlet oxygen. The latter is one of the reactive oxygen species (ROS) capable of non-selective oxidation of biomolecules inside cancer cells, causing their apoptosis. The challenges faced by PDT include design of photosensitizer structure that is simultaneously (i) effectively generating ROS, (ii) exhibiting low toxicity without irradiation (low dark cytotoxicity) and (iii) can be excited within range of the so-called “therapeutic window” (800–1000 nm, NIR). [1]

Attractive approach to reach therapeutic window is to facilitate two-photon absorption phenomenon.[2] This can be achieved by designing 2PA-PS dyads composed of photosensitizer (PS) moiety responsible for generating ROS and antenna showing two-photon absorption properties (2PA) in the NIR range linked by non-conjugated linker. By selecting an optimal distance between spatially separated fragments of PS and 2PA, as well as tailoring absorption and emission properties of the components, resulting molecular architecture will allow energy transfer from the antenna to the photosensitizer via Förster resonance (FRET). FRET mechanism and separation of the molecular building blocks allows for preservation of the photosensitizer structure, without risking negative impact on the ROS generation efficiency derived from applied modifications.

Herein, we present a BODIPY-coumarine dyad linked by an aliphatic ester linker. Obtained COU-BDP dyad as well as reference compounds were thoroughly characterized using diffraction methods, spectroscopic measurements and assessment of ROS generation efficiencies. Special attention was devoted to confirm non emissive energy transfer between coumarine and BODIPY moieties.

Research was funded by the Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) programme (YOUNG PW).

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EFFECT OF DRY-MILLING COATING METHOD ON STRUCTURAL PROPERTIES OF LITHIUM IRON PHOSPHATE

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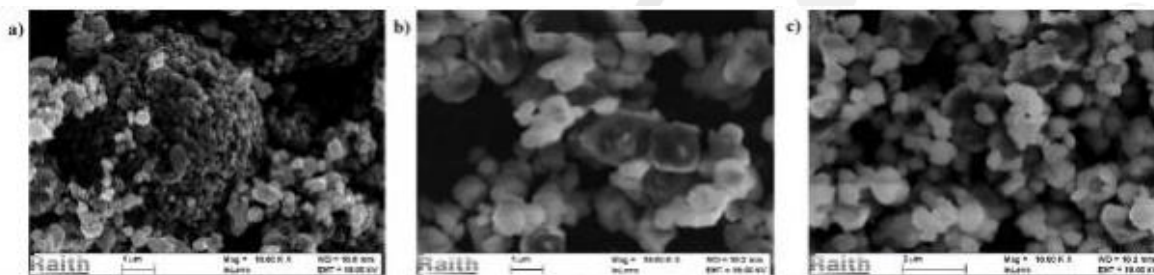
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A Cathode material in the form of Lithium Iron Phosphate (LFP) offers numerous advantages. This includes good retention of gravimetric capacity in function of the next cycles of charging and discharging additionally, it consists of non-toxic elements what is beneficial for the environment. One of the challenges that this material presents is its incompatibility with one of the most well-known solid electrolytes Li₇La₃Zr₂O₁₂ (LLZO). This material in comparison to liquid electrolyte offers high thermal stability, and low safety hazards. It also has fairly high ionic conductivity on the level of 10⁻³ S/cm [1]. The incompatibility between battery components is attributed to high reaction energy between them on level of -1.75 eV/atom [2]. The reaction of LFP and LLZO leads to degradation of LLZO cubic structure to low conductivity tetragonal structure. However, it is implied in numerical papers [3] that there exists the possibility of coating application, which would result in a decrease of reaction energy between the cathode and electrolyte by forming a buffer layer.

There are a few methods of material coating, one of which is the dry-milling method, which is a simple and accessible process. In this work, we examine the impact of the dry-milling method on the properties of active cathode material in the form of lithium iron phosphate. The process as simple as it is has a lot of parameters that can be altered throughout the method. We studied the impact of different rates of milling as well as different coating materials. The results of milling process on LFP and LFP milled with coating material are shown on Fig. 1.



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BODIPY COMPLEXES DEMONSTRATING TWO PHOTON ABSORPTION AS EFFICIENT PHOTOSENSITIZERS

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Photosensitizers are currently one of the intensively developed classes of compounds due to their potential application in anticancer photodynamic therapy (PDT) posing an alternative approach to currently used invasive methods such as chemotherapy or radiotherapy [1]. For a compound to be used as a photosensitizer it must be an efficient generator of reactive oxygen species (ROS), exhibit low cytotoxicity in the absence of light and, most importantly, be excited in the near-infrared range to minimize the possibility of radiation absorption by surrounding tissue [2].

In our previous work, we have introduced donor-acceptor architecture in BODIPY complexes, simultaneously allowing for orthogonal arrangement of individual molecular components. Such strategy significantly increases the probability of intersystem crossing (ISC), thereby allowing for efficient generation of excited triplet states capable of energy transfer to oxygen molecules and as a result ROS production [3]. Current studies are focused on functionalizing BODIPY compounds in terms of near-infrared criteria. The classical approach to obtaining compounds exhibiting a bathochromic shift in absorption spectra requires a significant elongation of conjugated π bonds system, which is unfavourable for PDT application due to decreased photosensitizer solubility in aqueous media. Therefore, as an alternative, photosensitizers exhibiting two-photon absorption (2PA) phenomenon have been designed, allowing the excitation of the molecule using two low-energy photons, hence longer wavelengths [4].

Herein, we present series of BODIPY complexes modified in meso position with aromatic donor molecules enabling 2PA properties. We have characterised all compounds using spectroscopic methods, diffraction techniques and theoretical computations. Conducted experiments allowed us to confirm two-photon absorption properties. Finally, 2PA-BODIPY complexes have been successfully used as potential photosensitizers in selected test reactions.

Research was funded by the Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) programme (YOUNG PW).

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AGING PROCESSES OF SECONDARY ORGANIC AEROSOL IN THE ATMOSPHERICAL WATER USING KINETICS AND TANDEM MASS SPECTROMETRY

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Recently, an increasing amount of experimental and modeling data confirms that an important, although poorly understood, pathway for the formation of secondary organic aerosol (SOA) are the aqueous phase process.[1] One of the important precursors of SOA formation are monoterpene compounds (C₁₀H₁₆), whose oxidation products easily dissolve in atmospheric waters.[2]

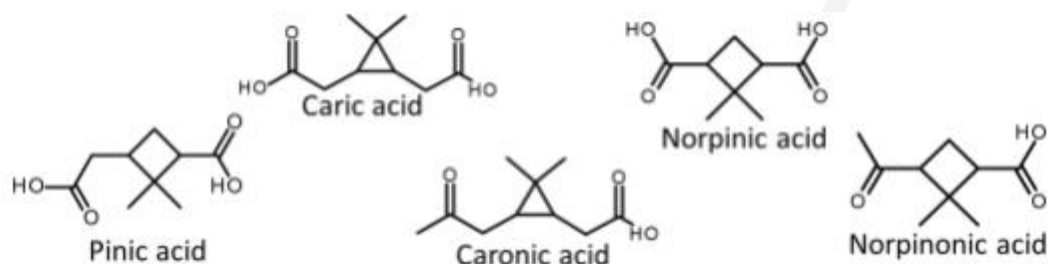


Fig. 1 Oxidation products of α -pinene chosen for analysis

Table 1. Reaction rate constants measured for analysed acids with OH radicals (pH=2) for five different temperature points ($287\text{ K} \leq T \leq 318\text{ K}$)


T (K)	$k_{OH} (10^9 \text{ L} \cdot \text{mol}^{-1} \cdot \text{s}^{-1})$				
	Norpinic acid	Norpinonic acid	Pinic acid	Caric acid	Caronic acid
288	0.96 ± 0.09	1.06 ± 0.20	1.85 ± 0.13	2.87 ± 0.15	2.23 ± 0.26
293	1.28 ± 0.19	1.18 ± 0.09	1.93 ± 0.68	2.83 ± 0.50	3.11 ± 1.42
298	1.17 ± 0.10	1.10 ± 0.06	2.07 ± 0.08	3.22 ± 0.13	3.33 ± 0.31
303	1.44 ± 0.36	1.35 ± 0.15	2.50 ± 0.17	3.51 ± 0.26	3.70 ± 0.81
308	1.59 ± 0.34	1.61 ± 0.33	2.47 ± 0.15	3.86 ± 0.60	3.84 ± 0.58

The presented project aimed to investigate the reaction of the oxidation products of α -pinene and δ -3-carene (Fig. 1) with OH radicals in the aqueous phase. The reaction rate constants (k_{OH}) of these products with OH radicals were determined using the relative reaction rate measurement method. The tested terpene acids showed a higher rate constant in the reaction with OH radicals at pH = 10 than in the pH = 2 environment. Additionally, it was shown that the reaction rate constants of the tested compounds increase with increasing temperature. (Table 1)

Thanks to the National Science Center for funding the research. Project OPUS 21 nr: 2021/41/B/ST10/02748

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SYNTHESIS, POLYMORPHISM AND SHAPE COMPLEMENTARITY-INDUCED CO-CRYSTALLIZATION OF HEXANUCLEAR CO(II) CLUSTERS

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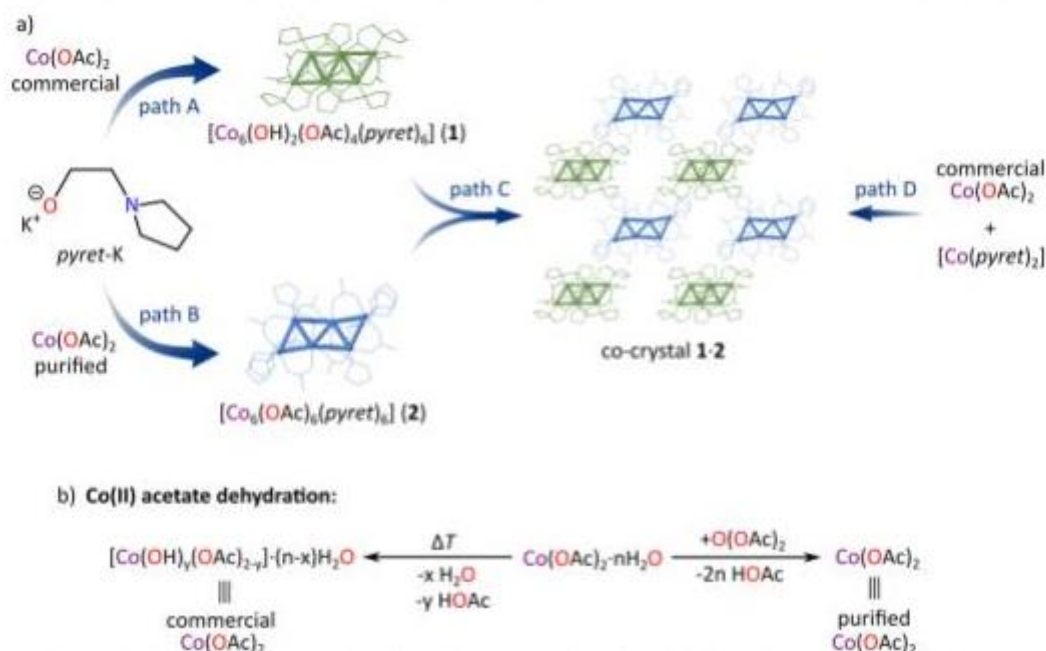
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The introduction of organic or inorganic additives either deliberately as materials dopants or serendipitously as impurities in reaction systems may significantly alter the characteristics of the products, leading to their new unique properties. Notably, many groundbreaking discoveries have been initiated by accidental contamination of the reaction systems, such as the development of Ziegler–Natta catalysts for olefin polymerization originated from the observation of catalytic effects of nickel impurities from the steel reaction vessel,[1] the first syntheses of ferrocene by passing hot cyclopentadiene vapor through an iron pipe,[2] or even development of the first controllable synthesis of colloidal quantum dots by Bawendi, who used old batches of n-butylphosphine contaminated by its oxidated form.[3]



Herein, I present our studies about synthesis and characterization of two new heteroleptic hydroxido-acetato and acetato Co(II) clusters $[\text{Co}_6(\text{OH})_2(\text{OAc})_4(\text{pyret})_6]$ (1) and $[\text{Co}_6(\text{OAc})_6(\text{pyret})_6]$ (2) incorporating auxiliary 2-pyrrolidinoethoxylate (pyret) ligands.[4] On this occasion, we revealed that the commonly used thermal procedure for dehydration of

cobalt(II) acetate leads to a reagent comprising substantial contamination by cobalt hydroxido moieties.

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THE STUDY OF NEWLY PROPOSED WORKING FLUIDS IN ABSORPTION REFRIGERATION TECHNOLOGY

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The search for alternatives to various energy-intensive traditional technologies has recently become extremely desirable in both academia and industry. One such technology is refrigeration technology.

Currently, the most widely used and main type of cooling is compressor refrigeration, which the devices consist of three main elements: evaporator, condenser, and compressor in. However, a mechanical compressor requires a significant amount of electricity to operate. An alternative to this type of refrigeration is absorption refrigeration, which instead of a mechanical compressor, the so-called thermal compressor composed of an absorber and a desorber is used in. The movement of the refrigerant is therefore initiated by the process of absorption and desorption under conditions of changing pressure and the supply of heat. The heat required to separate the absorbate from the absorbent may be waste heat, which is generated as waste in various types of industrial plants. This means that overall electricity consumption and operating costs are lower, unlike compressor refrigerators.

Absorbent and absorbate make working pairs necessary for the operation of an absorption refrigerator. Currently, two commonly used working pairs are {lithium bromide + water} and {water + ammonia}. However, both pairs are not without numerous disadvantages. In aqueous lithium bromide there is a problem with salt crystallization in the circuit and salt corrosion, and in the case of {water + ammonia}, the initial cost is a significant problem due to the need for a rectification column as both components are volatile and the need to monitor the tightness of the device as the mixture of air and ammonia is explosive. Moreover, absorption refrigerators based on both systems have lower coefficients of performance (COP) values and thus lower cooling efficiency than compressor refrigerators.

Our goal is to find new, problem-free working pairs with high coefficients of performance. We have proposed new working pairs consisting of diethyl- and dimethyl ionic liquids as the absorbent and ethanol as the absorbate. We have performed several studies, which included measurements of density, viscosity, vapor-liquid equilibria (VLE) [1], and excess enthalpy of mixing [2]. We also have performed calorimetric analysis of ionic liquids and calculated coefficients of performance values [3] based on procedure proposed by Yokozeki [4]. In our research, we have checked how the influence of structural elements of ionic liquids, i.e. the length of the alkyl chain in the cation and anion, or the presence of various functional groups affects the tested values. The obtained results indicate that the newly proposed working pairs can be an alternative to conventionally used working pairs.

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TRIBLOCK COPOLYMERS PREPARED THROUGH RAFT, COMPRISING CYCLIC ANHYDRIDE MOIETIES, ACTING AS RECYCLING ENHANCERS FOR POLYAMIDES

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Polyamides (PA) are a group of semicrystalline thermoplastics with high melt temperatures and excellent mechanical properties. [1] They are utilized in the production of fabrics, carpets, airbags, nets, etc., but also in the manufacturing of construction elements, photovoltaic panels, blood bags, and many more. [2] They are widely used, but unfortunately not widely recycled, as reprocessed PA have worse properties than virgin materials. [1] This is due to the polymer degradation occurring during the recycling process. [3] At elevated temperatures, polyamide chains are cut to shorter moieties, most often with the aid of water (hydrolysis) or by radical processes (thermooxidative degradation), which results in lowered melt viscosity and mechanical properties.

In this work, we designed, synthesized, and studied five macromolecular block copolymers with polycarbonate or polyether cores and poly(styrene-co-maleic anhydride) side chains. The side chains' purpose is to act as PA chain extenders, while the core's is to modify tensile and impact strength. The additives were synthesized by the Reversible Addition Fragmentation chain Transfer (RAFT) polymerization method. The copolymers, when processed with PA in the melt state, could join together short PA chains by the reaction of maleic anhydride moieties with PA end groups, hence compensating for the hydrolytic degradation. Therefore, the additives could improve PA's mechanical recycling. This was proven by much higher viscosity values during reactive extrusion of PA-additive blends than neat PA. Moreover, since those macromolecules bond covalently with PA chains, the ability of the additives to migrate and leech out is limited to the minimum.

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SYNTHESIS OF AZO DERIVATIVES OF CHALCONES

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From a biological point of view, chalcones with different structures are important natural and synthetic compounds that find application in many fields of science and technology. They exhibit a wide spectrum of biological activities [1], such as analgesic [2], anti-tuberculosis [3], antipyretic, antibacterial, antifungal [4], anti-HIV [5], as well as anti-inflammatory and anticancer [6] properties. The health benefits of natural chalcones can be attributed to their redox properties and their ability to eliminate radical oxygen species. Chemically, a chalcone consists of two aromatic rings (ring A and B) connected by a strongly electrophilic three-carbon α , β -unsaturated carbonyl system ($-\text{CO}-\text{CH}=\text{CH}-$) (Fig. 1).

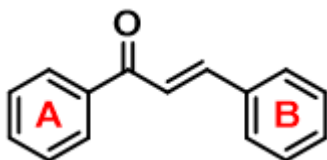


Figure 1

Due to the biosynthetic pathways occurring in plants, chalcones derived from them have -OH and MeO- substituents on rings A and B. Introducing an azo bond into the stilbene structure of the chalcone creates a system capable of reversible transition between two thermodynamically stable states possessing different molecular structures - E and Z states. These are so-called molecular switches. They can be used to deliver drugs to infected cells, known as molecular photoswitches (photopharmacology). This can be achieved, for example, by incorporating the molecule into a membrane channel and then, under the influence of light, opening the channel in the cell and introducing the therapeutic substance [7].

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STUDIES ON THE AIE EFFECT IN MECHANOCHEMICALLY SYNTHESIZED POLYAROMATIC AMIDES.

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Aggregation-induced emission (AIE) effect, described for the first time in 2001 [1], has significantly changed the perception of the design of light-emitting materials [2]. Unique light-emitting properties in the aggregated state make these compounds very promising molecules from the viewpoint of applied sciences. Particular interest has been focused on the AIE-active to chemoreceptors. Mechanochemistry, although known since ancient times [3], is considered a modern and attractive synthetic tool in organic chemistry. It allows a significant reduction in the use of harmful reactants and waste generation, as well as the synthesis of compounds impossible to obtain by standard methods.

Despite mechanochemical synthesis and design of AIE-active compounds are emerging fields of chemistry, the reports dealing with merging these concepts are extremely sparse [4]. In this poster, the results of mechanochemical synthesis of series of novel polyaromatic amides will be presented. Mechanochemical synthesis was carried out using a house-made milling system in a glass tube. The attractive AIE-related optical properties of the designed compounds will be discussed.

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