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Book of Abstracts

The 11th Torunian Carbon Symposium

Copernican revolution in carbon science



Welcome

It is a great honor to welcome you to the XI th Torun Carbon Symposium. It has been organized since 1992 by the Polish Carbon Society (ptw.edu.pl). The eleventh edition (TCS 2024) falls one year after the celebration of the Copernican year (2023) and one year before the 40th anniversary of the discovery of fullerenes (1985). The theme of the conference - Copernican Revolution in Carbon Science - is a reference to these anniversaries. The concept of fullerenes was difficult for skeptics to accept because it required acceptance of the presence of complex carbon structures in nature. The fullerene hypothesis and experimental evidence of its existence changed the way of thinking about carbon, which in "the pre-Copernican paradigm" could only exist in two allotropic varieties - diamond and graphite. "The post-Copernican paradigm" in carbon science has resulted in the synthesis of new carbon materials with reduced dimensionality, including nanotubes and graphene, exhibiting a spectrum of impressive properties, so to speak, opening up the field of nanotechnology. The change in thinking has led to development of a wide spectrum of materials with reduced dimensionality that revolutionize science and technology.

The conference will discuss achievements and new challenges facing carbon materials in various allotropic forms, from 0-dimensional to 3-dimensional structures, as well as other synthetic carbon materials used in aerospace, automotive, construction, energy conversion and storage, electronics or optics. Issues related to modern applications of carbon materials in medicine or environmental protection will be discussed, as well as topics aimed at working towards reducing the negative impact of carbon-related industries on the natural environment. We really hope you enjoy the conference and that you make lots of new friends!

Paweł Schroeder

Chairman

Aneta Frączek-Szczypta

Vice Chairman

Mirosława Pawlyta

Vice Chairman



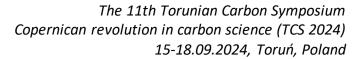




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Invited Talks





Carbon nanostructures: Revolutionary objects for tackling real-world challenges

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Carbon nanostructures cover a rich family of objects in two, one, and zero dimension. Conceptually, they have in common a hexagonal network of sp2 hybridized carbon atoms, forming the 2D sheet of graphene [1]. Introducing structural defects and curvature, provides the base for the revolutionary extension into closed hollow 1D nanotube [2] and 0D fullerenes [3]. Their beautiful and highly perfect structure endows each of these low dimensional objects a whole bunch of unpreceded functional properties with world-record characteristics. Having found their way into the market, they offer unique opportunities for the fabrication of novel, high performing device structures and sustainable technologies contributing to tackle major challenges mankind actually is facing.

This presentation will provide a travel through the revolutionary aspects of carbon nanostructures. First, it will cover the fundamental aspects on the relationship between structure and properties. Second, it will concentrate on processing issues and pathways towards sustainable electronic device fabrication. Third, at hand of selected examples of own latest research findings on nanoscale, processing and device performance [4-10], it will lay out the contribution of carbon nanostructures to the field of energy applications as emerging solution to face the challenge of clean and sustainable energy production.

- [1] K.S. Novoselov, A.K. Geim, et al, Science 306, 666-669 (2004)
- [2] S. lijima, Nature 354, 56-58 (1991)
- [3] H.W. Kroto, J.R. Heath, S.C.O'Brien, R.F. Curl, R.E. Smalley, Nature, 318, 162-163 (1985)
- [4] M. Peláez-Fernández et al., Carbon 178 477-487 (2021)
- [5] E. Palacios Lidón et al., ACS Mater. Lett. 3, 1826-1831 (2021)
- [6] S. Victor-Román, Catal. Today 357, 350-260 (2020)
- [7] J.M. González-Domínguez et al., Nanomaterials 11, 1435 (2021)
- [8] A. Ansón-Casaos et al., Int. J. Hydrogen Energy 46, 12180-12191 (2021)
- [9] E Colom et al., Chem. Mater. 35, 3522-3531 (2023)
- [10] C. Martínez-Barón, Green Chem. (submitted 2024)





Catalytic graphitization of non-graphitizing carbons

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Keywords: non-graphitizing carbons, catalytic graphitization, graphite, lithium-ion cells.

The slowdown of climate change requires vast utilization of "green", bio-derived carbon materials. In fact, a growing number of biomass pyrolysis plants have come in recent years, and this may be a great source for the production of graphite for applications in energy storage and conversion. Current graphite production, whether obtained through high temperature (3000 °C) transformation (synthetic graphite) of graphitizing carbons or mining (natural graphite), is highly deleterious to the environment. Recently, many studies have demonstrated that biochars derived from pyrolyzed biomass and other non-graphitizing carbons could be converted to high purity, highly crystalline graphite [1,2]. Additional reports have shown the potential for the conversion of biomass to anode active materials of lithium-ion cells [3,4].

The most efficient method for the production of graphite from non-graphitizing carbons is catalytic graphitization. Typically, this process turns amorphous carbon into graphitic structures with the assistance of a transition metal catalyst such as Fe, Ni, Co, Mn, and Cr. Also, semi-metals, such as Si, cause a catalytic graphitization effect. What is more, the presence of catalyst particles can lower the temperature of the structural transformation towards graphite in both non-graphitizing and graphitizing carbon precursors.

This contribution will present recent progress in the catalytic graphitization of non-graphitizable carbons. The advantages and weak points of this technology and the resulting graphitic materials will be discussed. The poorly understood phenomena, such as the mechanism of the catalytic graphitization and the porosity collapse during the process, will be exposed. Finally, the potential of utilization of the catalytically-graphitized bio-carbons in the sodium-ion and lithium-ion technology will be evaluated. The literature achievement will be confronted with the experimental results (X-ray diffraction, small-angle scattering, Raman spectroscopy, scanning and transmission electron microscopy, electrochemical tests) obtained for catalytically-graphitized saccharides and furfuryl resins.

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- [1] Z. Shi, S. Wang, Y. Jin, L. Zhao, S. Chen, H. Yang, Y. Cui, R. Svanberg, C. Tang, ..., T. Han, SusMtt, 3 (2023) 402415.
- [2] A. Gomez-Martin, Z. Schnepp, J. Ramirez-Rico, Chemistry of Materials, 33 (2021) 3087-3097.
- [3] L. Lower, S. C. Dey, T. Vook, M. Nimlos, S. Park, W. J. Sagues, ChemSusChem, 16 (2023) e202300729.
- [4] N. A. Banek, K. R. McKenzie Jr, D. T. Abele, M. J. Wagner, Scientific Reports, 12 (2018) 8080.





Electrochemical energy storage with carbons

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Keywords: carbons, metal-ion batteries, electrical double-layer capacitors, metal-ion capacitors.

Energy management is an unavoidable strategy in the panel of solutions to reduce fossil consumption and greenhouse gases emissions. To manage the fluctuations of renewables and on-board energy in vehicles, electrochemical energy storage can be used to adapt the delivery to the demand. Two main systems may be applied, batteries and electrical double-layer capacitors (EDLCs), which store energy through faradaic and electrostatic processes, respectively. Due to these mechanisms, batteries store high amount of energy, whereas EDLCs are perfectly adapted to harvest energy in small amount during short periods of time, for example during braking of vehicles. Presently, all the research efforts are guided by enhancing the electrochemical performance of both systems, while implementing environmentally friendly materials and reducing the production costs.

Graphite has been early recognized as the material of choice for anodes of Li-ion batteries. To enhance the power delivery of these systems, hard carbons have been implemented, especially for the sodium-ion systems where graphite displays a poor performance. Fashionable materials, such as carbon nanotubes (CNTs) have been also proposed, yet their large mesopore volume favours a high irreversibility of metal insertion, leading to a poor cycle life of the batteries. Nonetheless, CNTs added in small proportion in the formulation of electrodes might be very useful to enhance their conductivity and thereof power of the devices.

Nanoporous carbons (especially activated carbons — ACs) owing to their versatility of structure/texture, morphology, low cost and highly developed surface area are the basic electrode material for EDLCs [1]. New forms of carbons, e.g., carbon nanotubes and graphene, as well as carbon black are applied for the percolation of electrodes or as support for electroactive materials. In all cases, these various carbon forms are designed to enhance the specific energy of EDLCs, while developing safe and environment friendly solutions. High energy EDLCs can be realized with ionic liquids by the implementation of hierarchical porous carbons having i) mesopores produced by silica templating carbonization of glucose and ii) micropores simultaneously created in the pore walls by ZnCl2 activation. Appropriate glucose/SiO2/ZnCl2 proportions enable to optimise simultaneously the micro-/mesopore volume ratio and the density of carbons, and develop high volumetric energy EDLCs able to operate at high power with ionic liquid from -40 to 100 °C.

Despite their interesting features, EDLCs come nevertheless with limitations, such as notably low specific energy and a significant rate of self-discharge compared to other types of energy storage systems. These disadvantages may hinder their application as a primary power source in hybrid vehicles and their integration into the electrical power grid. Therefore, metal-ion capacitors (MICs) combining an electrical double-layer positive electrode and a battery-type negative electrode have emerged as a promising energy storage technology [2] due to two notable features: i) the negative carbon electrode operates at low potential, thus, the maximum operative voltage of MICs is significantly higher than that of an AC//AC capacitor, reaching generally 3.8 V; ii) the EDL positive porous carbon electrode operates in a wider potential range than the positive electrode of an EDLC, typically between e.g., 2.5 V and 4.1 V vs Na/Na+ for a sodium-ion capacitor [2], thus the capacity/capacitance of the device is larger than in a conventional EDLC. This unique configuration enables MICs to achieve up to ca. four times higher specific energy than EDLCs at comparable power levels, which makes them very promising for applications in electric vehicles. The operando track of ion population changes in the EDL carbon electrode of a lithium-ion capacitor will be presented during its charge/discharge.

- [1] A. Frackowiak, F. Béguin, Carbon, 39 (2001) 937-950.
- [2] A. Chojnacka and F. Béguin, Electrochem. commun., 139 (2022) 107305.





Carbon-based electrocatalysts for energy generation reactions

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Keywords: carbon materials, electrocatalysts, oxygen reduction reaction, non-precious electrocatalysts.

Carbon materials possess unique properties that make them valuable for a wide range of technological applications. This diversity in properties arises from their different structures. Surface chemistry, influenced by the concentration of intrinsic defects and the presence of heteroatoms, plays a crucial role in determining the properties of the carbon materials. Then, the combination of structure and surface chemistry results in an enormous collection of materials with properties that can be tailored for many different applications.

Recently, the development of electrochemical energy storage and production devices has significantly increased interest in carbon materials. In this field, the role of carbon materials as catalyst or catalyst support is outstanding and strong research and technology development efforts are being done trying to optimize the performance of electrochemical technologies, which are still far from industrial requirements.

In the specific context of energy generation using fuel cells or metal-air batteries, a significant challenge arises from the sluggish kinetics of the oxygen reduction reaction (ORR) at the cathode. This limitation needs substantial quantities of precious metals, hindering widespread adoption of the technology. Consequently, extensive research efforts are focused on developing alternative catalysts, such as metal-free carbon materials or non-precious metal-based catalysts, capable of replacing precious metals. Carbon materials properties enable them to play various roles in the ORR, including acting as catalysts, catalyst supports, and promoters of catalytic activity. In this presentation, we will explore examples illustrating these three functions of carbon materials in ORR. Our discussion will highlight the growing interest in finely tuning the structure and chemical composition of materials at the nanoscale to enhance catalytic properties. Specifically, we will examine N-doped carbon materials as catalysts, emphasizing the nature of their active sites. We will also showcase Fe-phthalocyanine catalysts supported on functionalized carbon nanotubes to illustrate the role of carbon as a catalyst support. Finally, we will discuss the pivotal role of carbon materials in enhancing the catalytic activity of perovskite-type metal oxides.

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Carbon as a pollutant and a nanomaterial: spectroscopic and chemical diagnostics for unveiling its structure

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Keywords: carbon pollutants, carbon nanomaterials, soot, particulate, advanced diagnostics.

While reducing carbon particulate matter emissions from transportation engines is a pressing challenge for modern societies, recent findings regarding the extraordinary properties of carbonaceous functional nanomaterials have opened up new possibilities for the large-scale, flame-based synthesis of these otherwise undesirable combustion products. In both cases, the elusive character of combustion-formed carbon particulate—which is primarily caused by its complex structure that is highly variable with temperature, residence time, and fuel identity—limits our capacity to research novel, optimum solutions based on the particular industrial end-user needs. Indeed, our current understanding of this intriguing yet intricate subject is still lacking.

Because of the complexity of carbon particulate matter, a broad range of diagnostic instruments tailored to the identification of structure, size, and chemical composition are needed, and often not enough, for its thorough characterization. This is particularly true when considering ultrafine and nano- particles, which have a size of less than 100 nm.

In order to create innovative nanomaterials and for achieving clean transportation in the future, a better understanding of the structure of carbon particulate matter will enable improvements in engine design, fuel reformulation, or industrial process optimization. These improvements will have a significant positive impact on the economy, the environment, and citizen standards of living.

The main characteristics of ultrafine and nanocarbon particulate matter generated under controlled combustion conditions and collected by batch sampling methods are briefly reviewed in this keynote, along with an overview of the analytical methodology employed by our team. Advantages and drawbacks of the techniques more recently developed have been analyzed, for building and resolving the analytical puzzle represented by carbon particulate matter characterization. Its optical properties, which make it appealing as a material for application in the fields of imaging, electronics or sensors, have been also highlighted.

References

- [1] Russo, C., Apicella, B., Ciajolo, A. (2023) Hydrogen, sp2 Carbon Hybridization, and sp2 Clustering as Pieces of the Puzzling Nanostructure of Soot: A Closer Look. Energy Fuels, 37, 17, 12525–12540; https://doi.org/10.1021/acs.energyfuels.3c01194
- [2] Russo, C., Ciajolo, A., Stanzione, F., Tregrossi, A., Apicella, B. (2023) Separation and online optical characterization of fluorescent components of pyrogenic carbons for carbon dots identification Carbon, 209, 118009 https://doi.org/10.1016/j.carbon.2023.118009
- [3] Russo, C., Carpentieri, A., Tregrossi, A., Ciajolo, A., Apicella, B. (2023) Blue, green and yellow carbon dots derived from pyrogenic carbon: Structure and fluorescence behaviour Carbon, 201, pp. 900–909, https://doi.org/10.1016/j.carbon.2022.09.062
- [4] Russo, C., Apicella, B., La Rocca, A., Sirignano, M. (2023) Fluorescent carbon dots synthesis in premixed flames: Influence of the equivalence ratio Carbon, 201, 659–666,

https://doi.org/10.1016/j.carbon.2022.09.061

[5] Apicella, B., Russo, C., Carpentieri, A., Tregrossi, A., Ciajolo, A. (2022) "PAHs and fullerenes as structural and compositional motifs tracing and distinguishing organic carbon from soot" Fuel, 309, 122356, https://doi.org/10.1016/j.fuel.2021.122356.





Engineered Diamond Surfaces & Heterostructures: Sensors for Environmental Monitoring and Life Science Applications

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Keywords: CVD diamond films, surface-termination, field effect transistor, chemical sensing, biosensing.

Diamond films grown by chemical vapor deposition exhibit a remarkable combination of properties advantageous for sensing applications, including tunable surface functionalities, high chemical stability, semiconductor behavior, and biocompatibility. This study briefly reviews recent advances in tailoring the plasma properties, gas composition, pressure, and temperature during microwave plasma CVD growth of diamond films to control the resulting film properties for gas and biosensing [1].

Hydrogen-terminated diamond surfaces induce a highly sensitive two-dimensional hole gas that enables room-temperature detection of oxidizing (NO2) and reducing (NH3) gases [2,3]. The influence of nanostructured surface morphology on the gas sensor response will be discussed. Benchmarking against commercial SnO2 layers elucidates the distinct sensing mechanisms operative for H-terminated diamonds, especially in a heterostructure with 2D materials (MoS2 or GO).

Furthermore, diamond surface terminations and morphologies critically impact the patterned adhesion of cell lines, a crucial consideration for bioelectronic applications. Label-free cell detection is demonstrated using diamond-based field-effect transistors, providing insights into real-time monitoring capabilities and sensor performance metrics like sensitivity, stability, and reliability. Novel biosensing principles based on impedance, optical, and mass transduction modes using diamond devices will be presented [4,5].

The scientific findings highlight the potential of engineered diamond films as a multifunctional material platform for advanced chemical and biological sensing [6,7] by elucidating key structure-property relationships that govern sensing performance.

- [1] M. Varga et al., ACS Omega, 2019, 4, 8441.
- [2] M. Davydova et al., Beilstein Journal of Nanotechnology, 2014, 5, 2339.
- [3] M. Kočí et al., ACS Applied Materials & Interfaces, 2023, 15, 34206.
- [4] A. Broz et al., Journal of Biomedical Materials Research Part A, 2017, 105, 1469.
- [5] M. Krátká et al., Colloids and Surfaces B: Biointerfaces, 2021, 204, 111689.
- [6] R. Pfeifer et al., ACS Applied Engineering Materials, 2023, 1, 1446.
- [7] M. Augustín et al., Bioelectrochemistry, 2024, 158, 108691.





Copernican revolution(s) in carbon science

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Keywords: fullerenes, carbon nanotubes, graphene, graphite, negative magnetoresistance, superconductivity.

A series of breakthroughs in carbon science, such as fullerenes (1985) [1], carbon nanotubes (1991) [2], and graphene (2004) [3], would not have been possible without the efforts of many generations of researchers. These were preceded by research on graphite oxide and graphite intercalation compounds, dating back to Schafheutl's reports on graphite intercalation and exfoliation in the 1840s. In these compounds, electron decoupling leads to extraordinary electronic properties. The term graphene was first proposed by Boehm in 1962 [4], who studied the phenomenon of electron decoupling in graphite exfoliated by chemical methods. Electron decoupling leads to extraordinary electronic properties of low dimensional sp2 carbons, such as high charge carrier mobility and high conductivity. For heat transport in isolated graphene layers collectively excited phonons with an average free path of hundreds of micrometers are responsible, leading to high thermal conductivity. In some cases, superconductivity is observed in these systems.

Superconductivity can be found among the phenomena that are revolutionizing the carbon science. The possible superconductivity in carbon materials was first reported by Prof. Antonowicz in 1974 [5]. The Antonowicz hypothesis is currently being developed in many centres around the world in fullerenes, HOPG and other carbon materials. The mechanism explaining the superconducting behavior is still not fully understood. All that is known is that the superconducting phase(s) exist in the graphene matrix.

- [1] H.W. Kroto, J.R. Heath, S.C.O'Brien, R.F. Curl, R. Smalley, Nature, 318 (1985) 162.
- [2] S. Iijima, Nature 354 (1991) 56-58.
- [3] K.S. Novoselov, A.K. Geim, S.V. Morozov et al. Science, 306 (2004), 666-669.
- [4] H. P. Boehm, A. Clauss, G. Fischer, U. Hofmann in Proceedings of the Fifth Conference on Carbon, Pergamon Press, Heidelberg, Germany, 1962, p. 73.
- [5] K. Antonowicz, Nature, 247 (1974) 358-360





Oral Presentations





Selective sorting of single-wall carbon nanotubes using conjugated polymers in organic solvents

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Keywords: Single-Walled Carbon Nanotubes, Conjugated Polymer Extraction, Solvents, Chirality

Single-walled carbon nanotubes (SWCNTs) with semiconducting characteristics find great utility in photonics, nanomedicine, and microelectronics, among other fields. Nevertheless, challenges in producing chirality-specific fractions with desirable properties continue to impede many exciting SWCNT-based concepts [1]. Numerous sorting strategies have developed over time to address this challenge.

Conjugated polymer extraction is a powerful, selective technique. Additionally, the method makes use of the isolated SWCNTs' pre-existing volatile organic solvents, which makes them perfect for the manufacture of devices. Although there are benefits, the sorting procedure is poorly understood, and only (6,5) and (7,5) SWCNTs are typically isolated using this method [2].

Here, we outline the process we used to extract specific SWCNTs from complicated mixtures utilizing a variety of organic solvents and conjugated polymers that were specially created. Monochiral suspensions of (7,3) SWCNTs were effectively synthesized by carefully adjusting the polymer properties and separation conditions [3]. We discussed the inverse connection between efficiency and purity, which is a common issue in the purification of nanomaterials. We used mixed solvent engineering using toluene and tetralin to create a substrate that exhibited both remarkable purity and great performance.

- [1] D. Janas, Towards monochiral carbon nanotubes: a review of progress in the sorting of single-walled carbon nanotubes, Materials Chemistry Frontiers 2 (2018) 36-63.
- [2] A. Dzienia, D. Just, D. Janas, Nanoscale, Solvatochromism in SWCNTs suspended by conjugated polymers in organic solvents, Nanoscale 15 (2023) 9510-9524.
- [3] A. Dzienia, D. Just, P. Taborowska, A. Mielanczyk, K.Z. Milowska, S. Yorozuya, S. Naka, T. Shiraki, D. Janas, MixedSolvent Engineering as a Way around the Trade-Off between Yield and Purity of (7,3) Single-Walled Carbon Nanotubes Obtained Using Conjugated Polymer Extraction, Small 19 (2023) 2304211.





Electrocatalysts, adsorbents for arsenic removal and components for polymer composite membranes based on pyrolytic carbon deposited on metals/metal oxides derived from hydrotalcite-like materials

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Keywords: oxygen reduction reaction, arsenic removal, poly(ε -caprolactone)-based composite membranes.

This presentation is devoted to N-doped carbon materials in combination with Fe- or Ni-containing species examined as electrocatalysts in oxygen reduction reaction (in alkaline medium), adsorbents for eliminating water pollutants such as inorganic arsenic species and as components for the preparation of conductive polymer-based composite membranes, in order to demonstrate their versatile properties.

A series of the composites of N-doped carbon materials and Fe or Ni species was synthesized via chemical vapour deposition (CVD) acetonitrile (as carbon and nitrogen source) at 600, 700 and 800 oC for 30 minutes in the presence of metal oxides derived from hydrotalcite-like materials (HTs) of various chemical compositions (MgAl, MgFeAl, NiAl). The samples were treated with hydrochloric acid in order to remove inorganic compounds such as metal/metal oxides, which were not anchored to the carbonaceous component. Acid treatment of the samples after synthesis did not completely eliminate inorganic compounds, there was still (~ 10 - 30 %) a non-carbon component tightly covered with a carbon deposit, e.g. iron or nickel nanoparticles involved in the formation of carbon nanostructures. The physicochemical features of the obtained composites were described by means of several techniques including powder X-ray diffraction (XRD), elemental analysis (EA), volumetric nitrogen sorption, X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, scanning electron microscopy (SEM). The carbon materials differed in the morphology of carbon grains, specific surface area and of micro- and mesopore volumes, nitrogen content. The concentration of Fe- and Ni-containing species in acid-treated samples also varied.

Judging by the values of kinetic current, onset potential and number of electrons the most active for ORR was the composite obtained at 700 oC using MgFeAl HTs. Its electrocatalytic performance seemed to be a result of a relatively high content of Fe species ($^{\sim}$ 0.77 at. %) covered with graphitic layers doped with nitrogen located at the edges of the graphene layer ($^{\sim}$ 2.79 at. %), in particular graphitic nitrogen ($^{\sim}$ 1.06 at. %), which could be responsible for generating active sites for ORR on the neighbouring carbon atom.

Depending on surface Ni concentration (determined by XPS), i.e. 1.0, 0.4 and 0.2 % at., the composites obtained at 600, 700 and 800 oC using NiAl HTs were able to adsorb various amounts of As (V), i.e. 9.69, 8.64 and 6.63 mg g-1.

The highest electrical conductivity of 10-4 [S m-1] was shown by the composite membranes prepared with the addition of 0.13 or 0.26% wt. carbon component obtained at 800 oC with the use of NiAl HTs. The carbon component in the form of lamellar grains contributed less to the improvement of the conductivity of the composite membranes than the one in which, in addition to the lamellar grains, tubular grains were present; the probable reason for this was that carbon materials made of lamellar grains were characterized by thinner graphite domains and contained more amorphous carbon compared to samples containing carbon nanotubes, and furthermore, tubular grains could be better dispersed in the polymer matrix in the composite material than lamellar grains, which were in the form of aggregates - difficult to dispersed by means of ultrasound; it is possible that metal nanoparticles (Fe or Ni) trapped in carbon nanotubes could also contribute to the electrical conductivity of the membranes obtained with their participation.

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Electroconductivity enhancement of electrospun PVDF fibers by selective MWCNT electrophoretic deposition

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Keywords: electrospinning, PVDF, MWNT, electrophoretic deposition (EPD), energy harvesting, electrospun fibers.

The rapid advancement of smart electronics and self-powered technologies has sparked a significant interest in piezoelectric materials, notably electrospun polyvinylidene fluoride (PVDF) fibers, recognized for their flexible and porous structure and high piezoelectric coefficients[1]. This study addresses the challenge of enhancing the electroconductivity of these fibers to better serve energy harvesting applications. We employed electrophoretic deposition (EPD) to deposit multi-walled carbon nanotubes (MWCNTs) onto electrospun PVDF fibers. Moreover, by optimizing the deposition parameters, we are able to ensure uniform coverage while maintaining the high porosity of mats, which is essential for their application in flexible smart textiles.

Our results indicate that the optimized EPD process not only preserves the intrinsic properties of the fibers but significantly enhances their electrical conductivity. This was achieved by maximizing the contact area between the carbon nanotubes (CNTs) and the polymer fibers, thereby drastically reducing their resistivity. The morphology of the resulting fiber mats was characterized by scanning electron microscopy (SEM), while the electrical conductivity was measured using a two-point probe setup. Such enhancements are crucial for the development of next-generation smart textiles capable of sensing and energy harvesting where electrospun fibers with conductive coatings can be used.

This research underscores the potential of combining traditional fiber electrospinning techniques with nanoscale material deposition to create advanced materials with tailored properties for specific technological applications. Our findings contribute to the broader field of material science by providing a scalable method to enhance the functionality of piezoelectric fibers, paving the way for innovative applications in smart devices and textiles[2].

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References

[1] Sukumaran, S., Szewczyk, P.K., Knapczyk-Korczak, J., and Stachewicz, U. (2023) Optimizing Piezoelectric Coefficient in PVDF Fibers: Key Strategies for Energy Harvesting and Smart Textiles. Advanced Electronic Materials, 9 (12), 1–12.

[2] Szewczyk, P.K., Taşlı, A.E., Knapczyk-Korczak, J., and Stachewicz, U. (2023) Steering triboelectric and mechanical properties of polymer fibers with carbon black. Composites Science and Technology, 243,0–10.



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Potential of using spent magnetic carbonaceous adsorbents in blast furnace coke blends

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Keywords: carbonaceous adsorbents, magnetic properties, coke

The presence of iron gives an opportunity to treat the spent carbonaceous adsorbent with magnetic properties in a copyrolysis process for metallurgic coke production. To make the blast furnace more environmentally sustainable, it is necessary to reduce its energy consumption and greenhouse emissions. This can be performed by using highly reactive coke. The reactivity of metallurgic coke can be increased by the addition of an iron catalyst.

The main aim of this work is to study the effect of the addition of a spent magnetic adsorbent on the parameters that characterise the properties of the coking mixture. The adsorbents have been obtained from polyfurphuryl alcohol [1] and sawdust. The proportions in which these admixtures can be used are determined to obtain the best parameters of coke reactivity while maintaining mechanical strength and a low content of ballast in the form of mineral impurities. To establish this, the following tests are performed: coking power by the Roga test and plastic properties by the Audibert-Arnu test. Furthermore, the determination of the hardness of cokes and the reactivity of coke towards CO2 was carried out. The selected coke blend was also characterised in terms of SEM-EDX, XRD, and TGA 8000 Perkin Elmer- FTIR .

The study showed that the type of starting material from which the carbonaceous magnetic adsorbents were obtained had no effect on the final strength of the coke. This characteristic was dependent on the amount of spent adsorbent added. The increasing addition of iron-containing composites amplify the reactivity of the obtained coke. However, the addition above 15 % leads to a drop in the degradability. The type of starting material from which the magnetic adsorbent was obtained had a significant effect on the plasticity properties of the coke mixture. The addition of adsorbents obtained from biomass reduced the dilatation to a high extent, but the polymer-based magnetic adsorbents did not induce such an effect.

This work shows that the spent carbonaceous magnetic adsorbents are promising additives for the preparation of the coke of the furnace.

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References

[1] E. Lorenc-Grabowska, O. Stasiak, K. J. Kordek-Khalil, Adsorption 30 (2024) 279–291.





Electrolytic water disinfection and hydrogen production from real wastewater

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Keywords: hydrogen evolution reaction, non-noble metal catalyst, hydrogen evolution overpotential.

Wastewater in urban areas is usually processed in municipal wastewater treatment plant before it enters the river. Water being an effluent of this process is devoid of majority of contaminants, however, it is still not fully remediated and drinkable. Electrochemical wastewater treatment might become an additional process to disinfect water from the organic pollutatnts hardly (or too costly) removable by conventional techniques. It can be realized by its oxidation using the hydrogen peroxide synthesized in the process of two-electron water oxidation. Simultaneously, production of hydrogen takes place at counter electrode, which can be further used as an energy carrier in fuel cells.

Two-electron water oxidation to hydrogen peroxide being a competitive process to four-electron water oxidation to oxygen is naturally less thermodynamically preferred, therefore an adequate catalyst is necessary to change this ratio. In this work, molybdenum-based catalyst deposited on nanostructured carbon was suggested for wastewater treatment to increase disinfective properties of the process and reduce the hydrogen evolution overpotential. This non-critical raw material catalyst makes the process more economically viable. Wastewater contaminants was simulated by methylene blue and its concentration was monitored in-situ using light absorption spectroscopy during electrolysis process at 3 V. We have noticed that electrode comprising molybdenum(VI) oxide was able to decolour the solution at higher rate than only carbon-based electrode. Although it was more efficient towards water disinfection, less amount of accumulated hydrogen peroxide was detected. Disinfective properties indicate that the lifetime of produced hydrogen peroxide is short and it immediately turns into hydroxyradicals decomposing organics in real time.

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Comparison of thermally and chemically reduced graphene oxide cryogels

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Keywords: graphene oxide, reduced graphene oxide, cryogel, regeneration of graphenic structure

Graphene oxide (GO), formerly considered mainly as an intermediate in wet chemical graphene production, has now become a widely applicable material with expanding possibilities. While traditionally used in a solid, dry form for the production of GO-based electrodes and optoelectronic devices, it is often processed in a suspended state. Despite its beneficial hydrophilic nature, GO tends to lose many of its remarkable graphitic properties. To compensate for this, various reduction methods are available.

Different reduction techniques restore the graphenic properties with different efficiencies. This study investigates the effect of a physical (thermal) [1] and a chemical (ascorbic acid) [2] reduction method on GO. Characterisation using conventional analytical methods highlights the advantages and limitations of each alternative approach. A comprehensive analysis was carried out to reveal the morphology and surface chemistry of the reduced cryogels. Powder X-ray diffraction (XRD) and nitrogen adsorption were used for morphological analysis, while the possible regeneration of the graphenic structure was followed by Raman spectroscopy. The chemical composition was investigated with thermogravimetry/mass spectrometry and photoelectron spectroscopy (XPS). The overall effect of the surface chemistry is demonstrated by water vapour adsorption.

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References

[1] S. Farah, A. Farkas, J. Madarász, K. László, J Therm Anal Calorim 142 (2020) 331–337.

[2] M.J. Fernández-Merino, L. Guardia, J.I. Paredes, S. Villar-Rodil, P. Solís-Fernández, A. Martínez-Alonso, J.M.D. Tascón, J Phys Chem C, 114 (2010) 6426–6432.





Enhanced energy density of nitrogen-doped reduced graphene oxide aerogel-based symmetric supercapacitor in aqueous electrolytes

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Keywords: reduced graphene oxide aerogel, nitrogen doping, hydrothermal synthesis, symmetric supercapacitors, redox electrolyte

The development of efficient and long-lasting energy storage devices is becoming an ever more urgent need in the present day. The unique structural and morphological features of reduced graphene oxide aerogels (rGO aero), such as a stable and mechanically robust porous network combined with high electrical conductivity, allowed them to store large amounts of energy [1]. One of the effective methods to improve the surface properties of graphene-based active materials in supercapacitors is to incorporate heteroatoms such as nitrogen, phosphorus, boron, and sulphur into their structure [2]. Among them, nitrogen is the preferred element to be doped for several reasons. First, nitrogen atoms have an atomic size and molecular weight comparable to that of carbon atoms, which reduces the risk that the introduction of nitrogen significantly disrupts the structure of the graphene aerogel. Second, the introduction of nitrogen-containing functional groups into the graphene lattice improves hydrophilicity of the carbon surface. It has a positive impact on the wettability of electrodes working in an aqueous electrolyte, generates pseudocapacitance, and improves electronic conductivity [3]. The electrochemical performance of the supercapacitor can be further boosted by the addition of redox-active species to the electrolytes. The redox additive is adsorbed on the electrodes and undergoes reduction and oxidation reactions at potentials, which ensures additional pseudocapacitance to the energy storage device. Some typical redox additives contain KI, hydroquinone (HQ), 1,4-dihydroxyanthraquinone, Ce2(SO4)3 and Fe3+/Fe2+ [4,5].

In this study we have determined the influence of nitrogen doping on the electrochemical behaviour of a hydrothermally reduced graphene oxide aerogel. A 7.4 at. % of nitrogen was introduced into the structure of the synthesized of N-rGO aero. Several instrumental techniques were applied to characterize materials prior to electrochemical tests: N2 sorption at 77K, X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), scanning electron microscopy (SEM) and thermogravimetry analysis (TGA). The materials obtained by straightforward synthesis were tested in symmetrical systems using two aqueous electrolytes: acidic (1 M H2SO4) and acidic enriched in redox-active species (1M H2SO4+0.2MHQ). When 1M H2SO4 electrolyte was used in supercapacitors with rGO aero and N-rGO aero electrodes, an energy density of 12.3 and 14.5 Wh kg-1 was revealed, respectively. The addition of HQ into the electrolyte does not affect the system's working window but ensures that it yields a specific capacitance of 302 and 397 F g-1 and much higher energy density of 20.6 and 27.0 Wh kg-1, respectively. The experimental results show that the combination of nitrogen incorporation into the rGO aero structure and the addition of hydroquinone to the electrolyte is a highly effective way to improve the energy density of the supercapacitors.

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- [1] S. Korkmaz, A. Kariper, J. Energy Storage, 27 (2020) 1-12.
- [2] M. Pathak, D. Bhatt, R. C. Bhatt, B. S. Bohra, G. Tatrari, S. Rana, M. C. Arya, N. G. Sahoo, Chem. Rec., 24 (2023) 1-37.
- [3] Z.-Y. Sui, Y.-N. Meng, P.-W. Xiao, Z.-Q. Zhao, Z.-X. Wei, B.-H. Han, ACS Appl. Mater. Interfaces, 7 (2015) 1431–1438.
- [4] L. Zhang, S. Yang, J. Chang, D. Zhao, J. Wang, C. Yang, B. Cao, Front. Chem., 8 (2020) 1-7.
- [5] A. Moyseowicz, G. Gryglewicz, Electrochim. Acta, 354 (2020), 1-10.





Fundamentals and implication of PZC determination for activated carbons in aqueous electrolytes for Electrochemical Quartz Crystal Microbalance (EQCM) applications

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Keywords: Electrochemical capacitor, activated carbon, aqueous electrolyte, electrochemical quartz crystal microbalance

The point of zero charge (PZC) is crucial for investigating molecular level charging mechanisms in energy storage systems, as demonstrated in electrochemical capacitors. In this work, three electrochemical techniques were studied for PZC determination in electrochemical quartz crystal microbalance (EQCM) applications: cyclic voltammetry (CV), staircase potentio electrochemical impedance spectroscopy (SPEIS) and step potential electrochemical spectroscopy (SPECS) for two activated carbons (ACs) with 0.1 mol L – 1 aqueous solutions of LiNO3, Li2SO4, and KI. The porous AC charging process in aqueous electrolytes is a complex phenomenon; the ion mixing zone covered a wide potential region. Inadequate PZC determination could lead to obscure data evaluation, which could further provide a misguided mechanism description at the molecular level. In the aqueous solutions studied, the adsorption of specific ions and active participation of all ionic species in the electrical double-layer formation were considered. The SPECS technique was determined to be the most beneficial for the PZC determination in electrochemical quartz crystal microbalance (EQCM) applications. The advantage of this technique includes a short implementation step time (in this case, 1 mV s-1). Moreover, the potential shift is quite gentle and enables detailed data to be recorded in the entire potential range, increasing the recorded data resolution and accuracy. These potential steps lead to a smooth behaviour of probable redox reactions and balanced ion redistribution in the pores. Additionally, this method provides insights into the charging mechanism via a detailed specific capacitance division into a porous and a geometric one.

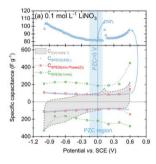


Fig. 1. Specific capacitance vs. potential calculated from the three electrochemical techniques: CV (gray shade), SPECS (blue triangular scatter) and SPEIS (red square and green circular scatter) for YP-50F and 0.1 mol L-1 LiNO3 in EQCM cell. The upper part of the plot represents the zoomed SPECS specific capacitance vs. potential in the Emin to Emax direction.

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Tailoring the properties of salt-templated carbons for energy storage systems

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Keywords: salt-templated carbon, electrochemical capacitor, aqueous electrolyte

Carbons with a developed surface area are typical electrode materials for electrochemical capacitors (ECs). However, activation process of carbon precursor allows to obtain texture without a strict control of pore size distribution. Here, novel approach so called soft- and salt-templated method [1,2] has been used to obtain attractive porous carbons with specific surface area ranging from 1450 to 2640 m2/g. In the present work, the various eutectic mixtures of alkali metal chlorides (CsCl, NaCl, LiCl, and KCl) have been used as salt-template. These salts can be easily washed out from the carbon samples using water. Such synthesis method is sustainable, ecofriendly, and provides fine control on carbon porosity.

The carbon material properties (structure, surface chemistry and porosity) were characterized in detail by different physicochemical techniques: XPS, Raman, TPD-MS, gas adsorption using nitrogen and carbon dioxide. Optimal carbon materials which combine large surface area and graphitic-like domains were achieved. All carbons were tested as electrode components for two-electrode ECs operating at 1.6V. Lithium sulfate (1M) served as electrolytic medium. Electrochemical performance was evaluated by cyclic voltammetry, galvanostatic cycling, floating, electrochemical impedance spectroscopy and self-discharge. High values of capacitance have been reached (125 to 250 F/g). Careful correlation of structural/textural/surface chemistry properties of carbons with capacitance values was examined and insightful correlations were observed. Ragone plot presents energy versus power density for all carbon samples used as electrodes of ECs (Figure 1).

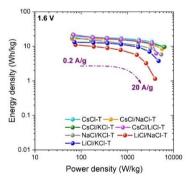


Figure 1: Ragone plot of salt-templated carbon materials in 1M Li2SO4

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- [1] A. Platek-Mielczarek, C. Nita, C. Matei Ghimbeu, E. Frackowiak, K Fic, ACS Appl. Mater. Interfaces 13 (2021) 2584.
- [2] C. Nita, M. Bensafia, C. Vaulot, L. Delmotte, C. Matei Ghimbeu, Carbon, 109 (2016) 227.





Diclofenac electrochemical detection: from modified glassy carbon electrode to miniaturized inkjet-printed setup

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Keywords: diclofenac, electrochemical detection, thermally reduced graphene oxides, inkjet-printing, miniaturized setup

Diclofenac (DCF) is an anti-inflammatory pharmaceutical product being an active compound in commercially available drugs, as for example Acoflam and Diclac. However, its overdose has negative impact on human health and can contribute to environmental pollution [1]. In consequence, there is a high interest on the development of an accurate and reliable methodology for DCF detection to meet EU regulations [2]. In this context, electrochemical techniques arise as potential alternatives for currently applied spectroscopic or liquid chromatography as they facilitate quick and easy measurements. Nevertheless, to improve sensors performance novel working electrode modifiers must be proposed. Among them, graphene-based materials have increased in interest due to their suitable properties as high electrical conductivity and enhanced surface to volume ratio. Moreover, miniaturization of detection setups is highly required to perform point of care measurements in low-volume samples [3]. Therefore, screen printed electrodes (SPEs), or inkjet printed electrodes (IPEs) are being evaluated.

In this work we propose facile, non-direct electrochemical DCF detection applying thermally reduced graphene oxides (TRGOs) as working electrode modifiers at neutral pH. Series of TRGOs obtained at different temperatures (400, 700 and 1000 °C) was tested as glassy carbon electrode (GCE) modifiers. Electrochemical measurements revealed a promising electrochemical response towards DCF when using TRGOs, achieving a limit of detection (LOD) of 61 nM. Moreover, selectivity studies in the presence of common interfering compounds (glucose, ascorbic acid and others) indicated their high potential application in real samples analysis. From these promising results, a novel miniaturized experimental setup based on IPEs was developed. IPEs were produced using cheap office printer, aiming to reduce cost of setup preparation. Inks formulation was optimized considering graphene oxide concentration, surfactant selection, carbon black addition and number of printed layers. They were subsequently printed on Kapton® flexible substrate and thermally treated at 400 °C to reduce oxygen content. According to the obtained results the optimized ink formulation was composed of GO (7000 ppm), Triton X-100, carbon black and 8 layers of print. The application of the as designed miniaturized electrochemical setup enabled to detect DCF at neutral pH in samples of volume as low as 50 μ L.

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- [1] W. Boumya, N. Taoufik, M. Achak, H. Bessbousse, A. Elhalil, N. Barka, Talanta Open, 3 (2021) 100026.
- [2] N. Vieno, M. Sillanpää, Environ. Int. 69 (2014) 28–39.
- [3] Y. Gao, X. Guo, Z. Qiu, G. Zhang, R. Zhu, Y. Zhang, H. Pang, ChemPhysMater. 1 (2022) 17–3.





Biomass based porous carbon and its potential in environmental application

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Keywords: biomass, activated carbon, coffee grounds, pyrolysis, adsorption from dilute solution

Activated carbon prepared from spent coffee grounds as biomass precursor shows great potential in several fields such as wastewater treatment, air purification, storage of various gaseous substances or as catalysts due to high reactivity, good physical and chemical stability, high specific surface area and excellent pore size distribution. The aim of this work was to investigate the possible biomass – porous carbon conversion routes for coffee grounds. Pyrolysis – GC/MS and TG/MS were used thermal analysis (TA) to study the thermal decay. Traditional pyrolysis and hydrothermal treatment was used to obtain intermediates for further activation.

The morphology of the carbon matrices was characterized by low temperature nitrogen adsorption, while the chemical composition was obtained from ultimate analysis and XPS.

Based on these results samples were selected for application related measurements, i.e., removal of organic molecules from water and energy storage/conversion tests.

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Functionalized Carbon Surfaces by Plasma: the Role of Surface Morphology

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Keywords: oxygen plasma, surface morphology, work function, stability of functionalization, DFT molecular modelling

Carbon materials have been used in various areas of physics, chemistry, biology and material science because of its exceptional properties and diversity in structure. However, for wide range of applications surface properties needs to be tunned as they are chemically inert and hydrophobic in nature. Functionalization of carbon surfaces by the introduction of the functional groups/heteroatoms on the surface has emerged as a powerful strat egy for tailoring their surface properties. At the same time carbon materials physical and chemical properties strongly depend not only on functional groups but also on the surface morphology. The aim of this work is to investigate the impact of surface morphology such as surface defects [1], presence of edges [2] as well as surface curvature [3] on the stability of functional groups on carbon materials. The extent of functionalization and its stability were monitored via XPS, SIMS, RS, TEM and work function measurements. The results are discussed in terms of various positions of surface functional groups, their stability and possible recombination pathways. For a comprehensive understanding on molecular level of the phenomena taking place at the oxygen-functionalized carbon surfaces, the experimental investigations were corroborated by theoretical modelling (DFT).

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- [1] J. Duch et al., Carbon 137, (2018), 425-432
- [2] D. Kumar et al., Carbon (submitted)
- [3] D. Kumar et al., (in preparation)





Investigation on N-doped and N, S-dually doped resorcinol-formaldehyde carbon xerogels for fuel cell applications

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Keywords: carbon xerogel; N-,S-doping; electrocatalyst; oxygen reduction reaction, fuel cells

It has already known that resorcinol-formaldehyde carbon xerogels have numerous advantageous properties which make them promising candidates as catalysts in anion exchange membrane fuel cells (AEMFCs) or catalysts supports in proton exchange membrane fuel cells (PEMFCs) [1, 2]. Incorporation of heteroatoms (such as O, N, S, P, B, etc.) into the carbon network can improve its certain features [3]. In this present work, two series of doped carbon xerogels were prepared by sol-gel polycondensation, using urea and thiourea as nitrogen- and nitrogen-/sulphur sources. In the seven-sample series, the molar ratio of urea/resorcinol and thiourea/resorcinol in the reaction mixture was varied from 0 to 1, in order to examine the effect of increasing doping.

The morphology and the surface chemistry of the xerogels were studied with low temperature N2 adsorption/desorption, scanning electron microscopy/ electron dispersive spectroscopy (SEM/ EDS), X-ray photoelectron spectroscopy (XPS), elemental analysis, pyrolysis-gas chromatography/ mass spectrometry (Py-GC/ MS), thermogravimetric analysis coupled to mass spectroscopy (TGA/ MS), water vapour adsorption and electrical conductivity test. Electrochemical measurements, such as cyclic voltammetry (CV), oxygen reduction reaction (ORR) and stability test were also carried out to study the materials catalytic behaviour in basic and acidic electrolytes. The results showed that the doping does not change significantly the morphological properties, but does have influence on the porosity. In the electrochemical experiments, the N- and N-,S-containing carbon xerogels performed enhanced activity with increasing heteroatom content.

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- 1. Job, N., Marie, J., Lambert, S., Berthon-Fabry, S., & Achard, P. (2008). Carbon xerogels as catalyst supports for PEM fuel cell cathode. Energy Conversion and Management, 49(9), 2461-2470.
- 2. Abidin, A. F. Z., Loh, K. S., Wong, W. Y., Mohamad, A. B., & Puspasari, I. (2018). Effect of carbon precursor and initial pH on cobalt-doped carbon xerogel for oxygen reduction. International Journal of Hydrogen Energy, 43(24), 11047-11055.
- 3. Barbosa, M. B., Nascimento, J. P., Martelli, P. B., Furtado, C. A., Mohallem, N. D. S., & Gorgulho, H. F. (2012). Electrochemical properties of carbon xerogel containing nitrogen in a carbon matrix. Microporous and mesoporous materials, 162, 24-30.



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Possibilities of using computer simulations and theoretical methods to model and explain adsorption phenomena on the example of adsorption of pyrrole, furan, and thiophene in the pores of activated carbons

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Keywords: computer simulation, GCMC, adsorption, carbon materials.

Furan is a well-known representative of a series of five-membered aromatic "heteroaromatic" compounds, which include many others, like pyrrole and thiophene - Fig. 1 [1]. Moreover, each member is the parent of a vast family of derivatives. Compared to its homologs, pyrolle and thiophene, furan displays the lowest aromatic and the highest dienic character, as illustrated in Fig. 1. Weak intermolecular interactions can be a subtle way to modify the properties of carbon materials. Over the last decade, several theoretical investigations of the compounds mentioned above and hybrid systems have also been performed [2,3]. The main goal of this report is to present selected theoretical methods used by the authors to model, analyze, interpret, and explain adsorption phenomena. Among them, an important place is occupied by Monte Carlo simulations, which not only generate adsorption isotherms but also provide insight into the enthalpy of the process [4]. The analysis of adsorption isotherms was discussed, in particular: values of Henry's constant (as a simple parameter reflecting the energetics of interactions of adsorbate molecules with the adsorbent surface) were determined, and adsorption potential distribution curves (as a way to gain insight into the mechanism of pore filling) were generated. The research used a series of model carbon structures with systematically changing porosity [4]. The combined use of molecular simulations and theoretical analysis methods allowed for a quantitative understanding of the relationship between the porous structure of activated carbons and their adsorption properties toward the studied compounds.

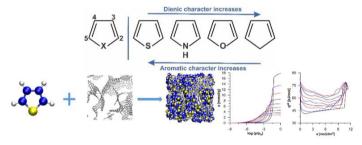


Fig. 1. The concept of the simulation.

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- [1] B.J. Levandowski, R.T. Raines, Chem. Rev., 121 (2021) 6777-6801.
- [2] Y. Zeng, P.Z. Moghadam, R.Q. Snurr, J. Phys. Chem. C, 119 (2015) 15263-15273.
- [3] P. Kamedulski, A. Kaczmarek-Kedziera, J. Lukaszewicz, Bull. Mater. Sci., 41 (2018), 76.
- [4] S. Furmaniak, Comput. Methods Sci. Technol., 19 (2013) 47-57.





Graphene and Borophene competing or plumbing to each other?

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Keywords: Multidimensional materials, 3D structures, Graphene, Borophene

Multidimensional materials, with their unique qualities that make them the materials of the future, would respond to humanity's growing needs in every field. Because of its unique characteristics, which include high intrinsic mobility, high electrical conductivity, and thermal conductivity, graphene is a significant advancement [1]. Researchers are getting access to the multidimensional world thanks to the development of graphene. After graphene, borophene is the most interesting multidimensional material with its unique properties.

Due to its electron-hole symmetry, the Fermi level in graphene is situated halfway between the valence and conduction bands. Depending on their nature, the electron band structures of borophene and graphene differ from each other [2].

We have examined the unique properties of borophene graphene and some other multidimensional materials in Table 1. Borophene is superior to graphene in electron mobility, making it promising in many applications. Also, theoretically calculated that there is a difference between graphene and borophene in thermal conductivity. According to Borophene, data is second on the list. It is not as high as graphene or borophene due to the nature of other multidimensional materials.[3]

Research should continue to develop forward steps for borophene synthesis methods to develop applicable production and sustainable methods.

Material	Electronic Mobility (cm ² V ⁻¹ s ⁻¹)	Thermal Conductivity (W m ⁻¹ K ⁻¹)
Graphene	180 000	3846
Borophene	280 000	1055
BN	0.05(insulator)	233.3(third)
Stanene	3000	2.9
Germanene	2800	9.87
Silicene	2100	9.4
Phosphorene	1000	180

Table 1: Specific properties of some multidimensional materials

Acknowledgements: P.A.G. acknowledge the use of the computer cluster at Poznań Supercomputing and Networking Centre (Poznań, Poland). P.K. special thanks to the National Center for Research and Development (Poland) for financial support of the research (contract project nr LIDER13/0303/2022).

- [1] P. Kamedulski, et al. Scientific Reports, 11, (2021), 22054.
- [2] H. Tang, et al. Physical Review B, 80 (2009), 134113.
- [3] P. Ranjan, et al., Advanced Materials, 32, (2020), 2000531.





Surface chemistry of carbon nanotubes governs their biomedical applications

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Carbon nanotubes (CNTs) possess some properties that make them extremely interesting from biomedical point of view. To name a few: photothermal, photodynamic and photoacoustic effects, fluorescence in the highly desired NIR-II region [1], high electrical and thermal conductivities or high mechanical strength [2]. Despite that, their application in biomedicine is still limited to the laboratory environment. Transition into the industry is being hindered by questionable cytocompatibility and some reports about possible carcinogenic effects. The controversies and unequivocal reports stem from the fact that the CNTs are often treated as a uniform material group with limited variability [3, 4]. Meanwhile, small and seemingly insignificant changes in their surface chemistry, dimensions, administration route or number of defects, can all govern the way cells and/or pathogens react [5, 6]. Tailoring the CNTs' surface chemistry is the key to obtaining materials with strictly desired properties.

This study proves that a careful selection of the CNTs oxidation state can yield materials that are cytocompatible, with the main determinant being the number of oxygen atoms exceeding 14% and a relatively high share of carbon atoms at a +3 oxidation state. Interestingly, such CNTs also possess innate anticancer and antibacterial properties, making them promising candidates for novel biomedical applications. Further substitution of some of the OH groups in the CNTs with ammonia boosts all of the positive properties even more [7]. Amazingly, these CNTs can then easily be used to produce electrically conducitve layers [8] or nanocomposites [9] that inherit these positive qualities from the CNTs – i.e., are cytocompatible, with detrimental effects against drug-resistant bacterial strains and cancer cells. These CNTs can also be used for assuring sustained and long-term release of bioactive compounds, while also protecting the latter from processing – induced damage.

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- [1] A.K. Mandal, et al., Scientific Reports 10(1) (2020) 5286.
- [2] A. Benko, et al., Cancer Drug Resistance 4(2) (2021) 264-297.
- [3] A.A. Shvedova, et al., Toxicology and Applied Pharmacology 261(2) (2012) 121-133.
- [4] M. Ema, et al., Regulatory Toxicology and Pharmacology 74 (2016) 42-63.
- [5] N. Chatterjee, et al., Carbon 108 (2016) 529-540.
- [6] K. Kostarelos, Nat Biotech 26(7) (2008) 774-776.
- [7] A. Benko, et al., Nanoscale (2023).
- [8] A. Benko, et al., Materials Science and Engineering: C 120 (2021)
- [9] S. Wilk, et al., Chemical Engineering Journal 455 (2023) 140617.





The effect of carbon fiber morphology on the cellular response of cells in fibrous substrates for tissue engineering application

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Keywords: cerbon fibers, carbon biomaterials, surface topography, surface porosity, cells-materials interaction.

Scaffolds for tissue engineering should be characterized by porosity that allows cell infiltration into their interior. Colonization of a substrate by cells and their effective adhesion to a surface of an elementary fiber gives a chance for rapid proliferation and full restoration of a defect. In this respect, the most promising are fibrous substrates that mimic a fibrous arrangement of collagen that builds an extracellular matrix of any tissue [1]. Low-modulus carbon fibers with proven biocompatibility may provide a good example of scaffolds for tissue engineering within bone and cartilage tissue defects. Here, however, morphology of the elementary fiber allowing first for adhesion and then for cell proliferation turns out to be very important [2]. Roughness and surface porosity of a carbon fiber can be controlled using such methods as the physical vapor deposition (PVD) with a special focus on magnetron sputtering (MS). In the study, oxidized, commercially available polyacrylonitrile (PAN) fibers (Zoltec) were bombarded with zinc, titanium, iron and copper atoms. Different exposure times were used to induce surface changes of the carbon fibers. The surface morphology of pure-carbon and after the PVD-MS modification was observed by scanning electron microscopy (SEM, Nova NANOSEM). Cross sections of the fibers were observed to determine their volume porosity (ImageJ). The total porosity and pore size distribution (space between fibers) were measured using the mercury porosimetry (PoreMaster 60, Quantachrome Instr., USA). The specific surface area of the fibers was determined using the BET adsorption isotherm method (ASAP2010, Micromeritics Instr.). The pore size distribution (PSD) of the nonwoven material was supplemented by the LF-NMR analysis. The T1 and T2 relaxation times were measured on a Rock Core Analyzer (Magritek), and were obtained from distributions calculated by applying the inverse Laplace transform. The use of this method makes it possible to supplement information as to the texture of the mesopores (2-50 nm). In addition, a numerical simulation of the size of the material surface was carried out, assuming an ideal pore structure in the form of cylinders of known diameter and length. The effect of partitioning of the nonwovens into smaller sections with the size of 1-2 µm for the BET adsorption measurements, was also evaluated. The experimental results showed, that the magnetron sputtering leads to the formation of roughness on the fibers exposed to the deposition of metals. The presence of mesopores on the surface of the carbon fibers has a positive effect on cell viability and proliferation (MG-63 osteoblasts and CHO-02 chondrocytes).

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- [1] M. Qian, et al. Acta Biomaterialia, 171 (2023) 308-326.
- [2] B. Baker et al. Nature Mater 14 (2015) 1262–1268.





Post-traumatic correction of the mechanokinetics of skeletal muscle contraction by administering water-soluble C60 fullerene

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Keywords: muscle gastrocnemius, muscle soleus, muscle injury, muscle contraction, biochemical indicators of blood and muscle tissue, C60 fullerene

Open injury of skeletal muscles is a complex pathology that accounts for more than 70% of combat wounds and leads to numerous complications. The initial phase of any post-traumatic muscle recovery is characterized by inflammation and further degeneration of the damaged tissue. Therefore, the therapy for the restoration of damaged muscles is ineffective without reducing the inflammatory processes in it. In this work, the biocompatible and non-toxic C60 fullerenes in the aqueous phase were used as powerful antioxidants [1].

The structural organization of C60 fullerene nanoparticles in an aqueous solution, as well as their stability were studied using the atomic force microscopy and dynamic light scattering techniques [2].

The biomechanical parameters of contractions of the fast (muscle gastrocnemius) and slow (muscle soleus) muscles of rats, as well as biochemical indicators of blood and muscle homogenates were studied 15 days after trauma caused by the destruction of muscle cells of varying severity. The introduction of C60 fullerene aqueous solution at a dose of 1 mg/kg into the damaged muscle improved its contractile function by $30-35\pm2\%$ and $15-20\pm1\%$ in the fast and slow muscles, respectively, compared to the control. A tendency to decrease the biochemical indicators by $15-17\pm1\%$ in the blood, as well as by $20-23\pm1\%$ and $15-17\pm1\%$ in the tissue of fast and slow muscles, respectively, was detected with the introduction of water-soluble C60 fullerenes.

The in vivo results obtained indicate the ability of C60 fullerenes to reduce the degree of muscle fibers damage and significantly weaken the course of the inflammatory process in them, which opens up the prospect of their use for the correction of pathological conditions of skeletal muscle that arise from its mechanical injury [3].

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- [1] C.A. Ferreira, D. Ni, Z.T. Rosenkrans, W. Cai, Nano Res., 11 (2018) 4955.
- [2] U. Ritter, Yu.I. Prylutskyy, M.P. Evstigneev, N.A. Davidenko, V.V. Cherepanov, A.I. Senenko, O.A. Marchenko, A.G. Naumovets, Fullerenes, Nanotubes, Carbon Nanostruct., 23 (2015) 530.
- [3] D. Nozdrenko, T. Matvienko, O. Vygovska, V. Soroca, K. Bogutska, A. Zholos, P. Scharff, U. Ritter, Yu. Prylutskyy, Appl. Nanosci., 12 (2022) 467–478.





Study of the suitability of selected phenolformaldehyde resins as precursors of carbon-carbon composite matrices

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Keywords: Phenol-formaldehyde resin, cross-linking, thermal and spectroscopic analysis, carbon-carbon composite matrix precursor

Wood composite adhesives, foams, mineral wool, fiberglass insulation binders, cutting wheels, brake pads are only few from many applications of phenolic resins. Particularly interesting, but more niche, are their special applications in the production of key components for the space industry, such as thermal shields, for which carboncarbon composites (CCC) are used. When selecting the appropriate resin for application in CCC, many criteria should be taken into account, the more important of which are viscosity, cross-linking process and carbon yield after pyrolysis [1]. The study investigated the cross-linking process of three commercial resole-type phenolformaldehyde resins in order to determine their application potential as CCC matrix precursors. The basic technique used in the work was differential scanning calorimetry (DSC). On the basis of DSC curves, the temperature, time and dynamics of the resin cross-linking reaction were determined. Additionally in this work, several coupled techniques, such as Thermogravimetry-Mass Spectroscopy (TG-MS) and Thermogravimetry-Fourier Transform Infrared Spectroscopy (TG-FTIR), were successfully used for deeper investigation of the crosslinking mechanism of selected resole type resins. Usefulness of TG-MS and TG-FTIR in testing phenolic resins was demonstrated in the detailed presentation of the emission of gaseous products of the cross-linking reaction. The analysis was supplemented with in situ FTIR as a function of temperature which allowed for the assessment of the structure of the tested resins during and after the cross-linking process. Samples of the three commercial resole resins were produced for their microstructure and mechanical properties assessment. Based on the resins tested in this work, composite rods reinforced with carbon fibers were produced, which differed significantly in the value of the stiffness modulus. The highest modulus was obtained for the prepared composites at the level of 140 Gpa.

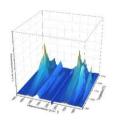


Figure 1. 3D spectrogram of TG-FTIR at 10oC/min for resole type phenol-formaldehyde resin

Acknowledgements: This work was supported by National Centre for Research and Development, project no. LIDER13/0108/2022.

References

[1] L. Pilato, Phenolic resins: 100 Years and still going strong, Reactive and Functional Polymers, vol. 73, issue 2, 2013, https://doi.org/10.1016/j.reactfunctpolym.2012.07.008



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Carbon-carbon composite rocket motor nozzles prepared by filament winding method

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Keywords: Carbon fibre reinforced carbon, filament winding, oxidation resistance, rocket motor, nozzle

Carbon-carbon composites are a group of materials consisting of carbon matrix reinforced uni- or multi-directionally with carbon fibre. These composites exhibit an excellent thermal stability, resistance to thermal shocks and good mechanical properties, which predispose them as a material for rocket motor nozzles [1]. Nozzle is a critical element of rocket engine, converting the internal energy of combustion products into the propulsive force by accelerating the gaseous products to high supersonic velocities. The combustion process taking place in engine produces an extreme thermal (up to 3000 oC), abrasive and oxidative environment, frequently leading to erosion of critical section of nozzle, which may result in pressure drops worsening the performance of motor or even its failure. Because of the above, it is extremely important to use materials providing the best possible resistance to erosion to hot, rapid outflow of gases and integral stability of nozzle.

One of the most popular and most effective methods of fabrication of carbon-carbon composites is the filament winding technique. The procedure involves winding carbon fibre wetted with resin around the mandrel, and subsequent curing of resin, thermal stabilization and carbonization in an inert atmosphere. Finally the material is subjected to cyclic densification by impregnating the product with resin or pitch and annealing until the desired density and mechanical properties are achieved.

In this work we demonstrate carbon fibre reinforced carbon composites obtained by filament winding method and subsequent carbonization and re-densification. As the precursor of carbon matrix phenolic-formaldehyde resin was used which allowed obtaining high carbon yield and good mechanical properties of composites. The composites were examined by measuring dynamic elastic properties, anisotropy and microstructure. Furthermore, we attempted to apply anti-oxidation layers by coating the composites with different anti-oxidation agents. The obtained results indicate that fabricated composites can be successfully used as a nozzles for rocket motors.



Figure 1. Filament winding of carbon– fibre on rocket nozzle form.

Acknowledgements

This work was supported by National Centre for Research and Development, project no. LIDER13/0108/2022.

References

[1] Li-na Peng, Guo-qiang He, Jiang Li, Lei Wang, Fei Qin, Effect of combustion gas mass flow rate on carbon/carbon composite nozzle ablation in a solid rocket motor, Carbon 50, 4, 2012, p. 1554-1562, DOI:0.1016/j.carbon.2011.11.034





Hard carbons and their application as anodes in Naion batteries

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Keywords: Na-ion batteries, hard carbon, active anode material, electron microscopy.

Batteries are an essential part of the smooth running of modern society and provide electricity on demand in many applications. Lithium-ion batteries were introduced to the consumer electronics market in the early 1990s and have successfully dominated it, mainly due to their high energy density. Due to issues related to the abundance and geographic distribution of lithium and some other components of lithium-ion batteries, creating new opportunities for future energy storage is of strategic importance. Sodium-ion batteries are a promising direction. Due to the size of sodium ions, hard carbon (hard carbons=disordered carbons that do not transform into graphite upon heat treatment) is used as the active anode material instead of graphite. Leading industry standard HCs can have capacities of 300+ mAhg-1 but lack in both area, volumetric and TAP densities when compared to their Li ion counterparts. 1 Therefore, research is undertaken on their discharge mechanism and its relation to the materials structure.2-4 The research material consisted of samples of commercial Hard Carbon characterized by different application properties. Advanced transmission electron microscopy techniques (HR TEM, EELS, HR STEM and electron diffraction) were used to show differences in their crystal and electronic structures.

- [1] Tapia-Ruiz, N. et al. 2021 roadmap for sodium-ion batteries. Journal of Physics: Energy 3, 031503 (2021).
- [2] Meng, Q. et al. Hard carbon anodes for sodium-ion batteries: Dependence of the microstructure and performance on the molecular structure of lignin. J Power Sources 581, 233475 (2023).
- [3] Youn, Y. et al. Nanometer-size Na cluster formation in micropore of hard carbon as origin of higher-capacity Na-ion battery. NPJ Comput Mater 7, 48 (2021).
- [4] Tan, S. et al. The Progress of Hard Carbon as an Anode Material in Sodium-Ion Batteries. Molecules 28, (2023)





Tailoring electrocatalytic properties of sp²-bonded carbon nanoforms by doping

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Keywords: carbon nanoforms, graphene, carbon nanotubes, doping, heterogeneous electron transfer.

A unique feature of graphene, which is structurally the simplest nanoform of sp2-bonded carbon, is the symmetry of the valence and conduction bands formed by bonding π - and antibonding π^* -orbitals near the Dirac points. In neutral graphene, the Fermi level intersects the Dirac points, the consequence of which is the symmetry of electrons and holes in the electronic density of states (DOS). This symmetry of electrons and holes in charge neutrality point (CNP) of DOS can be broken in graphene, carbon nanotubes, and other layered (2D) and cylindrical (1D) nanoforms of sp2-bonded carbon [1]. Introduction of adatoms [2], point defects and strain [3,4] cause changes in DOS that can result in p- and n-doping. By changing the concentration and distribution of defects, we can modify the electron structure, in particular adjusting the DOS of electrons (or holes) at the Fermi level to suit specific needs.

Based on the Gerischer-Marcus model [5], we discuss charge transfer reactions between graphene and nanotubes and the redox system in solution. As model electrodes, we consider 2D and 1D sp2-bonded carbons, in which the symmetry of holes and electrons is broken as a result of modification of the crystal lattice, i.e. electron or hole doping. As model redox systems we consider the Fe(CN)63-/4- and Ru(NH3)63+/2+ redox couples. We show that the reaction rate of heterogeneous electron transfer (HET) depends on the correlation between π -electron DOS of electrode and redox potentials of the electrolyte. The possibility of matching electrocatalytic properties of sp2-bonded carbon nanoforms by doping on HET is confirmed by exemplary results obtained from cyclic volta mmetry measurements.

Deeper insight into the relationship between the electronic DOS of the sp2-bonded carbon nanoforms and donor and acceptor states of redox species in solution will enable researchers to focus on the important design features of carbon based electrodes for electrochemical applications at the outset.

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- [1] I. Suarez-Martinez, N. Grobert, C. Ewels, Carbon, 50 (2011) 741-747.
- [2] T.M. Radchenko, V.A. Tatarenko, I.Yu. Sagalianov, Yu.I. Prylutskyy, P. Szroeder, S. Biniak, Carbon, 101 (2016) 37-48.
- [3] I.Yu. Sagalianov1, T. M. Radchenko, Yu.I. Prylutskyy, V.A. Tatarenko, P. Szroeder, Eur. Phys. J. B, 90 (2017) 112
- [4] P. Szroeder, I.Yu. Sagalianov, T.M. Radchenko, V.A. Tatarenko, Yu.I. Prylutskyy, W. Strupiński, Applied Surface Science, 442 (2018) 185-188.
- [5] H. Gerischer, Electrochemica Acta, 35 (1990) 1677-1699.





Steering triboelectric and mechanical properties of polymer fibers with carbon black

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Keywords: Electrospun fibers, Carbon black, Triboelectricity, Mechanical properties, Energy harvesting.

The rapid advancement of wearable electronics has increased interest in self-powered systems, particularly triboelectric nanogenerators (TENGs).[1] Previous research has predominantly focused on the mechanical enhancement of fibers without thoroughly addressing their triboelectric performance. The integration of conductive additives like carbon black (CB) into polymeric fibers has been suggested as a method to improve both mechanical strength and electrical output, but the effects of CB on different polymers have not been comprehensively explored. This study investigates how varying concentrations of CB influence the triboelectric and mechanical properties of electrospun fibers made from polyurethane (PU), polystyrene (PS), and polycarbonate (PC).[2] The addition of CB significantly altered the properties of the fibers: while it increased the mechanical strength of PU and PS fibers, it unexpectedly decreased their triboelectric output by over 90%. Conversely, CB addition enhanced the triboelectric output of PC fibers by 260%, demonstrating a materialdependent interaction. These results highlight the complex balance between enhancing mechanical properties and optimizing triboelectric output in electrospun fibers. The study provides new insights into the role of conductive additives in modulating the performance of materials used in energy-harvesting devices. Understanding the impact of CB on both mechanical and triboelectric properties is crucial for the design of more efficient TENGs, which are integral to the development of self-powered electronic devices. This research not only advances our understanding of fiber material science but also suggests the potential for tailored composite fiber formulations to meet specific industrial applications. Future studies could explore the integration of multiple conductive additives to further enhance the performance of electrospun fibers in various applications.

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References

[1] Szewczyk, P. K.; Busolo, T.; Kar-Narayan, S.; Stachewicz, U. ACS Applied Materials & Interfaces. 2023, 15, 48, 56575–56586.

[2] Szewczyk, P. K., Taşlı, A. E., Knapczyk-Korczak, J., & Stachewicz, U. (2023). Composites Science and Technology, 243, 110247.





Study of the graphitization trajectory of low- and medium-textured pyrolytic carbons under additional heat treatment

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Keywords: pyrolytic carbon, carbon fiber, CVD, heat-treated, C-C composites.

Pyrolytic carbon (PyC), also referred to as pyrocarbon, is a synthetic form of carbon produced through the pyrolysis of light hydrocarbons utilizing combined chemical vapour deposition (CVD) techniques [1]. PyC has traditionally been utilized in industry, particularly as a carbon-carbon (C-C) composite in space and aerospace technologies [2], and in the medical field as coatings for cardiovascular implants [3]. A novel application involves leveraging its mechanical and biological properties to interact with nerve tissue by forming composites of carbon fiber (CF) and pyrocarbon matrix, fabricated via an advanced CVD method involving direct resistive heating of the fiber bundle [4-5]. The study focused on examining the effects of additional thermal treatments (1600°C and 2000°C) on the composites initially obtained at 1100°C, assessing various morphological, microstructural, textural, structural, and mechanical properties. This investigation aimed to elucidate the relationships among these properties, including the graphitization and crystallinity trajectories within the fiber phase and PyC matrix, alterations in the orientation of crystalline and pseudocrystalline carbon domains, and the nature of discontinuities at the interfacial interface as functions of temperature. The analysis revealed that the graphitization trajectory of PyC indicated growth in crystallite size within the matrix material without significant ordering of the PvC structure. Furthermore, it was established that higher temperatures led to an increase in both the crystallite size and the number of microstructural defects at the interfacial interface. These changes were found to correlate with the mechanical properties of the composites. The findings underscore the impact of thermal treatment on the structural evolution of CF/PyC composites, highlighting the relationship between temperature-induced changes in crystallite size and the structure, and the microstructural defects, and the composites' properties.

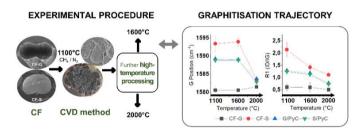


Figure 1. Scheme of the experiment and diagram of the graphitization trajectory of the composites examined as a function of temperature

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- [1] J.H. Je, et al., Carbon, N Y 22 (1984) 563-570
- [2] U. Gruber, et al., Industrial Carbon and Graphite Materials, Volume I: Raw Materials, Production and Applications (2021)
- [3] R.B. More, et al., Biomaterials science, (2013) 209-222
- [4] A. Fraczek-Szczypta, et al., Journal of Functional Biomaterials, 14(9):443 (2023)
- [5] R. Wielowski, et al., Diamond and Related Materials, 146, 111214 (2024)





Electrospun carbon-ceramic nanocomposites CNFs-SiC for environmental protection

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Keywords: carbon nanofibers, ceramics, carbon materials, nanocomposite materials, electrospinning

Broadly understood environmental protection aims to limit and counteract the harmful impact of human activity on the natural environment. One of the areas of environmental protection is water purification. Membrane techniques face many problems, making it necessary to search for new materials for the production of membranes. Due to the difficult operating conditions of the membranes, they must be characterized by high thermal, chemical and mechanical stability. In addition, they must show indifference to the environment. Another challenge is the phenomenon of biofouling, which involves the adhesion of micro- and macro-organisms on the membrane surface, creating a biofilm layer and thus reducing its efficiency and service life. Current trends in the search for new materials are directed towards carbon nanomaterials. One of the materials showing potential for use in membrane water treatment techniques are carbon nanofibers CNFs. Polymer nanofibers are obtained from the spinning solution in the electrospinning process and then thermally treated. CNFs are characterized by low density, low surface to volume ratio and chemical stability. The superiority of this method over other methods of obtaining CNFs is reflected in the possibility of controlling the process parameters, thanks to which we obtain materials with the desired properties, as well as in the profitability of the method. Moreover, electrospun CNFs can be easily modified. Modification of carbon nanofiber precursor solutions with silicon carbide SiC precursors allows obtaining nanocomposites with improved properties resulting from the combination of the carbon and ceramic phases. Obtaining carbon-ceramic hybrid materials combining the properties of carbon nanofibers with high chemical stability of silicon carbide, its resistance to high temperatures and oxidation allows the nanocomposites to work in difficult conditions. Nanofibrous carbon-ceramic composites exhibit some antibacterial activity, thus reducing the problem of biofouling of membranes. Mechanical damage to bacterial cell membranes with SiC nanostructures may result in oxidative stress and inhibition of bacterial growth or even death [1].

The work presents an attempt to obtain ceramic-carbon nanocomposites as a result of thermal treatment of electroformed modified PAN nanofibers. Various variants of the modification of carbon nanofibers with precerams have been prepared. The modified CNFs were prepared by electrospinning by adding SiC silicon carbide precursor at the PAN precursor preparation stage. Polysiloxane was selected as the silicon carbide precursor. The multi-stage heat treatment included stabilization, carbonization and high-temperature treatment of modified PAN nanofibers. Surface modification carbon nanofibers was also carried out. The obtained hybrid systems were characterized using SEM with EDS composition analysis. Their structure was analyzed using FT-IR and XRD analysis was performed to confirm the presence of SiC in the tested systems. The samples were tested for microbiological activity. The described method is a kind of novelty in carbon-ceramic composites. So far, the literature does not present nanofibers carbon-ceramic membranes obtained by electrospinning with potential applications in the field of water treatment.

Acknowledgements: This work was supported by the program "Excellence initiative—research university" from the AGH University of Krakow, project no. 1580.

References

[1] M. Szala, A. Borkowski, Toxicity assessment of SiC nanofibers and nanorods against bacteria, Ecotoxicol. Environ. Saf. 100 (2014) 287–293. https://doi.org/10.1016/j.ecoenv.2013.10.030.





Functionalization of graphenic surfaces via plasmas: surface electronic properties, wettability and biocompatibility

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Keywords: Graphenic surface, plasma treatment, electronic properties, wettability, biocompatibility.

Graphene-based materials have been extensively and intensively investigated for a wide variety of applications including electronics, CO2 capture, drug delivery and biomaterials, to mention a few. Surface properties like, electronic and wettability play crucial role for many specific applications and need to be modified as carbon surfaces are chemically inert and hydrophobic in nature. Several methods have been developed to achieve controlled tunning of the surface properties that can be achieved via the introduction of heteroatoms. Among these methods, oxidation through wet (using strong acids) or dry (plasma) treatments are commonly used. To preserve the bulk properties of the material, plasma modification is preferred for functionalizing the surface as it is environmentally friendly, energy-efficient and requires a short time for modification (seconds/minutes). The aim of this study is to investigate the possibility to tune the surface properties (electronic, wettability and biocompatibility) of graphenic surface by functionalization via different plasmas (O2, NH3 and SF6) [1,2]. The applied approach involves thorough characterization of the surfaces before and after plasma treatment (AFM, SEM, XPS, LDI-MS, RS, TG). Additionally, to investigate surface electronic properties, wettability and biocompatibility work function, water contact angle measurements and biological tests were performed (cell tests, bacterial adhesion). The experimental results are corroborated with the DFT calculations. Changes in work function and water contact angle of the graphenic surfaces are monitored to track the progress of modification, revealing a strong impact of the introduced functional groups on the surface properties. The results demonstrate that the plasma modification has been confined to the outermost surface while the bulk structure of the material remained intact. The introduced oxygen functional groups increase also the biocompatibility.

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- [1] M. Białoruski et al., Appl. Sur. Sci. 597, (2022), 153671
- [2] M. Golda-Cepa et al., J. Mater. Chem. B, (2023), 4946-4957





Posters





Adsorption of radon-222 inside carbon nanotubes - studies using molecular simulations

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Keywords: computer simulation, Monte Carlo method, adsorption, carbon nanotubes, radon.

Radon is a radioactive noble gas. Its most stable isotope (radon-222) is emitted due to transformations in the uranium series [1]. Radon adsorption in pores of carbonaceous materials is a phenomenon that can be applied to measure its concentration in the air [2].

All the results presented were obtained using computer experiments, i.e., the in silico method. The simulations used a series of twenty seven single wall carbon nanotubes, including eighteen of zig zag type (Fig. 1(a)) and nine of armchair type. The adsorption of radon-222 for T = 298 K was modeled using Monte Carlo simulations and the technique described by Yan and de Pablo [3], i.e., hyper parallel tempering Monte Carlo. The calculation scheme was analogous to the previously described [4]. The energy of interactions between various Rn atoms and between Rn atoms and C atoms in the structure of the adsorbents was calculated using the Lennard-Jones potential [5,6].

The computer experiments gave insight into the relationship between the geometric parameters of these materials and the efficiency of radon-222 capture. The highest relative differences occurred in the low-pressure region, which is the most important in practice. In this range, adsorption isotherms are linear — their shape and quantitative differences are precisely reflected by Henry's constant and the heat of adsorption at zero coverage (Fig. 1(b) and (c)). Even a slight reduction in the diameter of nanotubes can significantly improve the efficiency of radon capture.

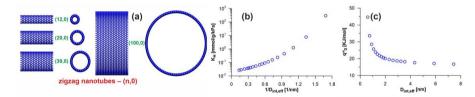


Fig. 1. (a) Selected carbon nanotubes. Comparison of (b) the Henry constant values associated with the adsorption isotherms and (c) the heat of adsorption at zero coverage qst0 associated with the isosteric adsorption enthalpy are presented as a function of the inverse of (or direct) the effective internal diameter of the zigzag nanotubes - Dint, eff.

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- [1] L.J.R. Nunes, A. Curado, S.I. Lopes, Appl. Sci., 13 (2023) 7460.
- [2] W. Poltabtim, C. Kranrod, S. Tokonami, Radiat. Environ. Med., 11 (2022) 41-49.
- [3] Q. Yan, J.J. de Pablo, J. Chem. Phys., 111 (1999), 9509-9516.
- [4] S. Furmaniak, A.P. Terzyk, K. Kaneko, P.A. Gauden, P. Kowalczyk, T. Itoh, Phys. Chem. Chem. Phys., 15 (2013) 1232-1240.
- [5] J.R. Mick, M.S. Barhaghi, J.J. PotoffJ., J. Chem. Engn. Data, 61 (2016) 1625-1631.
- [6] W.A Steele, The Interaction of Gases with Solid Surfaces, Pergamon Press, New York, 1974.





Single-walled nanoporous carbons as perspective adsorbents for removal of volatile organic compounds – a Monte Carlo study

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Keywords: computer simulation, Monte Carlo method, adsorption, benzene, acetonitrile, carbon disulfide.

The defining properties of volatile organic compounds (VOCs) are high vapour pressure and low water solubility. VOCs include a variety of chemicals. Some of them may have short- and long-term adverse health effects [1]. Several techniques have been used to reduce VOC concentration (e.g., sorption, condensation, thermal oxidation, and catalytic oxidation) [2]. Different adsorbents (i.e., silica, zeolites, carbon materials, MOFs) can be used [3]. The carbonaceous materials stand out for this application due to the vast and straightforward possibilities of controlling the sorption capacity and properties of these materials [3]. From an industrial point of view, it would be interesting to find a reliable correlation between the volatile organic compounds' adsorption and the properties of adsorbents.

The current study used Monte Carlo simulations to predict the adsorption properties of single-walled nanoporous carbons toward selected VOCs. Adsorption isotherms from the gaseous phase were simulated and analyzed for the series of nine carbons described by Nicolaï et al. [4] - Fig. 1. Computations were performed for three simple VOCs: benzene (C6H6), acetonitrile (CH3CN), and carbon disulfide (CS2) – Fig. 1. Adsorption isotherms were quantitatively analyzed using values of Henry's constant, adsorption potential distribution curves (APD) and values of adsorption capacity, respectively. The exemplary correlations are shown in Fig. 1. The results indicate that the main factor limiting adsorption capacity is the volume of available pores.

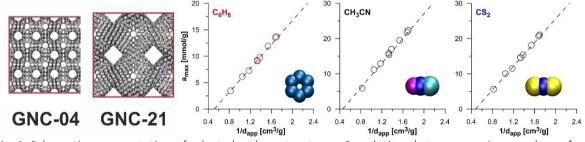


Fig. 1. Schematic representation of selected carbon structures. Correlations between maximum values of adsorption amounts - amax (observed for p/ps = 1) and reciprocals of apparent density (dapp) of carbon in the simulation boxes for all the studied VOCs and model carbons. The dashed lines are drawn to guide the eye.

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- [1] S. Anand, B. Philip, H. Mehendale, in P. Wexler (ed.) Encyclopedia of Toxicology. Elsevier; 2014. pp. 967–970.
- [2] Y. Yang, et al., Environ. Internat., 165 (2022) 107330.
- [3[X. Li, et al., Sep. Purif. Technol., 235 (2020) 116213.
- [4] A. Nicolaï, et al., J. Phys. Chem. C, 119 (2015) 2896-2903.





3D structured carbon nanomaterials – ways to add porosity

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Keywords: nanomaterials, 3D structures, carbon materials, electrode material.

This work presents results on the three-dimensional (3D) functionalization of commercial graphite—originated flakes to micro-mesoporous graphene by carbonization of specific precursors in the presence of a hard template, as illustrated in Fig. 1.

Nowadays, the subject of much research is to find new materials for energy storage that are environmentally friendly and highly effective at low production costs. This can be done thanks to supercapacitors, whose efficiency is determined, among other things, by using ultra-high-surface carbon materials in electrodes. The use of this type of materials in the oxygen evolution reaction (OER) or oxygen reduction reaction (ORR) will also provide an alternative to expensive platinum or ruthenium oxide catalysts. Thanks to this, it will be possible to carry out the water-splitting process and create the so-called "green energy" without CO2 emissions.

Graphene is a breakthrough due to its new properties, such as thermal conductivity, high intrinsic mobility, and high electrical conductivity [1-2]. The obtained materials were characterized using instrumental methods such as low-temperature nitrogen adsorption, Raman spectroscopy, SEM, EDX, and elemental analysis.



Fig. 1. The concept of the synthesis

Acknowledgements: P.A.G. acknowledge the use of the computer cluster at Poznań Supercomputing and Networking Centre (Poznań, Poland). P.K. special thanks to the National Center for Research and Development (Poland) for financial support of the research (contract project nr LIDER13/0303/2022).

- [1] P. Kamedulski, et al. Scientific Reports, 11 (2021), 22054.
- [2] P. Kamedulski, et al. Adsorption, 25 (2019), 631-638.





Chemical stability and electrical conductivity of diamond-filled polymers

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Diamond-filled polymers are gaining prominence due to their exceptional chemical stability and electrical conductivity. This study investigates the integration of diamond particles into polymer matrices to create composite materials with enhanced properties. By leveraging the inherent chemical inertness of diamonds, the composites exhibit significant resistance to chemical corrosion, making them ideal for harsh environments. Additionally, the electrical conductivity of the polymers is notably improved, resulting from the excellent conductive properties of diamond fillers.





Preparation of freestanding polyvinylpyrrolidone/carbon nanotube films for electrochemical applications

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Keywords: carbon nanotubes, polyvinylpyrrolidone, freestanding film, heterogeneous electron transfer.

Carbon nanotubes (CNTs) exhibit good electrical conductivity [1], which, combined with their large specific surface area [2], makes them a promising material for electrochemical applications. Chemical modification of the surface and combining nanotubes with other materials is a strategy for obtaining electrodes with specific electrocatalytic properties [3].

Freestanding polyvinylpyrrolidone/CNT films (buckypapers) were prepared by vacuum filtration from water suspension of pristine CNTs and hydroxylated carbon nanotubes (CNTs-OH). Polyvinylpyrrolidone (PVP) is water-soluble and additionally prevent the nanotube agglomeration. As a reference, freestanding films consisting of CNTs and CNTs-OH were used.

In the presentation, we compare the morphological properties of the obtained films (SEM), concentration of defects in CNTs estimated from Raman spectra, and electrical conductivity.

Electrochemical tests of the freestanding films were performed in three electrode configuration, where buckypapers served as working electrode. Fe(CN)63-/4- and Ru(NH3)3+/2+ couples were used as redox probes. Discussion of the obtained results of cyclic voltammetry includes specific areal capacitance and heterogeneous electron transfer kinetics. The electrocatalytic activity of the obtained films is crucial for future applications of this material in the design of electrochemical sensors.

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- [1] F. Vargas-Lara, A.M. Hassan, E.J. Garboczi, J.F. Douglas, J. Chem. Phys., 143 (2015) 204902.
- [2] A. Peigney, C. Laurent, E. Flahaut, R.R. Bacsa, A. Rousset, Carbon, 39 (2001) 507-514.
- [3]. P. Kamedulski, J.P. Łukaszewicz, Ł. Witczak, P. Szroeder, P. Ziółkowski, Materials, 14 (2021) 2448.





Influence of N,S-doping method on heteroatom groups distribution of doped rGO

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Keywords: reduced graphene oxide, thiourea, functionalization, hydrothermal process, thermal treatment.

Graphene is often subjected to various modifications to fully exploit its properties. Modification through doping is particularly significant as the resulting graphene materials exhibit high chemical stability due to the presence of covalent bonds within or beyond the graphene plane. Co-doping with two or more atoms, such as nitrogen and sulphur, is commonly employed, which imparts the graphene materials with properties characteristic of both atoms. Nitrogen enhances electrical conductivity, while sulphur, due to its lone pairs of electrons, contributes to catalytic processes. New properties also emerge from the mutual interaction of N, S dopants, positively affecting catalytic efficiency through synergistic effect. Doping the graphene structure is carried out through several methods such as hydrothermal treatment, chemical vapor deposition (CVD), or thermal processes [1, 2].

In this work, nitrogen- and sulphur-doped graphene materials (rGO-NS) were obtained through hydrothermal and thermal treatment. Graphene oxide (GO) was hydrothermally treated in the presence of thiourea (TH) serving as heteroatoms source. The syntheses were conducted at two temperatures 180 °C (rGO-NS/180) and 200°C (rGO-NS/200). For comparison, material obtained through high temperature treatment (rGO-NS/HTT) was obtained following thermal treatment of hydrothermally obtained rGO (180°C) in the presence of TH. Thermal treatment was performed at 850°C at an inert atmosphere. The characterization of the obtained graphene-based materials included determination of the elemental surface composition and distribution of functional groups (C, O, N, and S) using X-ray photoelectron spectroscopy (XPS). The morphology of the materials was determined using field emission scanning electron microscopy (FESEM). The nitrogen content was slightly higher in case of rGO-NS/200 (2.8 at.%) compared to 2.5 at.% for rGO-NS/180. Sulphur contribution for both materials was 2.7 at.%. Thermal treatment enabled to increase nitrogen contribution to 5.7 at.% and maintain sulphur content at the similar level as in case of materials from hydrothermal treatment (2.1 at.%). Nitrogen in rGO-NS 180 and rGO-NS 200 is primarily presented in amide/lactam/pyrrolic forms (72-76 %). In rGO-NS/HTT, similarly to rGO-NS 180 and rGO-NS 200, nitrogen mainly appears in the form of amide, imide, amine, and pyrrolic (54.3 %). The selected method of rGO doping heavily influence the sulphur species present in the graphene-based material, as well as its morphology due to the differences in the used graphene precursor.

In summary, we have confirmed that by employing different synthesis protocols we are able to adjust the N,S functional groups in the rGO materials.

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- [1] L. Giraud, A. Tourrette, E. Flahaut, Carbon, 182 (2021) 463-483.
- [2] W. Kiciński, M. Szala, M. Bystrzejewski, Sulfur-doped porous carbons: Synthesis and applications, Carbon 68 (2014) 1–32. https://doi.org/10.1016/j.carbon.2013.11.004.





Development of tailored Laser-Induced Graphene Electrodes for High-Performance Glucose Sensing

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Keywords: Laser-induced graphene; hydrogel membrane; electrochemistry; electron transfer kinetics; diffusion coefficient.

Carbon-based materials are extensively studied as electrode substrates for biosensing applications, with laser-induced graphene (LIG) standing out due to its excellent electrical conductivity, large surface area, and ease of fabrication. This study focuses on the development of a highly sensitive glucose sensor through the electrochemical deposition of Prussian Blue (PB) on tuned LIG electrodes. The best LIG electrodes in terms of electrochemical properties meticulously tailored by optimizing various lasing parameters to achieve the best possible substrate properties were coated with PB using different precursors. The structural and electrical properties of electrodes were characterized using techniques such as scanning electron microscopy (SEM), Raman spectroscopy, and electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV). These characterizations confirmed the successful creation of high-quality LIG substrates and the consistent, reproducible deposition of PB coatings.

The sensor's efficacy was tested by exposing the PB-coated LIG electrodes to H_2O_2 in phosphate-buffered saline (PBS). This interaction is critical for glucose sensing as PB mimics enzymatic activity, converting H_2O_2 generated from glucose oxidation into a detectable electrochemical signal. The resulting sensor configuration exhibited high sensitivity and specificity for glucose detection, with a response over a relevant concentration range.

The scientific novelty and significance of this work lie in its innovative integration of advanced materials science with electrochemical techniques on a laser-scribed platform. This novel approach not only enhances the sensor's sensitivity and specificity but also ensures its operational stability. The impedimetric signals provides insights into the concentration of target species and the interaction mechanisms between analytes and the electrode surface. By developing this biosensor, we aim to advance the field of biosensing for future innovations by offering a cost-effective, single-step fabrication method for a sensitive, reliable, and efficient tool capable of detecting various biomolecules.

References

[1] Yoon, H.; Nah, J.; Kim, H.; Ko, S.; Sharifuzzaman, Sensors and Actuators B: Chemical 2020, 311, 127866.



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The novel biopolymer-carbon nanocomposite hydrogel foils with a drug delivery mechanism based on carbon nanotubes

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Keywords: nanocomposite, collagen, carbon nanotubes, biomaterial, drug release.

There is a high and still growing demand for culturing cardiomyocytes in laboratories for drug testing, disease analysis, and obtaining parts of heart tissue for transplantation [1,2]. Unfortunately, maturing cardiomyocytes in in vitro conditions is time-consuming, comes with great financial expenses, and is characterized by low yield [3]. Therefore, it would be of significant benefit to improve the currently used culturing techniques. In this study, a new type of substrate, that can be used in the in vitro cellular cultures was obtained. Collagen type I-based hydrogel biomaterial was developed from a benign solution, based on DMSO and PBS. The surface-functionalized multi-walled carbon nanotubes were used as an electrically conductive modifier and a drug carrier. Dexamethasone and liothyronine were used as drugs to influence the maturation of human-induced pluripotent stem cell-derived cardiomyocytes [4,5].

Two main objectives were set in this study. The first was to obtain a collagen type I – MWCNTs nanocomposite hydrogel foil, that could be potentially used as a substrate in in vitro conditions. The second was to determine if surface-functionalized carbon nanotubes can influence the drug release profile from the biopolymer matrix.

Collagen foils were obtained by casting technique from 3% solution in DMSO/PBS (5:1), with a small addition of HCl and HF. The mixture was modified with the addition of glycerol (5% wt/wtcol), and either pure drug/s or the combination of functionalized MWCNTs (0,25% wt/wtcol) and dexamethasone and/or liothyronine. Materials were kept at 40°C, until fully dry, and later were kept in the fridge upon further use. The efficiency with which drugs attach to MWCNTs was evaluated with the use of the UV-VIS technique. Degradation studies were conducted to determine the collagen matrix decomposition rate in the wet environment. The samples were incubated in PBS for at least 21 days at 37°C. The mass change was controlled by periodic weight measurements, and the release of collagen was evaluated by the use of a BCA assay. The spectroscopic tools were also used to evaluate the drug release from the collagen matrix, in the case of liothyronine, with the additional use of an ELISA kit. Mathematical models were used to establish the release profile of tested materials.

Briefly, the study determined that the drugs can be successfully attached to the functionalized MWCNTs. The addition of carbon nanotubes to the collagen matrix does not significantly influence the degradation rate or water absorption capabilities. However, the release profile of the drugs from the collagen matrix varies in the presence of carbon nanotubes.

Overall, this study indicates that the drug release from the hydrogel substrate might be controlled with the use of MWCNTs.

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- [1] Eldad Tzahor and Kenneth D Poss, Science, 356(6342) (2017), P1035-1039.
- [2] Daniel Bernstein, Progress in Pediatric Cardiology, 46 (2017), P2-6.
- [3] Gaetano J. Scuderi et al., Front. Cell Dev. Biol., 5 (2017).
- [4] Chen Yu Huang et al., JMCC, 138 (2020), P1-11.
- [5] Cinsley Gentillon et al., JMCC, 132 (2019), P120-135.





Electrochemical Modification of Carbon Cloth as a Key to CNSs Synthesis for ORR/OER Electrocatalysts

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Keywords: carbon cloth, carbon nanostructures, electrocatalysis, Zn-air batteries.

Recent years have seen significant growth in ubiquitous electrical devices, increasing the demand for thinner, more efficient, and longer-lasting devices. Zn-air batteries offer a promising alternative to Li-ion systems due to their low cost, safety, environmental friendliness, and high energy density. The use of solid electrolytes and flexible air electrodes enables the creation of flexible systems suitable for flexible displays. One of the main limitations of this technology is the slow reaction kinetics at the air electrode, which affects discharge and charge efficiency. To improve efficiency, bifunctional electrocatalysts are being developed to increase the rate of oxygen reduction and evolution reactions (ORR/ OER) [1].

Although precious metals are considered the best ORR/OER electrocatalysts, their high cost and limited availability drive the search for new materials. Carbon materials, due to their unique properties such as chemical, thermal, and mechanical stability, are becoming attractive. Among them, carbon nanostructures (CNSs), such as nanofibers and nanotubes, are distinguished by their high electrical conductivity and large specific surface area. However, they are often produced as powders, which complicates their use as electrode materials. The solution is carbon cloth, which serves as a flexible, conductive, and easily modifiable substrate for the in situ synthesis of CNSs, combining the advantages of both materials. In addition, modification of the surface of carbon fibers in cloth (e.g., by electrochemical methods) allows control of the properties of CNSs and their electrocatalytic activity [2, 3].

The goal of the project was to synthesize electrocatalytic electrode materials for Zn-air batteries. In situ synthesis of CNSs on electrochemically modified carbon cloth was performed, and the effect of modification on the growth of nanostructures and their ORR/OER properties was studied. The work focuses on the effect of the position of the cloth during electrochemical activation on the size and structure of the nanostructures, and electrochemical tests revealed differences in their electrocatalytic properties.

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- [1] L. Bouleau et al., Carbon NY, 189, (2022), 349-361.
- [2] H. Jiang et al., Ceramics International, 48 20, (2022), 29695-29704.
- [3] W. Ding et al., Nano Research, 16 4, (2023), 4793-4802.





Conductive Carbon-Ceramic Foam Filters Modified by Oxide Nanofillers as Electrode Materials for Photoelectrolysis Wastewater Treatment

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Carbon-ceramic foam filters have been developed as cost-effective, efficient, and sustainable electrode materials for photoelectrochemical processes by incorporating photoactive fillers. The manufacturing process involves mixing α -Al2O3 ceramic powder with sintering coal, an organic coal binder, aqueous silicic acid sol, and sodium lignosulfonate. The mixture is further enhanced with 5% wt. of two types of nanoparticles - potassium hexavanadate and titanium oxide to boost electrooxidation activity. It is then coated onto polymer foams and baked at high temperatures in an oxygen-free environment. This treatment is a volumetric modification which promotes surface oxidation and generates turbulence within the open pore structure, significantly increasing the mass transfer coefficient, which improves current efficiencies and reduces energy consumption. The resulting anodes display high repeatability, reproducibility, and corrosion resistance, as confirmed by SEM images and Raman spectroscopy, which show well-dispersed photoactive fillers within the composite matrix.

These filters, modified with TiO2 and KVO, were tested as anode materials for electrolysis and additionally combined with photodegradation, using a Xe arc lamp to simulate sunlight. Caffeine degradation, facilitated by hydroxyl radicals generated via water oxidation on the anode surface, demonstrated their potential for wastewater treatment applications. The efficiency of caffeine degradation was analyzed using UV-Vis spectroscopy and differential pulse voltammetry. The carbon-ceramic foam filters' highly developed surface and effective modification make them a promising and valuable alternative for electrode materials in photoelectrochemical processes.

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Research on pultrusion as a method for obtaining carbon fiber reinforced rods in carbon-carbon composites

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Keywords: pyrolytic carbon, carbon fiber, CVD, heat-treated, C-C composites.

Carbon Fiber Reinforced Carbon (CFRC) composites are a group of advanced synthetic carbon materials dedicated to demanding applications, such as space technologies [1-3]. Mostly the intermediates for their manufacture are appropriately selected carbon fiber-based polymer composites. A special method for their manufacture is pultrusion. It allows to obtain reinforced profiles or precast, which, arranged in the appropriate directions, are preforms for the manufacture of CFRCs. The basic steps in obtaining pultruded rods are impregnation of fibers in polymeric liquids, forming in matrices with appropriately designated heating zones and their simultaneous curing [4]. These technological Dprocesses will vary depending on the type of raw materials or equipment used. A key aspect is the selection and use of thermosetting polymers, such as phenol-formaldehyde resins.

The experiment used carbon fibers (based on polyacrylonitrile) and a commercial phenol-formaldehyde resin. The goal of the work carried out was to obtain composite rods with a circular cross-section and a diameter of 2 mm with a reinforcement share of 70% by weight.

The rods were formed in a continuous manner. Studies were performed on the effect of crosslinking time and temperatures, the selection of temperatures in the heating zones, as well as the properties of the produced composite rods. The rods were characterized by a circular cross-section of a given diameter, fully reflecting the cross-section of the forming matric. The assumed share of reinforcement in the composite was also met. From the obtained semi-finished products, 3-axes preforms were produced in hexagonal and regular arrangements.

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- [1] U. Gruber, et al., Industrial Carbon and Graphite Materials, Volume I: Raw Materials, Production and Applications (2021)
- [2] E. Fitzer, The future of carbon-carbon composites, Carbon 25 (1987) 163-190
- [3] J. Chłopek J. et al., Mechanical properties of carbon-carbon composites, Ceramics International 19 (1993) 251-257
- [4] A. A. Nawaz, et al., Polyester Usage in Manufacturing of Electrical and Mechanical Products and Assemblies (2018)





Morphological properties of carbonized plastic waste for use as electrode material

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Keywords: carbonization, plastic waste, surface morphology, sp2-bonded carbon, specific surface area.

Controlled carbonization of polymer waste is a promising method for utilizing waste plastic and obtaining material that can find use as an electrode material [1].

We show results of carbonization of plastic waste carbonized in an inert atmosphere. Waste polypropylene (PP), acrylonitrile butadiene styrene (ABS), polyethylene terephthalate (PET), high-density polyethylene (HDPE), polyamide (PA), low-density polyethylene (LDPE) and waste containing a mixture of polymers were used as input material. The best carbonization efficiency (20%), by which we mean the mass of carbon material remaining after the carbonization process relative to the mass of the input material, was obtained for PET.

In the presentation, we discuss and compare morphological properties of carbon materials based on SEM images, surface distribution of elements based on SEM-EDX. The subject of comparative analysis is also the content of the sp2-bonded carbon phase, estimated from Raman spectra, and specific surface area obtained using BET.

A summary of the results gives clues as to which of the materials obtained are the most promising for use as electrodes in electrochemical devices.

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References

[1] J. Gong, X. Chen, T. Tang, Progress in Polymer Science 94 (2019) 1-32.





Determination of the adsorption mechanism on carbonaceous adsorbents with magnetic properties

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Keywords: carbonaceous magnetic adsorbents, adsorption, phenol, Congo red, chromium.

Waste-based carbonaceous magnetic adsorbents are huge prospective adsorbents because of their good adsorption performance, low toxicity, chemical stability, and ease of separation and recovery. Many common environmental pollutants, such as phenols, tetracycline, dyes, or heavy metals, have been removed from the solution by MAC adsorption [1-3].

In this work to obtain adsorbents with magnetic properties, different types of biomass, as well as different iron-containing compounds, that is, FeCl3, FeCl2 and FeSO4,, Fe2(SO4)3 were used. The iron compounds were chosen for several reasons: i) they are relatively inexpensive, ii) they are nontoxic, and iii) they are environmentally friendly.

The starting material for MAC is plant-based biomass obtained locally in Lower Silesia, such as sawdust from pine trees and sawdust from branches of ash-leaf maple. The excess solvent impregnation method was applied to introduce iron particles.

The obtained adsorbents have been characterised by: elemental analysis for C, H, N and S (Vario III Elemental Analyzer); porous texture determination from nitrogen adsorption isotherms at 77K (NOVA 2200 ,Quantachrome). Scanning electron microscopy (JSM 5800LV, Jeol) with energy-dispersive X-ray analysis (Link ISIS 300, Oxford) was applied to monitor the metal distribution of Fe-loaded char and the surface morphology of activated carbons. The crystalline structure of the electrodes was evaluated by X-ray diffraction (Rigaku Ultima IV diffractometer with CuKa radiation of λ = 0,1542 nm). The magnetic properties were evaluated on the laboratory neodymium magnet - balance test.

Adsorption of Congo red (CR) and phenol (P), antrazine (A), and chromium (Cr) from aqueous solutions was carried out at 24 C in a static system.

It has been found that magnetic properties are determined to a greater extent by the amount of iron introduced and not by the type of salt used. It has also been shown that only the mechanism of chromium adsorption is affected by the magnetic properties due to the presence of iron.

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- [1] S. Salem, Z. Teimouri, A. Salem, Adv. Powder Technol. 31 (2020) 4301–4309.
- [2] S. Tamjidi, H. Esmaeili, B. Kamyab Moghadas, Res. Express 6 (2019) 102004.
- [3] G.T. Tee, X.Y. Gok, W.F. Yong, Environ Res. B 212 (2022) 113248.



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Functionalized Carbon Surfaces by Plasma: the Role of Surface Morphology

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Keywords: oxygen plasma, surface morphology, work function, stability of functionalization, DFT molecular modelling

Carbon materials have been used in various areas of physics, chemistry, biology and material science because of its exceptional properties and diversity in structure. However, for wide range of applications surface properties needs to be tunned as they are chemically inert and hydrophobic in nature. Functionalization of carbon surfaces by the introduction of the functional groups/heteroatoms on the surface has emerged as a powerful strategy for tailoring their surface properties. At the same time carbon materials physical and chemical properties strongly depend not only on functional groups but also on the surface morphology. The aim of this work is to investigate the impact of surface morphology such as surface defects [1], presence of edges [2] as well as surface curvature [3] on the stability of functional groups on carbon materials. The extent of functionalization and its stability were monitored via XPS, SIMS, RS, TEM and work function measurements. The results are discussed in terms of various positions of surface functional groups, their stability and possible recombination pathways. For a comprehensive understanding on molecular level of the phenomena taking place at the oxygen-functionalized carbon surfaces, the experimental investigations were corroborated by theoretical modelling (DFT).

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- [1] J. Duch et al., Carbon 137, (2018), 425-432
- [2] D. Kumar et al., Carbon (submitted)
- [3] D. Kumar et al., (in preparation)





C60 fullerene nanoparticles improve the nerve conduction after achillotomy-induced muscle soleus atrophy

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Keywords: muscle soleus, muscle atrophy, muscle contraction, nerve conduction, C60 fullerene

The search for new means that would effectively influence the pathological consequences of skeletal muscle immobilization is an urgent priority request of modern biomedicine. Previously, the positive effect of C60 fullerenes, as the strong antioxidants, against the background of muscle ischemia, mechanical muscle injury, and other muscle dysfunctions was established [1-3]. These carbon nanoparticles reliably protected muscle tissue from damage caused by oxidative stress. The nerve conduction under stimulation of the rat muscle soleus after long-term immobilization of the hind limbs was studied using a clinical model - rupture of the Achilles tendon. The analysis of force muscle response was performed on day 45 after the initiation of atrophy by using tensometry. The water-soluble C60 fullerene was used as a therapeutic nanoagent at a daily oral dose of 1 mg/kg during the experiment. The delay in the time of muscle contraction caused by 1 and 2 Hz stimulations revealed a sharp increas e from 98 ± 6 ms in control to 443±8 and 487±7 ms after atrophy initiation, respectively (Fig. 1). This delay is associated with a decrease in the conductivity of the nerve stimulus due to destructive changes in the nervous tissue caused by muscle atrophy. In all the tests performed with the administration of water-soluble C60 fullerenes, an increase in nerve conduction by 31±2% and 36±2% at 1 and 2 Hz stimulation, respectively, was detected in relation to the atrophy group (Fig. 1). This indicates the presence of compensatory activation of the endogenous antioxidant system by C60 fullerenes in the process of dystrophic changes caused by prolonged immobilization. Thus, the obtained results demonstrate the prospects of using water-soluble C60 fullerene nanoparticles, which can alleviate pathological state in the muscular system that arises from skeletal muscle atrophy.

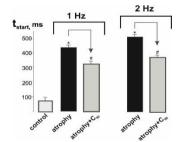


Fig. 1. The time of the start of contraction of the rat muscle soleus after atrophy when using 1 and 2 Hz pools of non-relaxation stimulation lasting 1800 s: atrophy and atrophy+C60 - contraction of the atrophied muscle soleus without the introduction of C60 fullerene nanoparticles and against the background of their introduction; *p<0.05 compared to control; #p<0.05 compared to the atrophy group.

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- [1] D. Nozdrenko, O. Abramchuk, S. Prylutska, O. Vygovska, V. Soroca, K. Bogutska, S. Khrapatyi, Yu. Prylutskyy, P. Scharff, U. Ritter, Int. J. Mol. Sci., 22 (2021) 4977.
- [2] D. Nozdrenko, T. Matvienko, O. Vygovska, K. Bogutska, O. Motuziuk, N. Nurishchenko, Yu. Prylutskyy, P. Scharff, U. Ritter, Int. J. Mol. Sci., 22 (2021) 6812.
- [3] D. Nozdrenko, T. Matvienko, O. Vygovska, V. Soroca, K. Bogutska, A. Zholos, P. Scharff, U. Ritter, Yu. Prylutskyy, Appl. Nanosci., 12 (2022) 467–478.





Carnosine-functionalized Carbon Dots as UV-protector for cornea regeneration

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Keywords: carbon dots, peptide functionalization, UV protection, biocompatibility, cornea

Long time performance of the cornea implant is determined by stability of an UV-protecting modifier. Among the most commonly used modifiers are peptides and polyphenols. However, their tendency to degrade under the UVR shortens time of efficient protection and therefore contributes to a shortened lifespan of the implant. Carbon dots (CDs) are promising modifiers as they are more stable when exposed to the UVR. Moreover, due to the presence of the various functional groups, CDs are easy to functionalize. Therefore, the objective of our study was to obtain the carnosine-modified CDs and evaluate their stability under the UVR [1], [2].

Carbon dots were obtained by the microwave method using citric acid and urea as precursors. To purify the CDs from unreacted synthesis substrates, they were heated to 370°C for 12h. To functionalize the carbon dots, equal amount of the CDs and carnosine were mixed and incubated in dark for 24h. Then, the morphology of the CDs was assessed with AFM (TopoMetrix Discoverer TMX 2000). The particles size was measured using the DLS method (Zetasizer Nano ZS, Malvern). The structural studies were carried out using the Raman spectroscopy (WITec Alpha 300M+ spectrometer). The Stability of the CDs particles was measured with the UV Vis (Shimadzu) and FTIR spectroscopy (Bruker Tensor 27). The fibroblasts viability was assessed after 3rd and 7th day of incubation.

The obtained results indicated the presence of the CDs with a size in a range of 6-20 nm. The Raman spectrum shows the presence of D and G band at the 1375 cm-1 and 1596 cm-1, respectively. The relation of relative ID/IG intensity was 0.95 which indicated the disordered nature of the CDs with poor crystalline framework. Further structural studies indicated the presence of N-H groups on the CDs surface. The UV-Vis studies showed the presence of absorption bands in a wavelength range of 280-440 nm. Subsequent in vitro studies showed no cytotoxic effect of the CDs.

The results of the studies indicates CDs as a promising UV-protecting modifier for cornea tissue engineering.

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References

[1] R. Lin, Y. Wang, X. Li, Y. Liu, and Y. Zhao, "pH-dependent adsorption of peptides on montmorillonite for resisting UV irradiation," Life, vol. 10, no. 4, pp. 1-13, 2020, doi: 10.3390/life10040045.

[2] H. Kaurav, D. Verma, A. Bansal, D. N. Kapoor, and S. Sheth, "Progress in drug delivery and diagnostic applications of carbon dots: a systematic review," Frontiers in Chemistry, vol. 11. Frontiers Media SA, 2023. doi: 10.3389/fchem.2023.1227843.





The influence of graphene addition on the thermal properties of flexible polyurethane coatings used in protective materials

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Keywords: graphene, protective materials, high-temperature environment, thermal properties, nanocomposites

Hybrid textile materials are multi-layered construction consisting of a textile carrier, often made by the combination of different yarns, and coating. Such materials are used for personal protective equipment (PPE) that provides complex protection against multiple hazards. The role of the coating is most often to transport contaminants away from the protective material and to provide protection against chemicals, heat and fire.

The use of carbon nanomaterials such as graphene as modifier for the coating of hybrid textile materials can significantly impact on the thermal properties of the materials [1 - 3].

The object of the study was a nanocomposite foil made from graphene-modified polyurethane paste, which was also intended to serve as a coating for a protective hybrid textile material. Nanocomposites were obtained by mixing polyurethane paste with two different weight contents of graphene nanoparticles in a planetary mixer. In the study, 0.25 and 0.5 wt % of graphene were used. Nanocomposite foils were produced using the Tape Casting method and then cross-linked in a dryer. In summary, three variants of the research materials were obtained: nanocomposite foils modified with 0.25 and 0.5 wt % graphene, respectively, and pure polyurethane without the addition of nanoparticles, serving as the reference sample. Thermal properties and microstructure of the samples were investigated. The impact of graphene on the glass transition temperature of the polyurethane paste was determined using differential scanning calorimetry. The thermal stability of obtained foils was assessed using thermogravimetric analysis in two atmospheres – air and nitrogen.

An increase in the glass transition temperature of rigid segments of polyurethane was observed with the increased content of graphene. Thermogravimetric analysis performed in an air atmosphere, showed an increase in the onset decomposition temperature of the polyurethane paste with the application of 0,25 wt% graphene, while a decrease of this temperature was observed with use of 0,5 wt% of graphene. The results of the thermogravimetric analysis performed in nitrogen atmosphere indicated an increase in the onset decomposition temperature for both graphene contents. Overall, no contraindications were demonstrated for the application of produced nanocomposite pastes as coating layers on textile carrier.

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- [1] S. C. Shiu and J. L. Tsai, Compos B Eng, vol. 56, (2014) 691–697.
- [2] D. Dandapani and K. Devendra, Indian J Sci Technol, vol. 15, no. 45. (2022) 2508-2514.
- [3] D. Wijerathne, Y. Gong, S. Afroj, N. Karim, and C. Abeykoon, International Journal of Lightweight Materials and Manufacture, vol. 6, no. 1, (2023) 117–128.
- [4] E. Irzmańska, A. Boczkowska, E. Żyłka, M. Jurczyk-Kowalska, K. Strycharz, and P. Szroeder, Przemysł Chemiczny, vol 1 (2024) pp. 117–123.
- [5] Sałasińska K, Leszczyńska M, Celiński M, Kozikowski P, Kowiorski K, Lipińska L, vol. 14 (5) Materials 1184.





Nano-Schottky junction in AgPt@GO composite and their role in ppb-level NO2 gas sensor

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Challenges in the area of gas sensors: low sensitivity, long reaction times and work-ing at elevated temperatures can be solved by designing sensors composed of various active materials. In the present study, the nature of the interface between core-shell AgPt nanoparticles and carbon structures (graphene oxide, graphene oxide doped with nitrogen, reduced graphene oxide) was analysed, followed by their sensing properties towards NO2. The best sensing properties showed the AgPt@GO, which responded to NO2 concentrations below 1 ppm at room temperature (RT). In addition, the tested material was characterised by stability and quick response (in the range of 1-50 ppm at RT). The excellent characteristics of AgPt@GO are attributed to the generated nano-Schottky junction, as demonstrated by dielectric spectroscopic experiments. The existence of a p-n junction was verified for the other material. In the sensor investigations, the impact of variations in humidity (RH 3–50%) and temperature (RT-250 C) on the response of the manufactured sensor systems and their selectivity (H2, CH4, H2S) was examined. Furthermore, the electronic structure of obtained composites was studied in detail.





Preparation of 3D carbon fibre reinforced carbon composites for rocket motor nozzles

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Keywords: Carbon fibre reinforced carbon, carbon fibre, composites, rocket motor, nozzle;

Carbon is widely known for its exceptional thermal stability and resistance to thermal shocks, and because of that carbon-carbon (C-C) composites are frequently used as refractory materials, heat shields, breaks and rocket nozzles. The C-C composites are characterized by excellent mechanical properties, light weight, great thermal stability, high thermal conductivity etc. [1]. Depending on the directionality of reinforcements they can be classified as a 1D – unidirectional, 2D – laminates and, 3- or more axis reinforced composites. The fabrication process consists of embedding carbon fibres in carbon rich resin or pitch matrix, which is subsequently carbonized and followed by densification through chemical vapor deposition or liquid impregnation cycles. The C-C composites due to its superior thermal characteristics and exceptional mechanical properties are particularly good candidates for rocket motor nozzles. These elements have to withstand the extreme thermal shocks, temperatures up to 3000 oC, and significant mechanical loads due to high pressure of gases and the high-speed exhaust flow. The main erosive mechanisms affecting the surface of nozzle are mass loss due to oxidation, ablation and tribological loss [2]. Such conditions necessitate materials that not only possess high thermal conductivity to dissipate heat effectively but also maintain structural integrity and resist oxidation and tribological wearing.

In this work we demonstrate the method of fabrication of 3D carbon reinforced carbon composite nozzle for rocket motors. The presented method involves the impregnation of arranged carbon rod frames with phenolic-formaldehyde resin and further heat processing - carbonization and re-densification. The velocity of ultrasonic pulse was measured in order to examine dynamic elastic properties, and to check the uniformity of materials. Preliminary results indicate that obtained composites can be successfully used in rocket motor applications.



Figure 1. Carbon fibre rod frame used for fabrication of 3D carbon-carbon composite.

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References

[1] Wenhao Du, Fanhao Zeng, Yu Dai, Yafang Gao, Meiyan Chen, Zhi Li, Oxidation behavior and thermal-shock resistance of AO20/Si3N4 coating for carbon/carbon composites, Ceramics International, Vol 50, 12, 2024, p. 21463-21472, DOI: 10.1016/j.ceramint.2024.03.257

[2] G.L. Vignoles, Y. Aspa, M. Quintard, Modelling of carbon—carbon composite ablation in rocket nozzles, Composites Science and Technology, Vol. 70, 9, 2010, p. 1303-1311, DOI: 10.1016/j.compscitech.2010.04.002





Polypropylene nanocomposites containing carbon nanofillers for MV and HV power cables

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Keywords: dielectric properties, polymer nanocomposites, polypropylene; MV and HV power cables

Cross-linked polyethylene (XLPE) is widely used as an insulation material in power cables. With recent advancements in medium and high-voltage power transmission and distribution, there is a growing need for new insulation materials that offer high performance, recyclability, and high operating temperatures as alternatives to traditional XLPE insulation. Polypropylene (PP) has shown excellent properties, making it an attractive candidate for medium and high-voltage direct current insulation and screening (Figure 1) [1,2]. It belongs to the group of polyolefins which can be obtained through the process of polymerization of propylene monomers. PP can be found in three stereo-specific configurations based on the attachment of methyl group (–CH3) on the polymer backbone (syndiotactic, isotactic, and atactic) [1]. The intrinsic high melting temperature of PP allows it to carry high voltages and withstand higher working temperature thus avoiding the use of crosslinking agents. Moreover, PP does not have impurities problems like XPLE and this favours the dielectric properties of PP [1]. Therefore, with respect to XLPE, PP shows the advantages of enhancing thermal and electrical properties, no by-product formation, no degassing treatment requirement, and is recyclable [1].

Thus, developing PP-based MV and HV power cable insulation and screens with enhanced electrical, thermal, and mechanical properties is crucial for finding a recyclable insulation material. The advancements in nanodielectrics suggest that nanotechnology could significantly improve the overall dielectric properties of PP-based materials. This work explores the key aspects of PP-based nanocomposites for MV and HV power cables, with a focus on how different nanofiller parameters affect the dielectric, and mechanical properties, as well as the water treeing effect. Based on the collected information, future directions for enhancing the properties of PP-based nanocomposites for MV and HV power cables will be discussed.

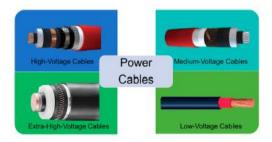


Figure 1. Different types of power cables used for electricity transmission and distribution [2].

- [1] M. Adnan, Z. Abdul-Malek, K.Y. Lau, M. Tahir, IET Nanodielectrics, 4 (2021), 84-97.
- [2] I. Plesa, P.V. Notingher, C. Stancu, F. Wiesbrock, S. Schlögl, Polymers, 11 (2019), 24.





Study of the oxidative thermal stabilization process of hard coal tar pitch for carbon-carbon composites matrix precursor

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Keywords: coal tar pitch, oxidative stabilization, carbon-carbon composites, thermal analysis

Coal tar pitch (CTP) is a derivative of coal tar produced in coke production processes. CTP is widely used in the synthetic carbon and graphite industry as a binder and impregnant. In addition CTP use as a binder in the production of coarse-grained products, it is useful also for lithium-ion batteries anode material manufacture; in the production of high-modulus carbon fibers; and in the production of carbon-carbon composite (CCC) matrices. Research on CTP treatment and modification is of great application importance, including attempts to modify its functional and processing properties, as well as to reduce the content of harmful CTP components, especially polycyclic aromatic hydrocarbons (PAHs).

The use of CTP, especially in its isotropic form, for obtaining carbon fibers and CCC matrices requires oxidative stabilization processes[1]. The stabilization process involves heating them in appropriately selected temperature conditions in an oxidizing atmosphere to remove volatile fractions of light hydrocarbons and to incorporate oxygen atoms into the CTP structure, which additionally stabilize its structure. The stabilization process changes the behavior of CTP during thermal processing, which no longer liquefies or liquefies in a limited way, depending on the need resulting from the technology in which it is used. Uniaxial hot pressing and subsequent pyrolysis, demand limited CTP viscosity and its reduced flow from the mold and from the formed material.

The study carried out tests on the stabilization of the currently widely used CTP with the trade name Carbores P in order to determine its usefulness in CCC manufacturing. Stabilization was carried out at 180 - 220oC for 0.5 - 360 h in an air atmosphere. The influence of the stabilization process on the softening process was examined using differential scanning calorimetry (DSC). Thermogravimetry (TG) was used to test thermal stability and residual mass after heat treatment for stabilized samples of CTP.

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References

[1] H.Niu,P. Zuo, S. Qu. Evaluating multi-step oxidative stabilization behavior of coal tar pitch-based fiber, Journal of Applied Polymer Science, vol.138, issue 11, 2021 https://doi.org/10.1002/app.50002





Study of activated carbon by differential scanning calorimetry

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Keywords: activated carbon, thermal analysis, differential scanning calorimetry

In studying activated carbons, it becomes necessary to characterise them accurately, including determining the specific surface area, pore size distribution, shape, and volume. The most commonly used analytical methods related to the pore-filling phenomenon are mercury porosimetry and techniques for measuring of adsorption/desorption isotherms. The complex structure of activated carbons and the presence of oxygen functional groups are responsible for the different adsorption mechanisms in different areas of the carbonaceous matter. Therefore, differential scanning calorimetry (DSC) can be a valuable and complementary research method for activated carbons.

This paper presents the results of a thermal analysis study of activated carbon with varying porous structures. Nitrogen adsorption/desorption measurements (77K) and thermal analysis studies by DSC using distilled water as adsorbate were determined. Activated carbon was saturated with steam in a vacuum desiccator at room temperature for 24 - 96 hours before testing. Measurements were carried out in the temperature range from - 50° C to 50° C, at a heating/cooling rate of 2° C/min, in a nitrogen environment. The reference sample was an empty crucible. During the measurements, crystallisation and melting curves were recorded, which were used to determine the characteristic temperatures Tmax (peak maximum temperature), Tonset (peak onset temperature) and the enthalpy of the processes ΔH .

DSC, in the thermal analysis of activated carbons, makes it possible to determine the freezing and melting points of frozen water in the adsorbed pores. The values of the freezing point of frozen water are in the range of -14.5°C to -12.5°C. Frozen water's melting temperature values are at -0.5°C to 3°C. Two peaks can be seen in the DSC curves, which show the melting of frozen water. The low-temperature peak represents the melting of water inside the pores, and the high-temperature peak represents the melting of water outside the pores.

- [1] G. Makomaski, Journal of Thermal Analysis and Calorimetry, 133 (2018) 1345-1352.
- [2] D. Majda, M. Zimowska, K. Tarach, K. Góra-Marek, B. Napruszewska, A. Michalik-Zym, Journal of Thermal Analysis and Calorimetry, 127 (2017) 207-220.
- [3] M. Landry, Thermochimica Acta, 433 (2005) 27-50.





Luminescence of tris(8-quinolinato)aluminum(III) (Alq3) adsorbed into activated carbons

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Keywords: adsorption, porosity, photoluminescence, Alg3

Tris(8-hydroxyquinoline)aluminum (Alq3) is well-known as a fluorescent complex showing electroluminescence with a significant quantum yield (Fig. 1). Since the pioneering report in 1987 by Tang and Van Slyke on efficient green electroluminescence using Alq3 [1]; this compound has been applied as an electron transport layer as well as a crucial light-emitting material for organic light-emitting diodes (OLED). The deposition process of Alq3 on various materials (including, in particular, carbon materials) in the form of thin films, just like the properties of these hybrid systems, has been widely described in the literature [2]. For a long time, less attention has been paid to the application/incorporation of Alq3 onto/into the porous materials. The problem may be the size of the Alq3 molecule, which is relatively small for this type of complex (~ 1 nm) [3], but on the other hand, its size may determine the choice of a porous medium [4,5].

The states of tris(8-quinolinato)aluminum(III) adsorbed in micro- and mesoporous carbon materials with different pore sizes were investigated. Alq3 was successfully occluded into the mesoporous carbons from the solution. The adsorbed amount of Alq3 was effectively controlled by changing the concentration of Alq3 the solution. The state of Alq3 in the mesopore varied depending on the pore size as well as the adsorbed amount of Alq3, as revealed by variation of the photoluminescence spectra. The pore size of the used carbon material allows for control of the guest–guest interactions between Alq3 molecules and the host-guest interactions between Alq3 and the mesopore.

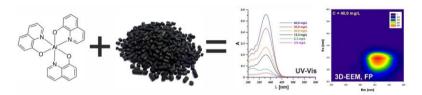


Fig. 1. The concept of the measurements.

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- [1] C.W. Tang, S.A. VanSlyke, Appl. Phys. Lett., 51 (1987), 913-915.
- [2] D. Zhang, K. Ryu, X. Liu, E. Polikarpov, J. Ly, M.E. Tompson, Ch. Zhou, Nano Lett., 6 (2006) 1880-1886
- [3] W. Xie, W.-W. He, D.-Y. Du, S.-L. Li, Chem. Commun., 52 (2016) 3288-3291.
- [4] M. Tagaya, K. Shinozaki, Y. Maruko, J. Appl. Chem., 2017, 1-10.
- [5] G.-S. Yang, M.-N. Li, S.-L. Li, Y.-Q. Lan, J. Mater. Chem., 22 (2012) 17947-17953.





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