ABSTRACT BOOK

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FOREWORD

It is a pleasure for us to offer you Abstract Book for the 9th International Conference on Materials Science and Nanotechnology for Next Generation; MSNG-2022. Our goal was to create a scientific platform that introduces the newest results on internationally recognized experts to local students and colleagues and simultaneously displays relevant Turkish achievements to the world. The positive feedback of the community encouraged us to proceed and transform a single event into a conference series. Now, MSNG-2022 is honored by the presence of over 200 colleagues from various countries. We stayed true to the original MSNG-2022 concept and accepted contributions from all fields of materials science and technology to promote multidisciplinary discussions. The focal points of the conference emerged spontaneously from the submitted abstracts: energy applications, advanced materials, electronic and optoelectronic devices. Further fields of interest include e.g. new advanced and functional materials, advanced-functional composites, biomaterials, smart materials, dielectric materials, optical materials, magnetic materials, organic semiconductors, inorganic semiconductors, electronic materials, graphene, and more.

Here now, we exultantly present you a freely accessable abstract book contain a good part of works presented in MSNG-2022 conference. We hope this abstract collection will be beneficial.

Our warmest thanks go to all invited speakers, authors, and contributors of MSNG-2022 for accepting our invitation

We wish you will be pleased by this abstract book of MSNG-2022 conference and look forward to meeting you again in one of the forthcoming MSNG-2023 event.

Prof. Dr. Şemsettin ALTINDAL
Conference Chair

Prof. Dr. Fahrettin YAKUPHANOĞLU
Conference Chair

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Plenary & Keynote & Invited Speakers Presentations

All Printed Perovskite Solar Modules Made Under Ambient Conditions for Next Generation Energy Production Devices

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Abstract: Inkjet-printing technology is anticipated to play a major role in the future prototyping of perovskite solar cells (PSCs) to enable their ultra-low-cost and scalable manufacturing. However, inkjet challenges related to fluid dynamics need to firstly be addressed so as to allow the fabrication of high-quality printed materials and competitive photovoltaics to the established market. PSCs with earth-abundant carbon as an effective replacer for unstable hole transporting materials and expensive electrodes is a proposed structure promising better air and moisture stability. In this presentation, we will report on the latest advances of perovskites used as absorbers in carbon based perovskite solar cells and also to their modifications for long term stability and simplicity of preparation methods. Some of their outstanding properties including low cost, high stability, ambient processability and compatibility with most up scaling methods will be also discussed. In brief, the results showed that by employing a facile and universal perovskite precursor ink concentration regulation strategy, the coffee-ring effect usually appear in inkjet printing technology is greatly suppressed, leading to the fabrication of much better-quality perovskite layers and correspondingly more efficient and stable photovoltaics. Finally, the development of all-printed carbon-based hole-transport-material-free perovskite modules will be demonstrated, along with low upscaling efficiency losses and outstanding stability after 1000 h of ageing.

Keywords: Perovskite solar cells, 3rd Generation PVs, carbon electrodes, monolithic PV module

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Nanotechnology: Pushing the Limits of the Universe

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Abstract: Although the famous physicist Feynman's talk which was titled "There is Plenty of Room at the Bottom" in 1959 is accepted as the beginning of nanotechnology, the roots of it is being traced to ancient times. In our era, nanotechnology which reshape our lives, a major driving force behind the technological revolution. The breakthroughs in nanotechnology recent years have shown that in few years, it will be possible that sci-fi matters become reality.

In the scope of this talk, examples of the revolutionary scientific innovations in nanotechnology are presented and it is mentioned how nanotechnology pushes the limits of the universe.

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Irreversibility Field and Upper Critical of MWCNT Added Single Crystal $FeSe_{0.5}Te_{0.5}$ Superconductors

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Abstract: After it was determined that the electrical conductivity properties of Multi-Wall-Carbon-Nanotubes were quite good, MWCNTs are used as a support material for electrical conductivity in many materials. A similar situation is also possible for superconducting materials, and MWCNTs have recently been used as additives in many superconducting materials.

In this study, 2 % and 4 % MWCNT added single crystal FeTeSe materials were produced using the self-flux method. The effect of the MWCNT addition on the electrical conductivity and magnetic properties was investigated. The results obtained show no significant change in the superconductivity phase transition temperature but changes both structurally and in terms of critical current density were obtained. In addition, it was observed that there were changes in the Irreversibility field and Upper Critical field properties which will be a significant advantage for technological applications.

Keywords: Multiwall carbon nanotube, superconductivity, single crystal superconductor, critical current density, irreversibility field, upper critical field

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Chitosan Based Hybrid Materials for Advanced Agricultural Applications

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Abstract: A chitosan-based hybrid nanocomposite system encapsulated with metal nanoparticles were developed to work as excellent super-absorbent system with take aim to fight against menace of drought, a serious and challenging threat to life of crops. The biodegradable polymeric shell/coating on plants seed heightens the adhesion of materials, protects the nutrients from degradation, slowing nutrients release and limiting loss of chemicals (Fertilizers/micro or macro nutrients). Controlled release regulates the nutrient dose and reduces wastes. The product material was analyzed by SEM and TEM to establish its nanometric dimension and morphological features. The biological tests of the material tested which showed the efficacy of the formulation in water storage, controlled nutrient release, biofertilization, seedling growth and germination. The study can provide inputs to devise an efficient plant nutrient management strategy for increasing crop production. The outcomes may possibly be applied to improve a possible replacement for designing a new delivery fertilizer system that is environmentally friendly.

Figure: Showing mechanism for activity and application of Chitosan based super- absorbents for improving crop water/nutrients efficiency and regulating growth

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Comparison between n-Type Doped Tin Oxide and Zinc Oxide as Transparent Conducting Oxides

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Abstract: Tin oxide (SnO_2) and zinc oxide (ZnO) are transparent conducting oxides of several applications in optoelectronics and solar cells. Both can be used as fore-contacts and antireflection coatings in solar cells. Both can be fabricated as thin films using low cost deposition techniques. In this work both of them were synthesized by the low cost spray pyrolysis technique as thin films. The fluorine doped tin oxide films (SnO2:F) and aluminum doped zinc oxide (ZnO:Al) films were characterized using X-ray diffraction (XRD), UV-VIS spectroscopy, and current-voltage (I-V) characteristics. The films showed polycrystalline nature, high transmittance, low resistance, wide bandgap energies, and linear I-V plots. A comparison between these properties of SnO_2 and ZnO was performed in the light of their suitability for use in solar cells.

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High Entropy Alloys: The Next Big Thing in Magnetic Alloys

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Abstract: The search for new functional magnetic materials has led to the exploration into multi-component alloys (MCAs), which contain 4 or more elements with percentages between 12.5 and 33%. These include the sub-class of high entropy alloys (HEAs) which often exhibit single phases, thought to be stabilized by the high entropy of mixing of these compounds amongst other competing thermodynamic contributions. The resulting alloys often have interesting functional properties, which are linked to their structure. In this talk, two different areas of our research into magnetic HEAs will be presented. The first is the development of combinatorial sputtering with high throughput experiments, allowing us to study over 50 different combinations within a couple of days, pinpointing compositions of interest for further study. The second shows the different compositions ($CoFeNi_{0.5}Cr_{0.5}Al_x$, $CoFeNi_{0.5}Cr_xAl$, $CoFeMn_{0.5}Al_x$, $CoFeNiCr_yCu_x$) studied in bulk form, to understand how the phases present in the alloys influence the magnetic properties. The research shows that magnetic HEAs have the potential to be competitive with existing soft magnetic materials.

Keywords: High entropy alloys, magnetization, soft magnetic materials, high throughput experiments

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Hydrogen Production and Role of Hydrogen in Renewable Energy

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Abstract: Hydrogen isn't a renewable energy, but it is a "fuel source", it's actually a "energy transport medium". It lets you store renewable energy or other form of generated energy from one place to another place for consumption. Hydrogen is the lightest element. At standard conditions hydrogen is a gas of diatomic molecule. It is the most abundant chemical substance in the universe, constituting roughly 75% of all normal matter and most of the hydrogen on Earth exists in molecular forms such as water and organic compounds. It's always in a chemical bond with something else, like Oxygen. It takes exactly as much energy to break that bond (to free the hydrogen) as is the amount of energy it can later produce by re-combining it with oxygen (either burning or in a fuel cell). The usual energy source to break those bonds is electricity, and there is some loss in efficiency.

There are several methods to produce hydrogen. In this talk, methods of hydrogen along with the ways of transportation to use it as fuel source will be presented

Keywords: Hydrogen, fuel, molecule, chemical, renewable energy, electrolysis, water, organic

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Influence of AC-Signal Amplitude on the Dielectric Properties of Al-TiW-PtSi/n-Si Schottky Diodes

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Abstract: Dielectric properties and electrical conductivity of TiW–PtSi/n-Si structures in the amplitude of ac-signal range of 5mV–1V (500kHz) and voltage range of (-2 V) to (4 V) have been investigated at the room temperature in detail by using experimental *C–V* and *G–V* measurements. Experimental results show that the values of ε' increase with increasing voltage, reaching saturation at a voltage of 2V. The values of ε' at (V_{ac}) = 200 mV are almost 3 times different from the others and also reach saturation. On all dependences on the applied voltage of the real and imaginary parts of the dielectric permittivity, real and imaginary parts of the electric modul *M'* and *M''*, resistance and ac-conductivity there is a sharp difference from other values when (V_{ac}) =200mV. For other values of V_{ac}, the dependence on the amplitude of the test signal is practically not observed. On all dependences on voltage, there is a jump in the value of the parameter in the range of voltage values 1-2V. It can be concluded that, at certain values, the amplitude of the ac-signal can significantly affect the interfacial polarization even at high frequencies.

Keywords: Silicide–silicon contact, PtSi/n-Si Schottky diodes, Dielectric properties, dielectric loss, Electric modulus, ac electrical conductivity, power dissipated

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Influence of Gamma Irradiation on Structure and Band Gap of Graphene Oxide (GO) and GO/PVA Nanostructures

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Abstract: Recently, extensive research has been conducted on the development of new types of composites based on graphene oxide (GO) and GO. This type of materials have a wide range of applications in various industries. They are used in energy storage devices, in the development of supercapacitors, in the creation of various types of sensors, in the process of photocatalysis, etc. is used. Such materials have a wide range of applications. It is possible to control their physical properties by exposure to various effects, as well as gamma radiation, which allows them to expand their field of application. Depending on the reduction degree, it is possible to control the band gap of the GO in the range of 0.02-2.2 eV. Researches show that the reduction rate of GO can be controlled depending on the intensity of gamma radiation. Another GO-based materials is GO/PVA-based composites. These types of composites are promising materials in the production of supercapacitor batteries. Therefore, the resistance of these materials to various effects, the dependence of their optical, electrical and other properties on these effects is of great interest.

In this study, GO was synthesized by the Hummers method. The sample was filtered through filter paper and washed several times with HCl (30%) and distilled water. GO was dried at room temperature and then added to distilled water. The solution was subjected to ultrasound for 1 hour and then centrifuged. The filtered solution was dried at room temperature. GO (1%, and 5%) of different concentrations were mixed with PVA and dried at room temperature.

In this study, graphite, GO and GO/PVA were exposed to gamma rays irradiation at different doses (1,50 and 150 Mrad). The power of the gamma source was 174.43 rad/sec. XRD measurements were performed using the Rigaku device. The results show that the crystal structure and particle size in GO and GO/PVA vary depending on the radiation dose. Changes are observed in the peaks of XRD charts. The value of the diffraction angles and the half-width of diffraction peaks vary depending on the intensity of the radiation. In addition, changes are observed in both the intensity and half-width of the diffraction maximums characteristic of PVA and GO. This indicates a change in the structure and composition of the particles and the polymer matrix. According to other literatures, it is thought that graphene oxide has been reduced by the effect of qamma rays It has been shown that the value of the reduction rate varies depending on the radiation dose.

UV-Vis measurements were conducted with Specord 250 Plus device. The width of the band

gap of the samples (graphite, GO, 1% and 5% GO/PVA) was determined optically. The results show that as the intensity of the radiation increases, the width of the band gap for all samples decreases. Thus, graphite, GO, GO/PVA samples with a concentration of 5% and 1% exposed to 1 Mrad intensity radiation and their band gap was resulted as following values 1.58, 1.60, 1.63 and 2.60 eV, respectively. In samples exposed to 150 Mrad radiation, these values were 1.33, 1.33, 1.20 and 2.00 eV, respectively.

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Interactions Between the Drug Molecules and Carbon-Based Nanostructures

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Abstract: Carbon-based nanostructures (CNS) with distinct and remarkable properties can be classified based on their hybridization, crystallinity and dimensions. Zero dimension (0D) such as carbon fullerene, Nanocages, 1D nanostructures such as pristine and carbon based nanotubes, 2D nanostructures such as graphene family based Nanosheets, are gaining increased interest in biomedical and tissue engineering as biosensors or drug delivery systems because of their unique and extraordinary physicochemical properties. Among several applications of CNS, the drug carrier role has been widely considered in recent years.

Here, the basic properties of CNS-drug complex systems investigated by density functional theory (DFT) for drug delivery and sensing study are presented. The parameters that defined the structural and adsorption properties of the system are reviewed. The analysis of thermodynamically parameters, Frontier molecular orbital and charge transfer analysis are examined. Quantum Theory of Atoms in a Molecule (QTAIM) analysis and the non-covalent interaction (NCI) analysis are given in a detailed discussion by comparing drug molecules' interactions with the CNS.

In this context, size and doping effect, covalent and non-covalent surface modifications on CNS –drug interactions are investigated to be defined the system, which can serve as promising sensors in practical applications to detect, recognize and carrier drugs for their medicinal applications.

Keywords: SWCNTs, Fullerene, C based nanocages, drug delivery, drug carrier, DFT.

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Molecular Modeling of Toxicology of DNA Adducts

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Abstract: A DNA adduct is a segment of DNA bound to a cancer-causing chemical. Carcinogens arising from many sources, including pesticides, industrial agents, agricultural contaminants, and environmental pollutants, are known to directly interact with DNA to form adducts. Although adduct formation most commonly occurs at guanine sites in DNA, adducts involving each of the four canonical nucleobases have been identified. Unfortunately, there is currently no clear molecular explanation for the diversity in the biological outcomes of DNA adducts. If structure–outcome relationships can be developed, it is plausible that the harmful effects of newly identified adducts could be accurately conjectured, which could in turn focus experimental studies geared toward understanding the toxicity mechanism of environmental contaminants and combating the effects of the associated DNA lesions. The current lack of a structure–outcome relationship for DNA adducts arises at least in part since experimental studies have typically concentrated on particular carcinogenic lesions. To complement experimental studies, computer modeling provides a unique approach for studying a range of lesions derived from known carcinogens. Moreover, calculations can be used to study methodically built analogues that may not have direct biological relevance, but are valuable probes for determining the influence of distinct chemical features of DNA adducts on observed biological outcomes. This presentation highlights the Molecular Dynamic and DFT methods to investigate the DNA lesions stemming from some more significant and prevalent adducts including PAHs.

Keywords: Toxicity, Carcinogen, DNA, PAH, MD, DFT.

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Quantum Photonics and Pattern of Light

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Abstract: We address the importance of structured light and its applications in different fields such as microscopy, quantum information, optical manipulation, and laser technologies. As an example, the self-healing characteristics of different kinds of structured light such as Bessel and Laguerre-Gauss, superposition of mirrored Laguerre-Gaussian beam have been presented. As an important results, the quantification and optimization of the self-healing characteristics were presented.

Keywords: Quantum photonics, Structured light, Self-healing

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Spectroscopic Ellipsometry Analysis of Polymethylmethacrylate/Perylene Dye Thin Films

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Abstract: A polymer solution of PMMA mixed with perylene dye was prepared to get spin-coated thin films. Two dye concentrations 10-2 and 10-8 wt % were used and the structure and optical properties have been studied using spectroscopic ellipsometry. Results have shown that the refractive index has an in-plane value of 1.696 while the out of plane value was 1.55 at wavelength of 632 nm. For the samples under investigation studied, the spectral dependence of the refractive index follows the anisotropic general oscillator model based on optical constants that were calculated using Cauchy point by point fitting. The results give a promising way for further investigations when analyzing such films for photo selective applications.

Keywords: PMMA polymer; Perylene; Spectroscopic ellipsometry; Refractive index; Thin films.

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Three Arguable Concepts: Point Particle Singularity, Asymmetric Action of EM on Quantum Wave Functions, and the Left Out Restricted Lorentz Gauge From U(1)

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Abstract: We address three concepts. i) The point particle assumption inherent to non-quantum physics is singular and entails divergent fields and integrals. ii) In quantum physics electromagnetism (EM) plays an asymmetric role. It acts on quantum wave fields (wave functions) but the wave fields do not react back. We suggest to promote the one sided action of EM on quantum waves into a mutual action-reaction partnership. By so doing, the quantum wave shares its analyticity with the EM field and removes the latter's singularities and divergences. iii. The conventional U(1) symmetry leaves quantum dynamics invariant under a 'general' Lorentz gauge and imposes the standard minimal coupling of the quantum wave to the EM 4-vector potential. One, however, has the option to ask for invariance under the 'restricted' Lorentz gauge. This in turn invites in a coupling to the derivatives of the vector potential in addition to the minimal coupling and, so to say, enlarges the U(1) symmetry. We examine the Dirac electron in this context and find that the electron exhibits distributed charge and current densities. The enlarged symmetry is expected to bring in its own constant of motion. Indeed it does. The anomalous g-factor of the so designed electron emerges, up to order as the new constant of motion in agreement with the QED theorized values.

Keywords: Point particle singularity, Asymmetric role of EM in quantum physics, Restricted Lorentz gauge, anomalous magnetic moment, U(1) symmetry enlarged, Non-minimal coupling.

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Tungsten Based Functional Nanoparticles from Recycling for Thermosets, Thermoplastics and GFRP - Industrial Applications within Reach

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Abstract: For decades, there seemed to be no alternative as using very high temperatures and strong acids for the recycling of tungsten scrap, due to the high melting points and strong abrasive resistance of the tungsten containing material.

Here, a different approach to tungsten recycling is utilized that is called bacteria-based recycling or bioleaching. As an innovative, sustainable biological process, it can be used to gain tungsten from scrap and to manufacture tungsten nano powders on an industrial scale. The gained tungsten nano powder can be pure nano tungsten or nano tungsten carbide, depending on the used scrap. Further the tungsten can be easily oxidized to receive tungsten oxide / tungsten trioxide. The tungsten nano materials can be dispersed in thermosets, thermoplastics and glass-fibre reinforced plastics (GFRP) to manufacture a “masterbatch” which is easy to handle for a production line. The tungsten containing masterbatches are known to improve the physical and chemical properties of the matrix (as for example polyester or vinyl ester resin). As little as 0.5-1% by weight of the masterbatches in GFRP are sufficient to significantly increase properties such as pressure or wear resistance, elasticity, or stiffness and to save material in product manufacture.

Keywords: Tungsten nano particles, Tungsten nano powder, Tungsten recycling, bioleaching, glass-fibre reinforced plastics, GFRP, masterbatches, wear resistance, pressure resistance

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A New Method in Molecular Dynamics Simulations: Nonequilibrium Free Energy Calculations

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Abstract: In this study, the Jarzynski equation, Crooks' fluctuation theorem and phase space method was employed to use the outputs of molecular dynamics simulations. Within this process, the results of the steered molecular dynamics simulation data were resolved by using weighted histogram analysis method to obtain the probability density distributions to be used in the phase space method. To test these non-equilibrium methods, a non-physical system in which a single ion is pulled in water was designed. In this simple system, Jarzynski equation, phase space methods and Crooks' fluctation theorems are tested. After obtaining the potential applied to this simple system and confirming that our non-equilibrium approach worked, calculations were repeated for more complex biomolecular systems.

As a result, a method has been developed and applied in simple and complex systems using phase space and Crooks' method. Moreover the work done by the dissipative force is calculated and free energy surfaces depending on the path are obtained. Hence, the first study, which calculates the work done by the dissipative force in molecular dynamics simulations, and enables the calculation of the friction force at nanoscale, has emerged.

Keywords: Dissipative force, Nano-friction, Jarzynski equality, Phase space method, Crooks theorem, Molecular Dynamics simulations

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A Study on Estimation of Material Properties to be Synthesized for Wideband Wide-Angle Ml-Ram Design

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Abstract: Stealth technologies are an essential issue that maintains their importance in military warfare applications and has gained popularity in recent years. The main purpose of this technology is to reduce the radar cross section (RCS) of the targets. For RCS reduction, either the incoming wave is directed to the other sides with geometric approaches, or the backscattering energy is reduced by covering the target with a special radar absorber material (RAM). Multi-layer (ML) RAM designs have been very popular in the last quarter century as they provide wide-angle, polarization-free, and broadband requirements. The most critical parameter that will advance the ML-RAM design process is the synthesis of different materials. However, to avoid redundant materials while performing material synthesis, the permittivity (ε) and permeability (μ) of the most commonly used material structures in the design of ML-RAM should be known, and synthesis processes should be performed accordingly.

In this study, ML-RAM structures designed from 16 different virtual materials are examined and the most selected material types are determined as a result of optimization. Thus, it has been revealed what kind of material development processes should be chosen in order to design full performance (thin, wide band, wide angle, min reflection, and polarization-independent) ML-RAM.

Keywords: Optimization, Permittivity, Permeability, Wide angle RAM, Wide band RAM.

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Altering Electric, Magnetic, and Optical Features of $LuFeO_3$ Via Substitution of Ir into Fe Sites

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Abstract: The electrical, magnetic, and optical properties of $LuFeO_3$ (LFO) and $LuFe_{1-x}Ir_xO_3$ (LFIO) (x = 0.05, 0.10) compounds were studied. X-ray diffractometer was utilized to identify the crystal nature of the samples. The scanning electron microscope was exploited to examine the surface topography of the samples. X-ray photoelectron spectroscopy was employed to determine the valence states of Lu, Fe, and Ir. The Raman investigations unveiled the Raman peak intensity reduces with Ir doping and the peaks shift toward the smaller wavenumbers. Dielectric studies demonstrated the LFO has a higher dielectric constant than the LFIO. Such decrement in dielectric was related to reduction in the ratio of Fe^{2+} ions and defects in the LFIO. The Magnetic measurements revealed the spin re-orientation transition temperature is around 47 K for all the samples. Furthermore, 5 mol % LFIO demonstrated the highest magnetization owing to the existence of magnetic impurities. M-H loops unveiled the Ir doping advances both H_c and M_r values, which could be due to the variation of the canted angels of Fe^{3+} moments, the advancement of energy of magnetocrystalline anisotropy, and formation of secondary phases. Furthermore, the optical band gap of LFO reduces from 2.19 eV to 2 eV by Ir doping.

Keywords: Solid-state reaction; orthorhombic $LuFeO_3$, Ir doping; dielectric properties, Raman spectroscopy; Magnetic properties; Optical band gap

Acknowledge: *This work was supported by The Scientific and Technological Research Council of Turkey (TUBITAK) through Grant No: 116F025.*

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Biophotovoltaic Devices

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Abstract: In the globalizing world, information transfer is very easy. Ideas about solving new generation problems are gaining popularity day by day. To offer solutions to these problems in the shortest way and to develop existing problems are done by scientists. There are many methods to obtain electrical energy from solar energy. Organisms such as bacteria or chlorophyll create a few of the mechanisms called biophotovoltaics. Although the efficiency of these mechanisms, which work like a solar cell, is low, they are suitable for development. These studies, which are seen as artificial photosynthesis, are quite interesting.

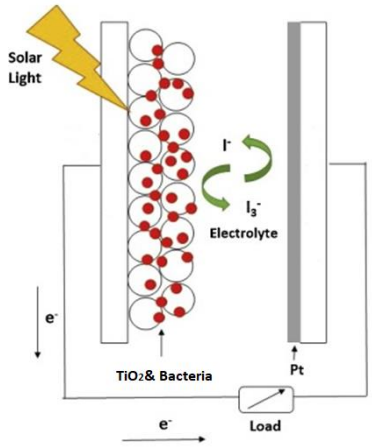

Figure 1. Scheme of classical biophotovoltaic cell

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Characterization of Anti-Nematodal Potential of Synthetic Compounds Using C.Elegans as Modal Organism

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Abstract: Parasitic nematodes infections in humans, livestock and agriculture become a major global issue. synthetic drugs are used against nematodes infections, due to nematodes resistance to these drugs and toxicity, we need to develop drugs which are environment friendly and high efficacy. Current Investigations determined the nematicidal activities of synthetic organic compounds (Thiazine derivatives SS-1 to SS-15) using *C.elegans* as modal organism. Synthetic compound SS-7 and SS-11 showed LD_{50} at 40µg/mL hence considered most potent. Most of the synthetic compounds showed excellent anti eggs hatching activity. At 20µg/ml concentration compounds SS-3, SS-4, SS-5, SS-7, SS-11, SS-13, SS-14 and SS-15 showed EC_{50} vales (50% unhitched eggs). In all synthetic compounds SS-4, SS-8, SS-9 and SS-13 showed high apoptotic/necrotic response confirmed through fluorescence microscope. RT-PCR results expressed the gene expression quantitatively in normal and affected *C.elegans*. In synthetic compounds the gst-4 was highly expressed by SS-13 (111.80±3.31 fold), SS-14 (127.43±6.19 fold) and SS-15 (134.14±6.06 fold), hsp-4 and hsp-16.2 were highly expressed by SS-15 (17.58±2.15 and 27.26±2.15 fold) and gpdh-1was highly expressed by SS-4 (32.45±2.03 fold), SS-5 (18.95±0.17 fold), SS-7 (17.29±2.88 fold) and SS-12 (18.17±3.73 fold) respectively. This study confirmed that most synthetic compounds are very effective because they showed changes on gene level and determined the mechanism of action of synthetic compounds within the Phylum Nematoda conserved pathways. The synthetic compounds (SS-1 to SS-15) showed different mechanism of action due to structural modification in Thiazine derivatives. The most potent synthetic compounds are good candidate(s) for novel broad scale anthelmintic drug(s).

Keywords: Parasitic nematodes, Nematicidal drugs, Synthetic compounds, Gene expression, Eggs, Humans, Livestock, Agriculture, *C.elegans*, pathways.

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Controlling the Electrical Characteristics of Au/p-Si Diodes by the ZnO: Ag_2WO_4- PVP Interfacial Layer

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Abstract: Current-voltage (I-V) characteristics of Au/p-Si diodes with and without ZnO:Ag_2WO_4-PVP interfacial layer were analyzed to get more information on the conduction mechanisms and barrier formed at the interface. The *I-V* characteristics have rectifying behavior with the rectification ratios 6.95 and 332.49 for Au/p-Si and Au/ ZnO:Ag_2WO_4-PVP/n-Si. It is clear that interfacial layer improves the device performance in terms of ideality factor, barrier height, and shunt resistance with values of 7.72, 0.56 eV and 2 kΩ whereas those of Au/n-Si diode are found as 4.83, 0.68 eV and 96 kΩ, respectively, as well as the high rectification ratio. The mechanism of space charge formation has been also investigated. The ln(I)-ln(V) curves show two regions corresponding to ohmic and space charge limited conduction. Experimental results reveal that the current flow is influenced by the space charges and the traps at the interface.

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Identification of the Negative Capacitance Effect in the Interlayered Metal-Semiconductor Structures and Distinct Electronic Devices

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Abstract: Negative Capacitance (NC) behavior, which can be explained as the material exhibiting an inductive behavior, is often referred to as "anomalous" or "abnormal" behavior in the literature. Especially in the forward bias/deposition region, the presence of surface states (N_{ss}) and their relaxation times (τ), series resistance (R_s), minority carrier injection, interface charge loss in occupied states under the Fermi energy level, parasitic inductance, or poor measuring equipment calibration problems can be counted among the causes of this behavior. Studies on NC behavior have shown that this behavior can be observed for different frequencies, temperatures, and such related parameters at forward biases. However, the NC behavior, which appears as an unidentified peak in admittance spectroscopy data, is not yet fully understood. Ultimately, the goal of this study is to compile and analyze the NC behaviors reported in selected scientific studies and to investigate the source of this behavior.

Keywords: Negative Capacitance; Metal-Semiconductor Structures; Interlayer; Data Mining; NC Devices.

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Iron Phosphide Electrocatalyst for Renewable Production of Value-Added Products

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Abstract: The electrochemical reduction reaction of the nitrate ion (NO_3^-) to valuable ammonia (NH_3) is a promising green approach. Herein, we report for the the electrocatalytic reduction of NO_3^- using different phases of iron phosphide. Particularly, FeP and Fe_2P phases were successfully demonstrated as efficient catalysts for NH_3 generation. The Fe_2P catalyst exhibits the highest Faradaic efficiency (96%) for NH_3 generation with a yield (0.25 mmol h^{-1} cm^{-2}) at −0.55 V vs. reversible hydrogen electrode (RHE). The recycling tests confirmed that Fe_2P and FeP catalysts exhibit excellent stability during the NO_3^- reduction at −0.37 V vs. RHE. These results indicate that the Fe_2P phase exhibits excellent performance to be deployed as an efficient noble metal-free catalyst for NH_3 generation. In addition to NO_3^- reduction the iron phosphide phases were used in electrocatalytic H2 generation using water electrolysis. The electrocatalytic activities of heat-treated Fe_2P−450°C, Fe_3P−500°C, and Fe_2P/FeP−500°C catalysts were studied for hydrogen evolution reaction (HER) in 0.5 M H_2SO_4. The lowest electrode potential of 110 mV vs. a reversible hydrogen electrode (RHE) at 10 mA cm^{-2} was achieved with a mixed Fe_2P/FeP−500°C catalyst.

Keywords: iron phosphide, electrocatalysis, NH_3 generation, H_2 evolution, water electrolysis

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Outlook of Fundamental Components Utilized in Cost-Effective Dye Sensitized Solar Cells

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Abstract: Dye-sensitized solar cells (DSSCs), which belong to the third generation of solar cells, have sparked fascinating scientific research in the solar energy sector throughout the past three decades. DSSCs are very popular because of their inexpensive manufacturing materials. A photoanode, redox electrolyte medium, dye, and counter electrode components make up a conventional DSSC device. By adjusting the characteristics of these parts, numerous tests have been carried out with an emphasis on the technological context-dependent photovoltaic performance of DSSCs. This study aims to describe the manufacture and characterization of DSSCs with different variations of these components utilizing a simple coating approach to fabricate a unique device structure.

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Past and Future of Emerging PV Technologies

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Abstract: Recently, most of the energy needs are met from fossil fuels. Since fossil fuels are on the verge of depletion and cause global warming and climate change there is no other choice but to turn to renewable energy sources. Among the renewable energy sources, the sun is important because it is environmentally friendly, free, abundant and peaceful. Solar energy can be converted into electrical energy using solar cells. Emerging PV technologies are counted as rising photovoltaic technologies that enable to produce electrical energy from solar energy in a cheap, easy and clean way, and it has become very important in terms of producing light, flexible and inexpensive solutions.

In this study, the past and future of emerging technologies will be reviewed. The scientific studies based on emerging PV technologies from past to present in YTU Organic Electronics Laboratory will be summarized.

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Perfect Raw Materials Metallic Glasses and Some Applications

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Abstract: In this study, general production techniques of metallic glasses were explained. The advantages of metallic glasses were given if compere with crystalline alloys with same composition. As mentioned headline, "why metallic glasses are perfect raw materials for some applications?" were given in detail. Magnetic properties of metallic glasses were compared with metallic alloys and the advantages were investigated. Some experimental results were given in figures, pictures and tables. We can be sure that near future bulky glasses will widelly take place in industry. For this reason, bulky metallic glasses will get significant place in this presentation.

Keywords: Metallic glasses, magnetic properties, coercivity, anisotropy, bulky metallic glasses.

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Polyaniline Membranes for Electrochemical Application: Some New Dimensions

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Abstract: Polyaniline (PANI) is an intrinsically conducting polymer that assumes different oxidation/doping states by varying synthesis conditions and external stimuli that results in various tunable electrochemical, mechanical, morphological and electronic and electrochromic properties. PANI has been used in various membranes applications for its switchable electrochemical and morphological characteristics. The low-cost raw material and easy water based (green) synthesis make PANI as one the prime materials of interest in various application. Owing to its brittleness and intractability in almost all solvents, PANI has been used as a composite membrane material such as through blending with other film forming polymers and through *in situ* chemical and/or electrochemical deposition on membrane substrate. Various deposition techniques and variation in parameters within these influence composite membrane morphology and other performance characteristics.

This paper discusses the recent work of polyaniline membranes for electrochemical applications supervised by the author. These membranes include novel polyether sulfone (PES)-PSS/DVB-PANI membranes for fuel cell applications where PANI coated PSS/DVB (polystyrene sulfonated-divinyl benzene) cation-exchange resin particles were incorporated in PES matrix. This PANI modification resulted in improved ionic conductivity as shown by EIS and reduced hydrogen cross-over through these membranes. In another study, PANI based Gas Diffusion Layer (GDL) was developed where effects of various PANI dopants such as HCl, dodecyl benzyl sulfonic acid (DBSA) and p-toluene sulfonic acid (pTSA) were studied on GDL morphology, 4-probe conductivity, water and gas permeation. The charge transport processes were characterized using EIS and further to this, the degradation behavior of these PANI based GDLs was also characterized using impedance spectroscopy. In third ongoing research on PANI electrochemical membranes in the group on polyaniline coated sulfonated polyvinyl alcohol (sPVA)-sepiolite composite membranes, effects of sepiolite content in in-house sulfonated PVA matrix and subsequent PANI layering using novel vapor-phase *in situ* deposition were elaborated. Dynamic mechanical analysis showed a shift in glass transition depending on sepiolite content indicating strong bonding of backbone polymer chains with sepiolite particles. The modelling of the EIS results showed a strong dependence of membrane transport processes on sepiolite content and PANI layering at the surface.

All these electrochemical and other membranes research in author's group show PANI as an influencing constituent of these composite membranes contributing to morphology, mechanical properties, thermal stability and membranes' transport processes.

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Polymers of Intrinsic Microporosity Membranes and Their Applications

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Abstract: The replacement of conventional separation processes by membrane processes has led to a search of membrane materials with improved separation ability. Polymers dominate the market of membranes owing to their easy processability. Polymers of Intrinsic Microporosity (PIMs), a novel class of polymers, have attracted considerable attention from the membrane community.[1] PIMs possess remarkable properties owing to their highly rigid and contorted polymer backbones, which frustrate efficient packing and provide high free volume. Their high thermal and chemical stabilities and high surface area make them promising for various applications.[2] They could be produced in many different forms such as powder, film and fibrous membrane forms due to their solution-processability. In addition, they are selective, organophilic materials, and their selectivity could be tailored by simple chemical modification methods for desired molecules. Therefore, we have developed wide range of PIM membranes for various applications, including adsorption, separation and electrochemical applications.[3]

Keywords: Polymers of Intrinsic Microporosity, PIMs, membrane, nanofiber, electrospinning.

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Production and Characterization of Flexible Dye Sensitized Solar Cells

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Abstract: Dye-sensitized solar cells (DSSCs) have been studied intensively, considering that they will be a promising energy source in the future due to their low cost, efficiency in low light conditions and absorption in the visible light spectrum. The development of DSSCs based on plastic flexible substrates such as polyethylene terephthalate (PET) and polyethylenenaphthalate (PEN) has become necessary today to reduce costs in solar cell manufacturing and make DSSC more practical. Flexible plastic substrates have created a new alternative for solar cells with very important advantages such as light weight, good flexibility, impact resistance, low cost, lower temperature and large-scale production. However, when DSSC is produced using a flexible plastic backing, is only processed at a low temperature of around 100-150^{o}C. As a result, DSSC performs poorly due to poor interconnection of TiO_2 particles. Methods such as sol-gel, microwave irradiation, electrophoretic deposition, and chemical vapor deposition are used to produce flexible photoanodes at low temperatures. In this study, flexible DSSCs developed by making new TiO_2 paste will be examined.

Keywords: Flexible DSSC, TiO_2 paste, chemical reduction method, fill factor, power conversion efficiency

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Roles of Nanotechnology in Solar Applications

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Abstract: A nano ceramic coating was used as passive radiative self-cooling layer on the rear side of a small PV module. The passive radiative self-cooling layer was prepared by blinding (Alpha) Al_2O_3 nanoparticles with water glass, then the formed glue was painted over the rear side of a small 10W PV module. The coating was applied using regular paint brush in two directions (horizontal and vertical). The test was done at an ambient temperature of 50°C. The layer showed a noticeable effect on reducing PV module temperature in the hot weather for up to 5°C, where the panel surface temperature was 63°C then dropped after coating to 58°C. In the same way this paint was also used to reduce the disadvantage of passive solar energy in hot regions such as heat sink for water tanks, as well as heat exchangers and vehicle radiators.

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The Study on The Wide Frequency Range of Electrical Characteristics in Al/(Coumarin-PVA)/p-Si Structures at Room Temperature

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Abstract: Coumarin-PVA is deposited on p-Si wafer using spin coating method. The main electrical parameters of the Al/(Coumarin-PVA)/p-Si type Schotkky barrier diodes (SBDs) have been investigated by capacitance-voltage-frequency (C-V-f) and conductance-voltage-frequency (G/ω-V-f) measurements at room temperature and they were performed in the frequency range of 10 kHz- 1 MHz and at (±5V) by 50 mV steps. The effects of (Coumarin-PVA), series resistance (Rs) and surface states (Nss) on electrical characteristics have been investigated in detail. In order to eliminate the effect of Rs on high frequencies these measurements, the measured Cm and Gm/ω values were adjustment. The high values of Nss at low frequencies are responsible for the non-ideal behavior of C-V and G/ω-V characteristics. The obtained value of ND exponentially decreases; the value of $\Phi_{B(C-V)}$ exponentially increases with increases frequency. Such behavior of N_D and $\Phi_{B(C-V)}$ are expected behavior and it is attributed to the particular density distribution of Nss, polarization processes and interfacial layer. Experimental results show that the C-V and G/ω-V characteristics of SBDs are affected not only in Nss and Rs but also interfacial polymer (Coumarin-PVA) layer.

Keywords: Al/p-Si SBDs with (coumarin-doped PVA) interfacial layer; Surface states and series resistance; Frequency and voltage dependence

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Theoretical Modeling of 2D Ferromagnetic Material

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Abstract: In this talk, after talking about my project about 2D ferromagnetic materials, I will also talk about the results of a study we have just completed since it is about 2D ferromagnetism which we study the electronic, magnetic and transport properties of the CrN/P/CrN heterostructure, composed of two hexagonal CrN monolayers and a blue-phosphorus monolayer. This system represents a minimal model for a CrN-based spin valve, schematically shown in Fig.1.

In the present study, we first use DFT to investigate both the structural and the magnetic stability of the CrN/P interface. We then analyze its electronic properties and study the spin-dependent transport properties of the CrN/P/CrN heterostructure by means of Boltzmann transport theory. We find the most-favorable stacking pattern and determine its Curie temperature. The transport properties of CrN/P/CrN are found to be strongly dependent on doping.

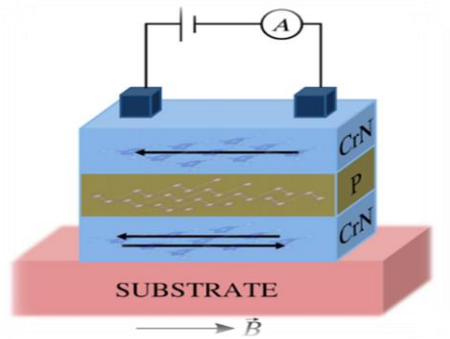

Fig. A lateral spin-valve device

Keywords: 2D materials, electronic properties, ferromagnetic material, spin-valve device.

Acknowledge: This work was supported by the Scientific and Technological Research Council of Turkey (TUBITAK) under Project No. 119F361. I acknowledge Ankara University for use of the high-performance computing facility through the AYP under Grant No. 17A0443001. I also acknowledge support from the FLAG-ERA JTC 2021 Project "MNEMOSYN", 221N400 Project No. (TUBITAK).

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Weak Ferromagnetism in a Double-Exchange Model for Cerium-Oxides

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Abstract: Cerium oxides exhibit weak, room-temperature ferromagnetism without d-electrons. A possible explanation for this is the Zener double-exchange, where itinerant electrons polarize the localized spins via Hund-coupling as they hop from site to site. Here, we report magnetization and spin-spin correlation results using various values of the Hund-coupling in a one-orbital double-exchange model with Ising spins. Our results at 50% spin concentration show ferromagnetic tendencies at low carrier densities (n=0.25). However, ferromagnetism is lost at intermediate carrier concentrations (n=0.50) due to charge localization at high temperatures, as evident from the density of states calculations and Monte Carlo snapshots. To our knowledge, our study based on a realistic Zener-type double exchange mechanism is a first in the study of magnetism in cerium oxides. Our results are also consistent with previous studies using similar Hamiltonians in the context of diluted magnetic semiconductors, where Heisenberg spins were used. We will further comment on possible improvements to our models and techniques.

Keywords: ferromagnetism, cerium oxides, Monte Carlo, diluted systems, strongly correlated electrons

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Oral Presentations

1-(2-Fluoro-3-(Trifluoromethyl)Benzylidene)-2-(Pyridin-2-Yl)Hydrazine and 1-(2-Fluoro-4-(Trifluoromethyl)Benzylidene)-2-(Pyridin-2-Yl)Hydrazine: Synthesis, Spectroscopic, Structural Properties

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Abstract: *Hydrazones* are organic compounds with the formula, $R_1R_2C=NNH_2$, where R_1 and R_2 represent different substituent groups. Hydrazones are the condensation product of hydrazines or hydrazides with aldehydes or ketones. When hydrazones are used as intermediates for the synthesis of other substances, the -CONHN=CH- azomethine group plays an active role. The chemical properties of hydrazone derivatives have been widely studied in many fields such as chemistry, technology, and medicine for long years. Of these, studies in biomedical applications have become very popular in the last few decades. Hydrazones possessing an azomethine -NHN=CH- proton constitute an important compound in new drug research. Therefore, many researchers have synthesized these compounds and evaluated their biological activities by elucidating their structures. In this first phase of this research, 1-(2-fluoro-3-(trifluoromethyl) benzylidene)-2-(pyridin-2-yl) hydrazine and 1-(2-fluoro-4-(trifluoromethyl)benzylidene)-2-(pyridin-2-yl)hydrazine have been synthesized. The purity of the synthesized compounds have been proven by elemental analysis and melting point assay. The crystal structure of this compound was resolved with the XRD method. Its structure was characterized using elemental analysis, FT-IR, ^{1}H-NMR, ^{13}C-NMR, and UV–VIS spectroscopic methods. In the second phase of this research the synthesized compounds' antioxidant activities were compared with the standard antioxidant BHT upon having assayed DPPH free radical scavenging activities.

Keywords: Crystal structure, X-Ray diffraction, Spectroscopic analysis, DPPH, Hydrazone

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A Comparative Study That CdS Thin Films Obtained with CBD on Different Substrates

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Abstract: Cadmium sulfide (CdS) is a semiconductor that belongs to the II-VI group family. CdS thin films are used as an important material in optoelectronic, photovoltaic, and piezo-electronic devices due to their suitable band gap (~2.42 eV), relatively high absorption coefficients, special optical properties, and ease of fabrication. In this study, CdS thin films were deposited on glass, ITO, and FTO substrates by chemical bath deposition (CBD) which is a simple and low-cost technique. The morphologic, optical, structural, and electrical properties of the CdS thin films were investigated comparatively on different substrates by scanning electron microscopy (SEM), UV-vis, X-ray diffraction (XRD), and Hall-effect measurement, respectively. It was seen that all films were deposited on substrates smoothly, homogenous, and consisted of nanoparticles. Also, they have a crystalline structure that was determined in polycrystalline structure with cubic and hexagonal contents. The conductivity of the CdS thin film obtained on FTO was found to be higher than that obtained on other substrates.

Keywords: CdS; thin film; semiconductors; optical properties; structural properties, electrical properties.

Acknowledge: This study was supported by the Research Fund of Mersin University in Türkiye with Project Number 2022-1-TP2-4649.

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A Comparison Electric-Features of Al/p-Si (MS) and Al/(Al_2O_3:PVP)/p-Si (MPS) Structures Using Current-Voltage (IV) Measurements

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Abstract: Both the *Al/p-Si (MS)* and *Al/(Al_2O_3:PVP)/p-Si (MPS)* type Schottky diodes *(SDs)* have been grown on the pSi wafer to compare their both electrical parameters and conduction mechanisms by using *IV* measurements. The basic electrical parameters like zero bias barrier height *(BH)*, ideality factor *(n)*, series resistances *(R_s,)* and shunt resistances *(R_{sh})* of them were extracted from the forward-bias *(I-V)* data by using thermionicemission (TE) theory and Cheung's-functions. Energy-dependence profile of interface states *(N_{ss})* have been evaluated from the *IV* data by taken-into account voltage-dependent of BH and n. *Ln(I_R)-$\sqrt{V_R}$* plots were also show good linear behavior, and while conduction mechanism is governed by Schottky emission *(SE*) for *MS*, it is governed by Poole Frenkel *(PF*) for *MPS* diode. These results show that *(Al_2O_3-PVP)* interlayer can be successfully used in place of conventional insulator/oxide-layers and it has many advantages such as low-cost, high-dynamic stress, charge storages capability, and flexibility.

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A Comparison of Electrical Characteristics of Al/p-Si (MS) and Al/(PVP-TeO_2:Cu)/p-Si (MPS) Structures Using Current-Voltage Measurements

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Abstract: Both the Al/p-Si (MS) and Al/(PVP-TeO_2:Cu)/p-Si (MPS) structures were performed onto the same B-doped Si wafer to determine the organic (PVP-TeO_2:Cu) interfacial layer effect on the performance of MPS structure using forward/reverse bias current-voltage (IV) measurements. For this aim, some important electrical parameters of them such as reverse saturation current (I_s), ideality factor (n), zero bias barrier height (Φ_{Bo}), series/shunt resistances (R_s, R_{sh}), rectification ratio ($RR=I_{for.}/I_{rev.}$ at ±5V) and compared each other. Three basic electrical parameters (n, R_s, and BH) of them were also extracted from the Cheung' s functions and compared thermionic-emission (TE) theory. The observed some differences between of them were attributed to the voltage dependent of them as well as the used method. The energy dependent density distribution profile of interface-traps/states (N_{it}/N_{ss}) was also extracted from the forward bias I-V data using Card-Rhoderick method. Experimental results show that (PVP-TeO_2:Cu) interlayer leads to increase the performance of the MS structure in respect of lower values of leakage current, R_s, N_{ss}, and higher values of RR and R_{sh}. Therefore, we can say that the used thin (PVP-TeO_2:Cu) organic layer between Al and p-Si wafer improves the quality of MS structure and hence it can be successfully used instead of conventional insulators (SiO_2, SnO_2) in respect of low-cost, low-energy consumptions, easy grown-processes, and flexibility.

Keywords: (PVP-TeO_2:Cu) organic interlayer, A comparison of MS and MPS structures; TE and Cheung methods; Energy dependent density distribution of interface states.

Acknowledge: This study has supported by TUBITAK-121C396 Project.

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A Minor Batch of Zn and Mg Incorporated Quaternary CuAlZnMg High Temperature Shape Memory Alloy (HTSMA)

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Abstract: High temperature shape memory alloys (HTSMAs) are widely desired to be used in related smart materials applications and HTSMAs with different functional and characteristic properties are muchly demanded for different tasks to be done by these alloys or devices designed by these alloys. A common practical way to fabricate HTSMAs with different shape memory effect (SME) and other properties is to fabricate them with different alloying compositions and add different additive elements. In this work, a quaternary CuAlZnMg HTSMA with an unprecedented composition consisting minor amount of zinc and magnesium additives was produced by arc melting method. After applying post-homogenization in high β–phase temperature region and immediate quencing a microstructural SME mechanism was installed in the produced alloy. To examine SME characteristics of the alloy some differential thermal analysis (DTA), microstructural (XRD) and magnetization (VSM) characterization tests were carried out. The DTA results showed that the alloy is a HTSMA exhibiting reverse martensitic transformations at temperature range between 167 °C and 489 °C. The XRD pattern obtained at room temperature revealed the martensite phases formed in the alloy which phases are the base mechanism of the reversible martensitic transformation (the SME property) of the alloy. The VSM test showed the paramagnetic nature of the alloy.

Keywords: CuAlZnMg, HTSMA, Shape memory effect, Martensitic transformation, Enthalpy, DTA, XRD.

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A Novel Dye Sensitized Solar Cell Application of TiO_2/ZnO Nanocomposite

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Abstract: The world's energy needs are increasing day by day due to the increase in the rapid increase in the world population and the development of the industry. On the other hand, the rapid decrease of fossil fuels encourages scientists to develop new alternative energies. Renewable energy sources are energy types that can create an alternative to fossil fuels, and solar energy shines like a star among them. Dye-sensitized solar cells are cheap, environmentally friendly and easily applicable. In this study, the solar cell assembly was made up of the FTO@TiO_2/ZnO photoanode, N719 dye, I^-/I_3^- electrolyte and FTO coated Pt photocathode. The solar cell efficiency values of prepared TiO_2 and TiO_2/ZnO have been found at 8.56 and 9.12%, respectively. With the addition of ZnO to TiO_2, the solar cell efficiency value increased by 10%.

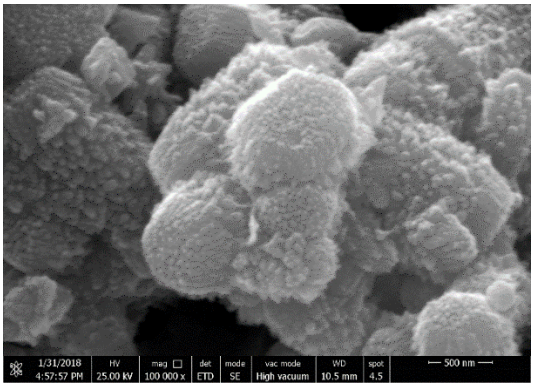

Fig. 1. The FE-SEM images of TiO_2/ZnO nanocomposites.

Keywords: TiO_2, ZnO, nanocomposites, DSSC.

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Ab-Initio Study of Effects of Na Doping on Hydrogen Storage Performance, Electronic and Elastic Properties of LiMg Compound

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Abstract: The energy demands of today's modern society increase due to rising populations. The fast consumption of fossil fuels will lead to the depletion of resources quickly. These concerns have promoted the search for sustainable,clean,practical, and environmentally favorable energy sources and carriers. Solid state storage of hydrogen such as metal or complex hydrides gives storing hydrogen with high gravimetric and volumetric densities [1-2]. Recently, experimental studies exhibited that Na-MgLi alloy has a suitable temperature range for hydrogen storage and lower dehydrogenization temperature [3]. In B2 intermetallics alloys, hydrogen generally shows a temporary alloying element due to its small atomic radius. The firstprinciples methods can be successfully employed to study the hydrogen storage performance of B2 intermetallic alloys [4]. In literature, it has been proved that element doping is an effective way to increase the performance of hydrogen storage. Here, the effects of Na-substituted dopants on hydrogen storage, electronic and elastic properties of LiMg alloy in B2 structure have been studied by the first-principles methods. Obtained results showed that Na atoms preferentially occupy the Mg atoms to form new Li_8Mg_7Na and $Li_8Mg_6Na_2$. The obtained formation energies of Li_8Mg_7Na, $Li_8Mg_6Na_2$ are higher than that of $Na_1Li_7Mg_8$, $Na_2Li_6Mg_8$ indicating better structural stability. The greater B/G ratio value of Li_8Mg_7Na shows that Na doping on Mg-site improves the recycling performance of LiMg alloy. The obtained results for the electronic structure, elastic properties and structural stabilities give the important knowledge for the design and improve of the hydrogen storage materials.

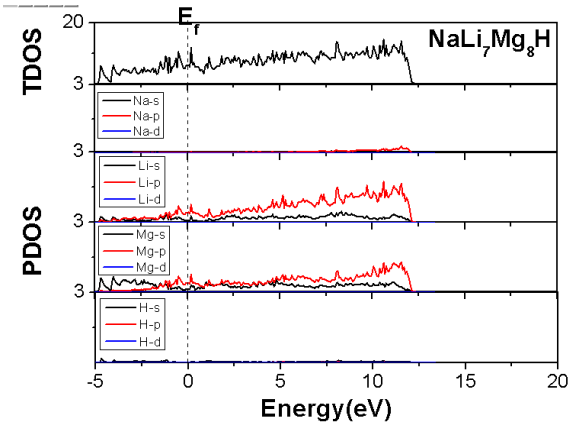

Figure 1. PDOS graphs for $NaLi_7Mg_8H$

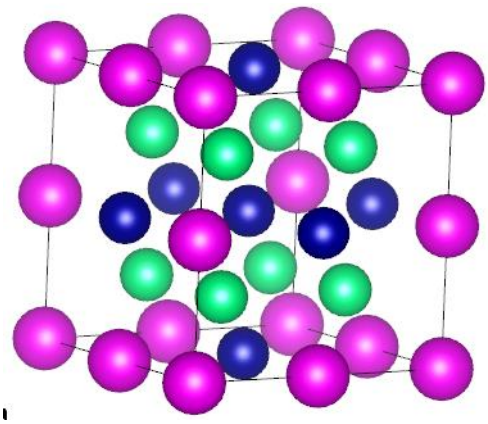

Figure 2. Unitcell of $Na_2Li_6Mg_8$

Keywords: 3D materials, B2 structure, hydrogen storage, density functional theory

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All-Dielectric Multi-Functional Optically Transparent and Flexible Microwave Metasurface

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Abstract: Metamaterial technology is advancing rapidly and opens new avenues to solve the inherent challenges of designing the parameters of wave-matter interactions, effective permeability, and effective permittivity structures with potentially broad applications in the field of antenna, radio frequency (RF) communication, and dual IR/RF windows. Here, we suggest a novel transparent multilayer structure as a radio frequency (RF) and infrared (IR) transparent composite meta-surface. For this aim, through sandwiching the periodic arranged Ge film between two dielectric layers, broadband microwave absorbers were designed with optically transparent and stable characteristics across the 8–18 GHz range. The metasurface design is also significantly flexible, and we showed that it could be adjusted to operate in different infrared frequency ranges thanks to its frequency scalability. Meanwhile, the geometric parameters of the metasurface were carefully chosen based on computational analysis and experimental evaluations, the absorption response shows two peaks at 2.4 μm and 7 μm wavelengths, and the maximum absorption is 96%. The suggested sandwich metamaterial absorber exhibits broadband microwave in the X and Ku bands and infrared absorption in the MWIR and LWIR bands while concurrently having high transmittance, indicating that it has a great deal of promise for creating optical transparent, absorbing devices.

Keywords: Microwave absorber, Infrared, Optically transparent, Metamaterial

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Analysis of the Electrical Characteristics of Al/ GaN/ p-GaAs Structure at High Temperatures

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Abstract: In the present work, electrical characteristics of Al/p-GaAs structure with GaN interfacial layer have been investigated by current-voltage (I-V) measurement at high temperatures. The main electrical parameters such as ideality factor (n), zero bias barrier height (Φ_{B0}) were found as 2.39, 0.444 eV at 300 K and 1.64, 0.562 eV at 380 K, respectively. The series resistance (Rs) of the structure was calculated from Ohm's law and values of the device were found to change from 10.38 Ω at 300 K to 5.92 Ω at 380 K at 0.5 V. In addition, the interface states (N_{ss}) as a function of energy distribution (E_{ss}-E_v) were obtained from the forward bias *I-V* measurements. The decrease of the values of N_{ss} with increasing temperature has been attributed to the molecular restructuring and reordering at the oxide/semiconductor interface, resulting in the more ordered interfacial layer and then lowering the values of N_{ss} under the effect of temperature. The experimental *I-V* characteristics confirmed that the distribution of N_{ss}, Rs and interlayer GaN are important parameters that influence the electrical characteristics of these devices.

Keywords: GaN, I-V characteristics, Interface states, Insulator layer

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Artificial Intelligence Classification of Crops and Weeds Using Impedance and Infrared Spectroscopy

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Abstract: Since herbicides, which are widely used to kill weeds, have many negative effects on the environment and people, it is very important to control weeds with automation based on artificial intelligence applications. In this study, we aimed to develop artificial intelligence applications that classify agricultural products and weeds in order to contribute to robotic applications to control weeds in hazelnut gardens. For this purpose, different data sets were created from the spectra obtained from the leaves of hazelnut tree and various weeds by electrical impedance spectroscopy (EIS) and Total Reflection-Fourier Transform Infrared (ATR-FTIR) spectroscopy techniques. EIS data provided the determination of the dielectric properties of plant leaves exposed to alternating current at different frequencies and ATR-FTIR spectroscopy data provided the determination of the differences in the molecular structures of plants. Using the obtained data, artificial intelligence training was performed with machine learning algorithms such as Support Vector Machine (SVM), k-Nearest Neighbor (kNN) and Partial Least Squares-Discriminant Analysis (PLS-DA). The success of the model created as a result of this training was tested and 80-97% accuracy was obtained. This study showed that artificial intelligence applications which enable agricultural products and weeds to be distinguished can be developed by using spectroscopic data.

Keywords: weeds, artificial intelligence, electrical impedance spectroscopy (EIS), Total Reflection-Fourier Transform Infrared (ATR-FTIR) spectroscopy, machine learning, Support Vector Machine (SVM), k-Nearest Neighbor (kNN), Partial Least Squares-Discriminant Analysis (PLS-DA)

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Calculating the Characteristics Parameters of a Schottky Diode from Forward Bias I-V Data: An Alternative Approach

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Abstract: We propose a diagnostic tool to determine the contact parameters for a Metal/Semiconductor (MS) diode using the forward bias current-voltage data, in cases where the dominant current carrying mechanism through the junction can be described by the Thermionic Emission (TE) theory. The method allows an accurate determination of the saturation current I_0 from *I-V* characteristics of the diode without any extrapolation procedure. Furthermore, a suggested plot of the experimental data in terms of a new variable $\Lambda(V)$ is almost linear in the whole data range and can be used to determine both the ideality factor *n* and series resistance R_s of the diode, without requiring the selection of a linear region. Effectiveness of the method has been tested and compared with some known methods on both artificially generated data and actual experimental *I-V* data of Re/*n*-GaAs/Au Schottky diode. The proposed method has been found to produce more accurate results throughout the whole data region.

Keywords: Schottky diode, parameter extraction, thermionic emission.

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Carbon-Coated Magnetite Nanoparticle Reinforced Magnesium Nanocomposites

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Abstract: In recent years, magnetite nanoparticles (Fe_3O_4 NPs) have received a significant attention owing to their have good stability, low cytotoxicity and high magnetic properties for excellent magnetism. Thanks to these properties, Fe_3O_4 has found its application in medicine, biology and many other fields. Recent studies also have focused on the effect of Fe_3O_4 NPs on the mechanical properties of nanoparticle-embedded matrices and remarkable results were obtained for the improvement of mechanical properties. However, insufficient corrosion resistance has limited its application areas. In order to make improvements in these restricted application areas, it may be a suitable solution method for Fe_3O_4 NPs to have a core-shell structure by creating a hybrid structure with carbon, and the application areas of metal matrix nanocomposites can be expanded. The production of Fe_3O_4 NPs can be achieved by using various methods such as co-precipitation, thermal decomposition, sonochemical synthesis, microemulsion technique and hydrothermal synthesis. Hydrothermal synthesis method offers ease of application, low cost, and environmentally benign method for the synthesis of Fe_3O_4 NPs, and this method is preferable because a hybrid nanostructure can be synthesized in single phase. In this study, it is aimed to synthesize carbon-coated Fe_3O_4 NPs and to evaluate their effect on the mechanical properties of magnesium composites. Nanoparticles were synthesized and characterized using SEM-EDX, FTIR and XRD methods. It is proposed that this type of magnesium nanocomposites can be a potential candidate in biomedical applications.

Keywords: Magnetite nanoparticles, hydrothermal carbon, magnesium nanocomposite.

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Characterization of Polycrystalline p-Si/CdS Thin Films Prepared by Chemical Bath Deposition

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Abstract: CDs thin film was deposited on p-Si substrates with the chemical bath deposition method at 85 °C for 25 minutes. Film thickness was proximate 230 nm in a single deposition. The film was observed by scanning electron microscope (SEM), X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDX) and Hall - effect measurement system. The optical band gap energy (Eg) value was estimated 2.33 eV, according to UV visible spectrometer measurements of on glass substrates thin films. The CdS thin film's surface morphology was as sphere-like grain. The film's structure was polycrystalline made of cubic, orthorhombic and hexagonal. The CdS thin film's had Cd:S element ratio 41:59. The film's conductivity was $1{,}83 \times 10^{5}\ (\Omega\text{-cm})^{-1}$ and n-type at room condition.

Acknowledge: This study was supported by the Research Fund of Mersin University in Turkey with Project Number: BAP 2020-1-TP3-4032

Keywords: CdS, p-Si, Thin Film, Chemical Bath Deposition.

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Colloidal stability of Fe_3O_4 Nanoparticles Synthesized by Hydrothermal Method

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Abstract: This study presents the results of preparation water-dispersible (Fe_3O_4) nanoparticles (MNPs) with a size range of 200 nm by one-pot hydrothermal method. These nanoparticles were prepared using tri sodium citrate as a crystal grain growth inhibitor and a stabilizer in ethylene glycol (EG) solution. When dispersed in water, the resultant MNPs exhibit poor colloidal stability. Their stabilities were confirmed to improve by addition of gelatin as a stabilizing agent. As the gelatin concentration was increased the resulting nanoparticle suspension displayed excellent long-term colloidal stability of at least one week without any agitation. They were also magnetic at room temperature. The interest in the stability of colloidal particles from the fact that some applications are not possible without achieving high stability rates in the medium term at least. Most important problems related to the preparation of nanoparticles can be pronounced as broad size distribution, easy aggregation. MNPs were characterized by X-ray powder diffraction (XRD), (SEM) Microscope, UV-vis spectra, (FT-IR). Also the effect of many parameters on the (MNPs) was studied, such as reaction temperature, reaction time, different glycols (EG, DEG). In addition, these MNPs may be useful in many fields, such as hyperthermia treatment of cancer, and targeted drug delivery, water treatment, based on their size-dependent magnetic property and excellent colloidal stability.

Keywords: Magnetite nanoparticles, colloidal stability, stabilizing agent.

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Comparison of Dielectric Properties of 1wt.% SmC* LC Doped Nematic LC

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Abstract: Chiral smectic liquid crystal ((S)-4-n-octyloxybenzylidene-4'-(3,7-dimethyloctyloxy) aniline) (Fig.1.) is used to dope the (4-cyano-4'-pentylbiphenyl) nematic liquid crystal (**5CB**). In this study, the dielectric properties of **5CB** doped with 1wt.% chiral smectic liquid crystal and pure **5CB** were compared. We have been used dielectric spectroscopy to determine the dielectric properties of the **1wt.% LC** doped with **5CB** liquid crystal. The real (ε') and imaginary components (ε'') of dielectric constant have been calculated by capacitance method. All dielectric parameters have been calculated and compared.

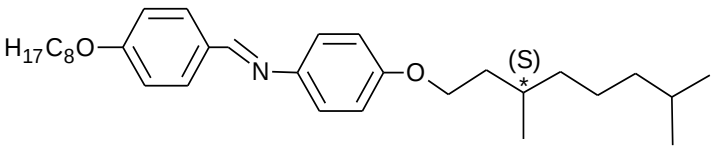

Figure 1. Molecular structure of chiral liquid crystal.

Keywords: Liquid crystal, Dielectric Spectroscopy (DS), Nematic (N)

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Comparison of the Low and High Frequencies Effect on the C&G/Ω–V Characterization of the Metal-Polymer-Semiconductor Structures

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Abstract: Frequency and voltage dependence of capacitance-voltage (C–V) and conductivity-voltage (G/ω–V) properties of Al/($ZnFe_2O_4$-PVA)/p-Si structure was investigated and compared for low (10 kHz) and high (1 MHz) frequency levels. The negative capacitance (NC) effect is observed at low frequency due to the minority carrier injection, surface states (N_{ss}) and series resistance (R_s). NC behavior loses its effect with increasing frequency and exhibits different behavior at low and high frequencies due to the special density distribution and relaxation times of N_{ss}. Also, the changes in C and G/ω were ascribed by the loss of charges in the surface interface states/traps, interlayer thickness and doping concentration. N_{ss} was acquired from Hill-Coleman method and barrier height (Φ_B), Fermi energy level (EF), and concentration of doped acceptor atoms (NA) were obtained from the inverse bias C^{-2} vs V plots at 10 kHz and 1 MHz frequencies. Consequently, it has been observed that C and G/ω are highly dependent on frequency and voltage parameters. The surface states and polarization effect are negligible at considerably high frequencies, and it can also be emphasized that the polarization and Rs should be considered for extracting basic parameters of the electronic devices.

Keywords: Metal-Polymer-Semiconductor Structures; Surface States; Negative Capacitance; Series Resistance; Frequency.

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Converted Molybdenum Oxide Intermediate Phases to Pure $\alpha - MoO_3$ Phase by RF Magnetron Sputtering

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Abstract: In this study, molybdenum oxide (MoO_3) thin films has been grown on Si(111) in different radio frequency (RF) powers and oxygen gas flow conditions. The substrate temperature kept constant at 300 ºC. To investigate the effects of oxygen flow rate, RF power supply was kept constant at 75 watt and the films were grown by changing the oxygen flow between 0.75-1.25 sccm. Also To investigate the effects of RF power supply we kept constant oxygen flow rate. It has been observed that by increasing RF power, the intermediate phases in the films and the MoO_2 phases due to oxygen deficiency, are decreased. Pure α-MoO3 phase was observed in all films with different oxygen gas flow. According to the atomic force microscopy (AFM) results, it was observed that all the films were coated as homogeneous and uniform surface. Optimum conditions for α-MoO3 phase thin films was 75 wat RF power supply and 1- 1,25 sccm oxygen gas flow rates.

Keywords: molybdenum oxide, thin films, $\alpha - MoO_3$ *phase*, RF magnetron sputtering, Coatings

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Copper Phthalocyanine- Perylene-3,4,9,10-tetracarboxylic dianhydride Supercapacitors

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Abstract: Perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) and copper phthalocyanine (CuPC were used to fabricated a supercapacitor. The present study reports the electrical properties of a supercapacitor based on PTCDA and CuPC. The active electrode, electrolyte, current electrodes used for the super capacitors are p-type and n-type organic semiconductors, copper chloride and Al-Cu metal electrodes, respectively. Black carbon was added to active electrodes f PTCDA and CuPc . The current-voltage and power-voltages characteristics of the prepared PTCDA and CuPC based supercapacitors were performed using Fytronix 9200 IV-CV analyzer. The Isc, Voc, and Pmax values for the Al/CuPc/PTCDA/Cu supercapacitos were 1.28 mA, 0.12 V, and 0.038 mW, respectively. Among the prepared supercapacitors, the supercapacitor with the CuPC ratio: BC=90:10 exhibited the highest electrical performance between all supercapacitors. It is evaluated that the organic semiconductor can be used for supercapacitor applications.

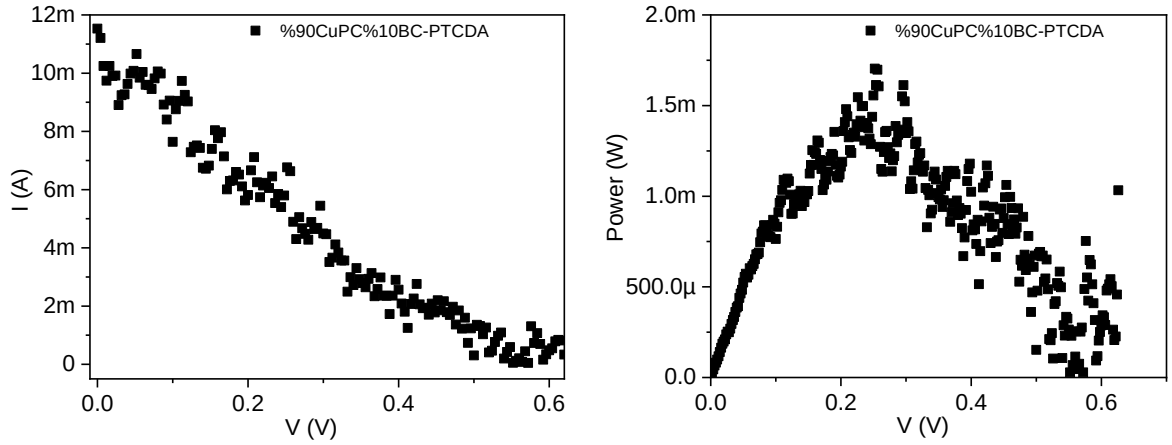

Fig.1. I-V and P-V curves of CuPc and PTCDA based supercapacitor

Keywords: Supercapacitors,

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Correlation of Rare Earth Element (REEs) Content in Turkey and World, and Contribution of Rare Earth Elements to Nano Technology

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Abstract: Rare earth elements come from the word unconventional rather than exactly rare, and there is a misnomer. The concentrations of the more abundant REEs in the earth's crust are similar to those of ordinary industrial metals such as chromium, nickel, copper, zinc, molybdenum, tin, tungsten or lead. In fact, some REEs are almost 200 times more abundant than gold. However, REEs are more difficult to obtain from ore deposits as concentrates, unlike ordinary base and precious metals. As a result, REEs obtained in the world are obtained from very few sources. Differences in individual REE abundances within the Earth's upper continental crust are represented by the superposition of both nuclear and geological effects. The Rare Earth Elements (REE) deposits and mineralization of Turkey can be divided into four types based on their geological setting and origin. These are deposits associated with carbonatite alkaline magmatic rocks, Triassic shales - the bauxites formed, the placer type and phosphorites. Although these rocks are home to the world's largest resources, it is an important issue that needs to be studied carefully for the country's economy, as there has not been enough work done in Turkey yet. In recent years, rare earth elements (REE) have become an essential part of advanced industries. Rare earth elements are used both in industries such as nuclear, metallurgy, chemical, catalytic, electrical, magnetic and optics, and in many futuristic industries such as lasers, fluorescent lamps, atomic batteries, motor turbines and super-magnets. However, its widespread use in these industries causes problems to enough obtain REE in geologic resources. Scientists are using nanotechnology to develop nano-cellulose that can effectively recover REE using a new and sustainable method.

Keywords: Rare Earth Element (REEs), geological setting, nanotechnology, nano-cellulose, industries.

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DC Characterization of GaN-Based HEMT for Fabrication Steps

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Abstract: Over the past twenty years, High Electron Mobility Transistors (HEMT) have been the focus of intense research. Gallium nitride (GaN)-based HEMT has advantages such as higher power density and breakdown voltage thanks to the wide band gap, saturated electron drift velocity and thermal conductivity [1]. In fabrication steps, AlGaN/GaN structure was grown on SiC substrate by MOCVD method with %24 Al concentration. Device fabrication begins with the mesa etching isolation step by Clor-based dry etch. Ohmic contact metals were formed by coating Ti/Al/Ni/Au metals respectively. Ni/Au Schottky gate lithography was performed in the electron beam lithography system. Fabrication was finished with a contact pad for characterization [2]. HEMT devices were investigated with maximum saturation current, on-resistance, transconductance, knee voltage, threshold voltage, gate turn on and breakdown voltage. DC measurements were done 2x125 um device periphery. Table 1 shows measurement results after the second metal metallization. In the results obtained, I_{dss} was 1.29 A/mm, g_m was above 300 mS/mm, and gate and drain leakages were below 100 uA/mm. Compared to the 0.25um gate technology in the literature, high drain current and low leakage current were obtained [3].

Device Type (um)	R_{on} (ohm mm)	I_{dss} (A/mm)	V_{knee} (V)	V_p (V)	g_m (mS/mm)	Id,leak (uA/mm) @70V	Ig,leak (uA/mm) @70V
2x125	2.51	1.29	5.2	3.45	317	96	60

Table 1. Measurement results after fabrication

Keywords: Transistor, GaN, HEMT, DC Characterization

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Design, Synthesis and Structural Characterization of Hydroxyurea Surface-Functionalized Five-Membered Heterocylic Carbon Quantum Nanodots

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Abstract: In developing pharmaceutical industry, green-based materials are known as the most attractive class of biomaterials useful for biomedical applications. However, nano-sized materials for example nanocomposites (NCs) have been gaining great attention in drug delivery systems. In this study, citric acid derived Carbon Quantum Nanodots (CNDs) synthesized by one-pot water-free green thermolysis of citric acid at 180 °C for 2 h, under open-air conditions by constant heating. Then the obtained drug carrier CNDs was chemically modified with an anticancer drug, Hydroxyurea (HU), which is currently used in the treatment of white blood cells called chronic myeloid leukemia (CML), by surface functionalization. Nanoscale conjugate, abbreviated as CNDs/HU, was synthesized in *N*,*N*-dimethylformamide (DMF) containing triethylamine (TEA) as a catalyst, at room temperature for 16 h, using an environmentally-friendly and low-cost experimental method. Structural characterization performed using spectroscopic [(Attenuated Total Reflectance-Fourier Transform Infrared ATR-FTIR), Nuclear Magnetic Resonance (^{1}H-NMR)] and chromatographic [Gel Permeation Chromatography (GPC)] methods. Results obtained concluded that synthesis of CNDs and its HU carbon quantum nanodots-drug conjugate successfully produced and structural identification performed. CNDs-drug conjugates produced from CNDs acting as drug carrier with green material properties have the potential to be developed as a promising candidate for cancer therapy in the future.

Keywords: Surface functionalization, Carbon Quantum Nanodots (CNDs), Ring-opening reaction, Attenuated Total Reflectance-Fourier Transform Infrared (ATR-FTIR), Nuclear Magnetic Resonance (^{1}H-NMR), Hydroxyurea

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Determination of the Radiation Shielding Performance of MoO_2 Addition on PbO_2 by Monte Carlo Simulation

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Abstract: Our study is to develop a composite material that can be used for gamma radiation shielding. Accordingly, the mass absorption properties of MoO_2, La_2O_3, PbO compounds and mixtures with different ratios were theoretically investigated. 50 keV, 80 keV, 120 keV, 662 keV, 1173 keV, 1332 keV gamma energies were used in the study. Radiation absorption properties of materials taken with XCOM database and GATE simulation programs at each energy value are given comparatively. By using the obtained mass attenuation coefficient, mean free path, half value thickness and linear attenuation coefficients were calculated. As a result, it is seen that the absorption property of all materials decreases with increasing energy value. The increase in the amount of La_2O_3 in the mixture increases the shielding property. Thus, alternative materials to PbO will be produced.

Keywords: Gama, XCOM, GATE, Shielding

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Development of Carbon Nanowall Thin Films Produced Using Pulsed Filtered Cathodic Vacuum Arc with Electron Cyclotron Resonance Microwave Method

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Abstract: Carbon nanowall (CNW) thin films were deposited on glass substrates at room temperature with Pulsed Filtered Cathodic Vacuum Arc Deposition (PFCVAD) system. The growth of carbon nanowall thin films was investigated by depositing films at different pulse rates. High purity graphite rod was used as carbon source and soda lime glass as a substrate. The vacuum chamber was closed and the working pressure was reduced to 10^{-3} Torr by means of vacuum pumps and production started. In the process of storing the films, 12kV was used as the trigger voltage and 500V was used as the cathode-anode voltage.CNW thin films are grown by the PFCVAD system at different pulse rate, followed by Electron Cyclotron Resonance Microwave Plasma (ECR-MP) system were employed to improve CNW structures. In the ECR-MP system, the reaction chamber is made of 304 stainless steel and has a cylindrical body structure with a height of 28 cm and a diameter of 39 cm. The system comprises of the microwave plasma generator and vacuum pumps. Before the deposition of CNWs the chamber is evacuated using turbo molecular pump down to the base pressure of $2x10^{-3}$ Torr. The deposition parameters were set to cyclotron frequency of 2.45 GHz and 150 W microwave powers. A magnetic field of 875 Gs is required for the system that produced by a group of excitation coils. Deposition was performed using high purity methane (CH_4, 99.999%). The growth pressure was $2x10^{-6}$ Torr and the substrate temperature maintained at 25°C. No bias is applied to the substrate during the growth. Flow rates measured with the Gas Flow-Pressure Control System were controlled as 6.9 sccm for CH_4. Optical, structural and surface properties of deposited CNW thin films were investigated.

Keywords: PFCVAD, ECR-MP, CNW

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Dielectric Properties of The Ag/GO-NiO/p-Si/Al Structures in The Frequency Range of 10 Khz-300 Khz

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Abstract: In this work, the frequency and voltage dependence of dielectric properties of the nanostructure NiO doped GO thin film on p-type silicon substrate, prepared by the sol-gel method, were analyzed. The dielectric properties of produced thin film samples were examined using capacitance-voltage (C–V) and conductance–voltage (G/ω–V) measurements occurred in the frequency range of 10 kHz-300 kHz under dark and light conditions at room temperature. As for the measurements findings, it was seen that the capacitance and series resistance (R_S) values descend with an increment of frequency. However, the conductance value was increased with the increment of frequency. This statement observed at higher frequencies can be sourced from the existence of interface state densities. Moreover, the other parameters being dependent on frequency such as dielectric constant (ε'), dielectric loss (ε''), loss tangent (tanδ), AC electrical conductivity (σ_{ac}) were researched with the help of the capacitance-voltage (C–V) and conductance-voltage (G/ω-V) surveys. Also, it was obtained that the parameters mentioned above were strongly frequency dependent.

Keywords: Silicon, dielectric properties

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Effect of Doping of the Rare Earth Elements on De-Hydrogenation Efficiency for ZrH_2 Compound: First-Principles Study

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Abstract: To provide our future energy demands, hydrogen is searched as one of the major energy carriers in developing new strategies. Because hydrogen does not produce any harmful gases, it has been considered as one of the most promising energy sources[1]. Materials-based -solid-state storage of hydrogen including the use of metal hydrides and complex hydrides have been investigated densly for it has high hydrogen density and safety[2]. In contrast to storing hydrogen in molecular form, it can also be stored as atomic hydrogen in metals and intermetallic compounds (MH), leading to higher volumetric density. Advantageously, MH provide relatively safe storage at ambient pressure conditions compared to compressed hydrogen gas, and these materials can therefore be handled relatively easily Doping of rare earth (RE) elements can improve the efficiency of hydrogen storage material in two way. One of them is that larger size of RE dopant increase the unitcell volume and thus increase the Zr-H bond length indicating that these results decrease the Zr-H correlation and desorption temperature. Second one is higher volume of RE element doped unitcell of ZrH_2 may store high hydrogen at interstitial spaces showing high specific capacity more than in pure ZrH_2. Using first-principles methods we have studied effect of de- hydrogenation efficiency on doping of rare earth elements La, Nd, Pr and Ce in ZrH_2. Specific storage capacity both in terms of volumetric and gravimetric capacity was also studied. To investigate clearly hydrogen storage capacity of ZrH_2 we have investigated elastic and electronic properties. Generally, obtained results exhibite that La, Nd, Pr and Ce doping on the ZrH_2 compound increase the hydrogen storage capacity.

Keywords: 3D materials, B2 structure, hydrogen storage, density functional theory

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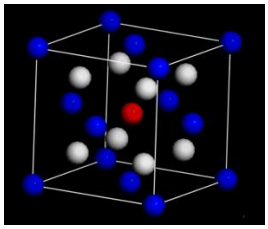

Figure 1. Unitcell of Zr4H8X (X=La,Nd,Pr, Ce red one)

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Effect of Metal Contact Selection on the Electrical Characterization of ZnSe Thin Film

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Abstract: The II- VI class of compound thin films are promising material for electro-optic applications. ZnSe which belongs to this group, receives considerable attention with its wide band gap and high electrical conductivity [1]. ZnSe thin films have a wide range of applications such as solar cells, light emitting diodes [2] and optical detection devices when deposited on silicon crystal substrates [3]. In this paper, ZnSe thin film was deposited with the RF sputtering technique, which is commonly used due to its high homogeneity and uniform thickness advantages of film deposition [4]. The effect of top metal contacts on the electrical characteristics of ZnSe metal-insulator-metal diodes is studied. The basic electrical parameters were observed strongly dependent on the metal contact selection [5]. The contacts were fabricated on the ZnSe thin film using the evaporation system with the help of a circular mask with equal thicknesses of Au, Ag and Al. From the result of the I-V characterization, the ideality factor (η), barrier height (Φ_{b0}) and series resistance (R_s) values, which are the main electrical parameters, were calculated. It was seen that the electrical parameters of the device with Au contact were more compatible with the literature than Ag and Al contacts.

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Keywords: ZnSe, thin films, metal contacts, I-V characteristic,

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Effect of Nickel Addition on Characteristic Properties of ZnO Thin Films

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Abstract: Among metal oxides, ZnO and NiO thin films are of particular interest. ZnO is widely studied for applications such as solar cells, chemical sensors, and photodetectors [1-3]. NiO and ZnO are intrinsically p- and n-type semiconductors, respectively, and their band alignments make them promising candidates for heterojunction thin film devices for optoelectronic applications such as LEDs and photodetectors (PDs) [4,5].In this study, different volumes of Nickel (Ni) doped Zinc oxide (ZnO) thin films were deposited on FTO by hydrothermal method. The films were characterized by SEM, EDS, UV-Vis Spectroscopy and X-ray diffraction. When SEM images are examined, it was shown that the nanoparticle sizes formed with the increasing volume of nickel decreased even more and the film surface had a homogeneous distribution. EDS spectra showed the increase in Ni by volume and its presence in the film composition. The results of UV-Vis Spectroscopy showed that the transmittance and band gap values can be changed by Ni doping, and thus the ZnO band gap can be adjusted by Ni doping. X-ray diffraction patterns revealed that in the crystal structure of ZnO and that no secondary phase was formed.

Keywords: Thin films, Hereronanostructures, Band gap

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Effect of Passivation on AlGaN/GaN HEMT for 5G Applications

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Abstract: AlGaN/GaN high electron mobility transistors (HEMTs) have demonstrated excellent device characteristics, making them excellent candidates for high power, high frequency, and low noise applications. However, the full potential of GaN HEMTs in large-signal operation at high frequency is limited by trapping effects and leakage currents at the interface between the epi-structure and passivation layer. A SiN_x passivation layer has commonly been used to mitigate electron trapping at the surface by providing extra positive charges to neutralize trapped negative electrons on the surface. In this paper, we present the results of the comparative study of two different passivation methods of AlGaN/GaN HEMTs. We studied the same epitaxial structure and fabrication steps but we only chance the first dielectric deposition methods. Sample 1 deposited 75 nm SiN_x with ICPCVD, Sample 2 deposited 75 nm SiN_x with PECVD.

Recipe	RF Power (W)	ICP Power (W)	Temperature (^oC)	Pressure (Pa)	SiH_4 (sccm)	NH_3 (sccm)	N_2 (sccm)	Ar (sccm)
ICPCVD	-	200	130	10	400	8.8	-	140
PECVD	30	-	275	75	140	6	500	-

Table 1: SiN CVD parameters

DC characterization of HEMTs shows that SiN_x by ICPCVD provides lower gate and drain leakage currents compared with SiN_x by PECVD. Prominent differences between the methods are temperature and pressure. In this study, results show that low temperature and low-pressure methods are more convenient for HEMT fabrication and ensure the deposition of good quality SiN_x films with low surface damage [1].

Sample ID	**Id, leak (uA/mm)**	**Ig, leak (uA/mm)**
Sample 1 (ICPCVD)	224	210.43
Sample 2 (PECVD)	602	736.98

Table 2: I-V results after gate bake

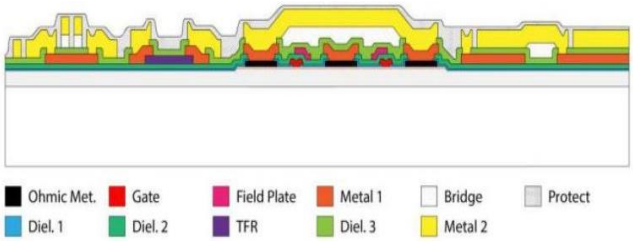

Figure 1: HEMTs layers cross-section [2]

Keywords: HEMT, GaN, SiN, Passivation

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Effect of Temperature on The Stress Softening and Damping Behavior of Phenyl-Vinyl-Methyl-Polysiloxane (PVMQ) Elastomers

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Abstract: The aim of this study was to identify the effect of temperature and co-agent type, stress softening, energy dissipation and damping properties of phenyl-methyl-polysiloxane(PVMQ) cured with peroxide curing system. To begin with, silicone blends were prepared by by using a Torque Mixer with banbury type rollers then the curing behavior was investigated by using Moving Die Rheometer and optimum cure conditions were determined. After that, the test specimens were molded in a hot press at 200bar. Prepared samples were conditioned for 30 minutes before testing at the same temperatures which the tests would be performed. The effect of these variables on the energy damping capacities of silicone elastomers was illuminated using hysteresis curves obtained by applying a 50% compression 10-repeat cyclic compression test using a universal test machine.We concluded that temperature and type of the co-agent are two important parameter controlling damping properties of polymers. Degrease of temperature slightly decrease of damping of silicone elastomer. Variation of co-agent type change the cross-link density of elastomer and in the presence of TAIC high crosslink densities was observed. Increase of crosslink density of elastomers also reduced the damping capacity of silicone elastomers.

Keywords: Phenyl-Vinyl-Methyl-Polysiloxane (PVMQ), Elastomers, The Stress Softening, Damping Behavior

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Effect of Type I and Type II Co-Agents on the Cure Kinetics of Silicone Elastomers

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Abstract: In this study, the effect of Type I co-Agents ZDA and ZDMA and Type II co-agents TAC and TAIC on the curing kinetics of VMQ and PVMQ elastomers was investigated. 2,5-Dimethyl-2,5-di(tertiary-butylperoxy)hexane(DBPH) was used as crosslinker. The rheological analyzes were performed with a Moving Die Rheometer(MDR) at four different temperatures. Cure curves were evaluated according to 1th and nth curing kinetics and curing rate constant (k), reaction degree (n) and activation energy(Ea) values were calculated. When the results were evaluated, it was seen that the k rate constant increased with the addition of TAC, TAIC and ZDA in the compounds, whereas the k rate constant value decreased with the use of ZDMA. It is thought that the reason for this is that ZDMA forms a more stable 3° radical due to the methyl group in its structure. ZDA was found to be the accelerator that increased the cure rate of PVMQ and VMQ. When the activation energies obtained were examined, it was seen that the activation energies for PVMQ were higher than energies obtained for VMQ. The reason for this was attributed stabilization of free radicals by the phenyl group in the structure of the PVMQ.

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Effect of Using Graphene Nanotube on Electrical Properties on Photo-initiators Containing Polymer Matrix Nanocomposites

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Abstract: It is becoming common to use environmentally friendly photo-initiators, to initiate and accelerate polymerization in polymer composite production, and the use of nanomaterials that improve materials' mechanical, physical, and electrical properties is becoming widespread recently. Therefore, in this study, a polyester resin containing photo-initiator at a rate of one in a thousand (0.1%) was evaluated in the production of polymer nanocomposites. In order to improve the electrical characteristics of polyester resins, Graphene Nanotubes (GNTs) containing 98% pure carbon were added to the resin (0%, 0.001%, 0.003%, 0.005%, 0.01%, and 0.015%) and blended with a high-speed mixer. Then, nanocomposites were placed into glass molds and cured under LED/UV light. Dielectric properties of the nanocomposites were analyzed by using impedance spectroscopy method including the capacitance-frequency (C-f) and conductance-frequency (G/ω-f) measurements. As a result, both the C and G/ω values increase with the increasing doping ratio. An increase in C with the addition of GNT is due to the filling of the charge traps in the composite with the GNT reinforcement and the charge deposition from the electrodes with AC frequency. Consequently, the dielectric properties have been increased by passivating the active charge traps with GNT doping and so the electrical properties of photo-initiated polyester nanocomposites have been improved.

Keywords: Photo-initiated polyester nanocomposites; Graphene nanotubes; Electrical characteristics; Frequency-dependent dielectric properties

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Effects of Protons on Photovoltaic Power Systems

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Abstract: Photovoltaic power systems are known an important power source that generates electricity by solar effect. It is important to examine the parameters that affect the performance of photovoltaic devices under different conditions, depending on the area of use. Especially the performance of solar cells plays an important role in space applications such as satellites. Solar cells as a long-term power source and optoelectronic components of satellites are exposed to irradiation by charged particles (protons, electrons, etc.) in the Earth's radiation belts. Due to the displacement damage caused by these particles, defective areas are formed. They cause some changes in the performance of the devices. In this study, it is aimed to examine the electrical parameters of the photovoltaic cells exposed to the proton beam. The characteristics of the performance parameters of the silicon photovoltaic device have analyzed before and after proton irradiation. The maximum power, short-circuit current, open-circuit voltage and power conversion efficiency have calculated from the current-voltage (I-V) and power-voltage (P-V) properties before and after proton radiation. The SRIM/TRIM simulation program has used to analyze the effects of radiation-induced displacement damage on the cell performance. Information about the performance of solar cells is given by examining the effects on the electrical properties of silicon cells irradiated with protons.

Keywords: Power systems, proton beam, photovoltaic.

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Effects of Substrate Temperature on The Structural and Optical Properties of RF Magnetron Sputtered NiO_x Thin Films

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Abstract: Nickel oxide (NiO) is a versatile wide band gap semiconductor material. It is a translucent p-type semiconductor material with an energy band of about 3.2-4.0 eV. Owing to its unique hole transport characteristics and good optoelectronic properties, it has great potential for application in perovskite solar cells, electrochromic devices, ultraviolet photodetectors, supercapacitors and gas sensors. NiO films can be deposited using many different chemical and physical methods such as magnetron sputtering, evaporation, sol–gel. Although some experimental studies at room and/or high temperatures of NiO film deposition have been published in recent years, the effect of growth temperature on the semiconductor properties of NiO film has not been strongly evaluated so far. In this study, NiO_x thin films were deposited on the glass substrate using a 99.999% purity and 0.250 inches thick NiO target by RF magnetron sputtering method varying substrate temperatures between room temperature and 300 °C. The structural analysis using X-ray diffraction data revealed that all films were exhibited a face-centered cubic (fcc) structure with a space group of $fm\bar{3}m$. The calculated band gap values of the film were found to be 3.72 eV. As a result, it has been observed that changing the substrate temperature of the films affects the optical and structural properties of the films.

Keywords: NiO_x, substrate temperature, magnetron sputtering, structural properties, optical properties

Acknowledge: This research was supported by Scientific Research Project Fund of Sivas Cumhuriyet University under the project number F-2021-640.

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Electrical and Ultraviolet Photo-Responsivity Properties of Au/Polyvinyl Alcohol Benzimidazole Copper Complex/n-Si Photodiode

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Abstract: The Abstract text cannot exceed the limits of one page. Au/PVA + benzimidazole Cu complex/n-Si metal/polymer/semiconductor (MPS) diode were fabricated and its main electrical properties compared with Au/n-Si metal/semiconductor (MS) diode. MPS diode's electrical and photo-responsivity (PR) properties were investigated by current-voltage (I–V) measurements under various ultraviolet (UV) (365 nm wavelength) illumination intensities at room temperature. The ratio between the dark and high UV illumination I(V) plots of the MPS diode was found above 105 times. Due to this higher response to UV illumination has caused the reverse bias current of the diode exceeds the forward bias current since the first UV illumination level. This ensures both the MPS diode has a very high PR value and allows that the diode working direction can be adjusted with UV exposure. The remarkably high PR values were obtained for P = 100 mW/cm2 as 11.01 A/W at −4.84 V, and 2.14 mA/W at 0 V. Also, main electrical parameters such as I_0, n, Φ_{B0}, Φ_B, R_s and N_{ss} of the MPS diode were obtained.

Keywords: Photodiode, benzimidazole Cu complex, photo-responsivity.

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Electrode Thickness and Wetting Optimization for $LiFePO_4$/Graphite Full Cells

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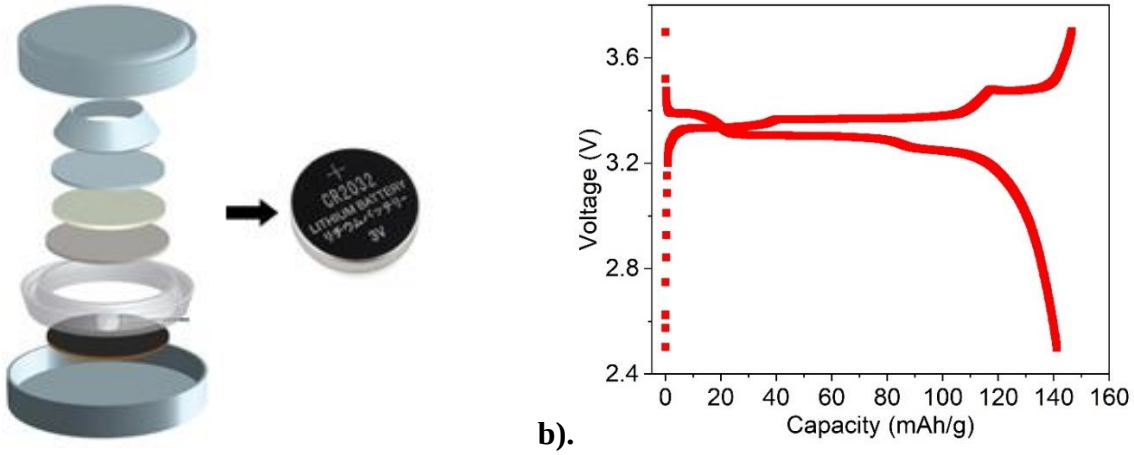
Abstract: In commercial batteries, the most time and cost is spent on the battery formation process. Efforts are still being made to reduce cost and time loss. In this study, electrode thickness and wetting process were studied to accelerate the battery formation stage in full-cell production. In this study, $LiFePO_4$ and graphite were used as the cathode and the anode, respectively. The cell design was presented in Figure 1.a One of the most important factors affecting the operating performance and life of the battery during the battery formation phase is the good wetting of the anode, cathode, and separator. To solve this problem, electrodes of different thicknesses were first studied and then different electrode wetting methods were used. EIS and cycle analyzes were performed to analyze the electrochemical performances of the produced batteries as seen in Figure 1b.



a). **b).**

Figure 1: a) CR2032 battery components and order, **b)** Capacity-Volt graph.

Keywords: Energy storage, Li-ion batteries, Full cell

Acknowledge: Authors would like to thank INONU University contract number of FBG-2020-2171 for their financial support.

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Electromagnetic Curves Related to Null Cone Fronts

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Abstract: When a charged particle enters a magnetic field, the velocity vector of the particle is affected by the magnetic field and a force called the Lorentz force is released. Under the influence of this force, the particle follows a new trajectory in the magnetic field. This trajectory is called the magnetic curve. When examining the geometric evolution of a linearly polarized light wave along an optical fiber, it can be assumed that the optical fiber is a one-dimensional object, that is, a curve embedded in a 3-dimensional space. Thus, in 3-dimensional space, a linearly polarized light wave curves the geometric phase equations and these curves can be studied with the help of Frenet apparatus. In this study, we consider space-like framed curves on a null cone. Next, we investigate a special kind of magnetic curve, called electromagnetic curves, which are produced by the electric field along the linearly polarized monochromatic light wave propagating in the optical fiber using the corresponding geometric phase equations. Then, we obtain the Lorentz force equations and magnetic field equations related to the obtained electromagnetic curves. Moreover, we give some motivated examples and visualize these curves with the help of mathematical programs.

Keywords: null cone, electric field, special curves, Minkowski 3-space, singularities.

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Electromagnetic Curves via Darboux Frame in Minkowski 3-Space

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Abstract: The force acting on the charged particle under the influence of the magnetic field is called the Lorentz force. With the effect of this force, the charged particle moves by following a trajectory. This trajectory is also called the magnetic trajectory or magnetic curve. In this study, we examine electromagnetic curves with respect to Lorentz force. Then we calculate electromagnetic equations and in this way we study this trajectory's geometric phase with Darboux frame field in Minkowski space. Furthermore, we investigate the electromagnetic curves three subsection for the three different cases of the polarization vector respect to Darboux frame's fields. Thus, we present the (EM-trajectories) related to the Berry phase model (geometric phase) obtained from the polarization plane of a light wave moving in an optical fiber. Then we research Killing magnetic fields for these three cases. Lastly, we show that some examples to assist the theoretical background via mathematical programs.

Keywords: Darboux frame fields, Vector fields, Electromagnetic theory, Magnetic field

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Electronic Transport Properties of WS_2 With Ensemble Monte Carlo Method

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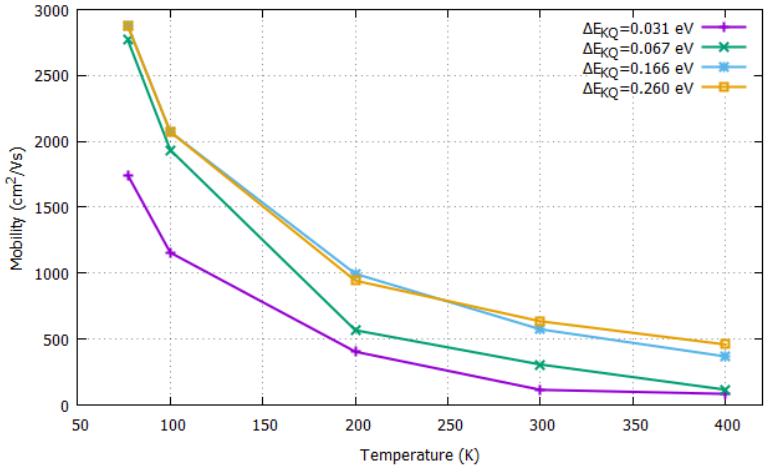
Abstract: The electronic transport characteristics of Tungsten disulfide (WS_2) sheets are studied by an Ensemble Monte Carlo (EMC) technique in the presence of phonon (acoustic, optic) scattering mechanisms where intra and intervalley scatterings are considered in a two valley model. Only intrinsic (WS_2) case is considered. The drift velocity of carriers is calculated as a function of time at a given value of applied field and from these, the steady state drift velocity-applied electric field curves are obtained for different temperatures in the presence of all scattering mechanisms just mentioned. It is found that the mobility of carriers sensitively depends on the energy difference ΔE_{KQ} between the minimums of the two valleys. The mobility of carriers is calculated as a function of temperature and the results are compatible with existing theoretical predictions.



Keywords: WS_2, Ensemble Monte Carlo, Scattering, Transport, Drift velocity, Mobility

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Environmental Effects on the Photovoltaic Properties of Silicon Solar Cells

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Abstract: Due to the increase in energy needs in our daily lives, current energy resources are being depleted rapidly. The use of alternative energy sources such as wind, solar, wave, geothermal, biomass, hydraulics and hydrogen has gained great importance in the near future due to the rapid depletion of fossil fuel sources and environmental pollution caused by fossil fuels. Solar energy generation is the most preferred alternative energy source applications. In this study, the emphasis is on the alternative energy sources used in the world and also solar energy 's current status,in developed countries and Turkey , types and working principles of solar power plants are evaluated. As it is known, solar energy systems have not reached the desired level in Turkey, it is known that the application areas are mainly solar energy systems applied to lands and roofs. These systems can convert solar energy into electricity by photovoltaic method.

In this study, the most preferred silicon solar cells among the types of photovoltaic solar cells are mentioned and ıt is focused on the environmental factors such as temperature, humidity, dust, and pollution which affect the silicon solar cells during the energy production stages. It has been focused on how to reduce the energy losses of the systems that generate electricity by using photovoltaic solar cells which its usage area is increasing day by day, how to increase the energy efficiency (Fig. 1) and how to minimize the environmental factors that affect the energy production stages.

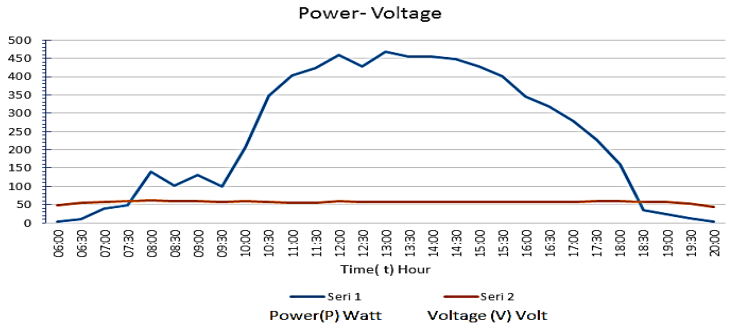

Fig 1.: The variation of Power and Voltage versus time

Keywords: Photovoltaic Systems, Environmental factors, Solar energy, Silicon solar cells

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Excellent Electromagnetic Wave Absorption Performance of PANI-coated YIG/CFO Hybrid Composites

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Abstract: Nowadays, escalating military requirements of developed countries and increasing electromagnetic pollution due to the abrupt improvement of technology draw the researcher's attention to develop broadband, lightweight and low-cost electromagnetic wave (EMW) absorbers. Magnetic and dielectric materials, together with their combinations, have been intensely investigated to meet these requirements and contribute to the absorption with intrinsic loss mechanisms. Ferrites have been extensively used due to their advantageous magnetic losses and cost-efficient manufacturing. Polyaniline (PANI) is combined with the ferrites to suppress its disadvantages, such as high density and low permittivity and actuate the dielectric loss mechanism in the absorber. In this study, PANI/[YIG_x/CFO_{1-x}] (YIG:$Y_3Fe_5O_{12}$, CFO: $CoFe_2O_4$) hybrid composite structures ($0.0 \leq x \leq 1.0$ with 0.2 steps) were synthesized by in-situ polymerization of aniline followed by the sol-gel route of magnetic particles. The magnetic particle and PANI weight ratio in the composites was adjusted to be 0.5:0.5. CFO and YIG crystal structures are determined as cubic symmetry with *Fd3m* and *Ia-3d* space group, and their average crystallite sizes were found as 35.3 nm and 42.9 nm, respectively. The results revealed that PANI/[$YIG_{0.2}$/$CFO_{0.8}$] hybrid composite could absorb the 99.99% of EMWs through X-band (8-12 GHz) frequency with a minimum reflection loss (RL) value of -47.34 dB at 8.14 GHz.

Keywords: Electromagnetic wave, Composite, Absorber, PANI

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Fabrication of Fe-Based Square Core Racetract Coil Prototype and Its Characterization

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Abstract: This study consists of three main steps. The first step is the production of Fe-Chalcogenide (Fe-Ch) core material by self-flux method by adding 3% Multi-Wall Carbon Nanotube (MWCNT). The second step is to produce wire with 1x1 mm square core with the Powder In Tube (PIT) method by filling the obtained core material in Fe and Ag tubes and convert it to the thin strip form. The last step is to produce the "racetract" coil prototype using the obtained strip. The structural and microstructural properties of the produced square core wire and strip were investigated. In addition, ~1153 A/cm^2 transport current value was obtained for the ~1x1 mm square core superconducting wire which is reasonably good for technological applications. Finally, 40 acres (winding) of Fe-Ch superconducting strip on the prepared Teflon mold was made into "racetract" coil form and electrical performance tests were carried out. It has been determined that for 40 windings, it can carry a current of 91.5A according to the criterion of 1 μV. The results obtained are extremely promising and reveal that the wire/strip form of Fe-based superconductors has technological application potential.

Keywords: Superconductivity, Fe-chalcogenide superconductos, square core wire, racetract coil.

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Features of Electrical Conductivity of Zeolite with A High Content of Silver Ions

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Abstract: Three features of electrical conductivity were experimentally observed:

1. The electrical conductivity has changed slightly, despite the high concentration of silver ions, embedded in the pores of zeolite as a result of the ion exchange process.
2. current stabilization was observed i.e. the current didn't decrease with time, which is typical for a zeolite with a low content of silver ions.
3. at normal (small) concentration of silver in zeolite, the electrical conductivity decreases to zero as air in pumped from atmospheric pressure to 10^{-2} Torr. At high concentration of neutralized silver in the pores of zeolite, the current does not depend on pressure

All three features are explained by the fact that due to the electroneutrality of the sample, the concentration of silver ions in the sample volume does not increase, but increases at the ends of the sample.

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First-Principles Study on Optoelectronic Properties of PtTiSn Under Pressure

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Abstract: One of the main challenges in materials science is the design of multifunctional materials where large responses are produced by applied fields and stresses. First-principle calculations of structures and properties are used to investigate the microscopic origins of functional properties of interest, and this knowledge is used to guide computational screening of many compounds in both equilibrium and metastable structures to identify promising candidate systems. Half-Heusler alloys have gained various practical applications in spintronic, superconductors, optoelectronic and thermoelectric devices. The study of new semiconducting materials with enhanced structural, electronic, mechanical and optical properties for the advancement of optoelectronic applications has high merits in material science. Some Half-Heusler ternary compounds offer several desirable semiconducting properties over the elementary and binary semiconductors. One important class of these ternary materials is the transition metal alloys (TMA), which are well-known to be stable and perfectly ordered. These TMA are crystalline in cubic MgAgAs-type structure with space group number 216 *F*43m. In particular, PtTiSn alloy fall within the class of TMA. This material has been subjected to both experimental and theoretical investigations. In order to describe the response of PtTiSn to electromagnetic radiation, we have calculated several optical parameters. Due to the technological importance of PtTiSn , we have investigated behavior of their structural, electronic, elastic and optical properties at both normal and high pressures. The response to the IR, visible and UV spectra is important from the view point of optoelectronic applications. The high absorption coefficient and low reflectivity in the visible to ultraviolet region make this compound a possible candidate for solar cell and optoelectronic device applications.

Keywords: DFT, Half-Heusler, optical properties, PtTiSn, electronic properties, mechanic properties

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FTO/CdS/CdSe Heterojunctions Synthesis and Investigation of Thicknesses Effect

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Abstract: The CdS/CdSe heterojunctions were produced at different thicknesses on FTO doped glass substrate by chemical bath deposition. The CdS/CdSe films were deposited on FTO for 4h, 6h, and 10h. The effect of thicknesses on the optical, structural, and electrical properties of the films was investigated by UV-visible spectrophotometer, Photoluminescence (PL), X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), and Hall-effect measurement. The electrochemical investigation of the CdS/CdSe heterojunctions was carried out by Mott-Schottky analysis and photoelectrochemical measurements. The band gap of the 4h, 6h, and 10h deposited CdS/CdSe films was determined. The electrical properties were determined with Hall-effect measurement, and it was compared with Mott-Schottky analysis. All films have polycrystalline structures mixed of hexagonal and cubic. It was seen from the morphological analysis that the nanowires started to form in small amounts at 4h deposition and were clearly formed in the 6-hour deposition. Then the surface was completely covered with CdSe nanowires in the 10-hour deposition. Photoelectrochemical measurements were performed using linear sweep voltammetry (LSV) in the range of -0.3V and 0.6V in dark and under light illumination. The photocurrent response of the films increased significantly as the deposition time increased.

Keywords: FTO/CdS/CdSe heterojunctions; Nanowire; SEM; Optical properties; Hall Effect, Photoelectrochemical measurements.

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Green Synthesis of Long-Term Stable Silver Nanoparticles via Artemisia Absinthium "Hairy" Roots Extract

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Abstract: Green synthesis of silver nanoparticles (AgNPs) attracts a lot of attention due to its effectiveness and environmental friendliness. This is due to the studied possibility of plant extracts exhibiting both reducing and stabilizing properties. This study used *Artemisia absinthium* L. "hairy" roots culture as a source of bioactive compounds with reducing activity, especially flavonoids. "Hairy" roots dry ethanolic (70%) extract was characterized by total flavonoid content (TFC) and reducing power. TFC was determined by the $AlCl_3$ method. The reducing power of the extract was measured by its ability to reduce Fe^{3+} to Fe^{2+}. AgNPs were obtained by adding 200 mL of 10 mg DW/mL plant ethanolic extract to 10 mL of 1mM $AgNO_3$ with subsequent incubating at 85ºC for 1h. AgNPs were characterized by UV-visible spectroscopy and transmission electron microscopy (TEM). The assay results indicated that the extract contained 134±8.4 mg/g flavonoids and has high reducing activity ($EC_{0.5}$=0.089 mg). According to the absorption results (fig.1), obtained AgNPs exhibited a strong, broad peak at 420 nm, which proves their silver origin. These AgNPs were round and oval-shaped (fig.2). Their size ranged from 20 to 60 nm. Moreover, they were stable for more than 9 months without a decrease in quantity.

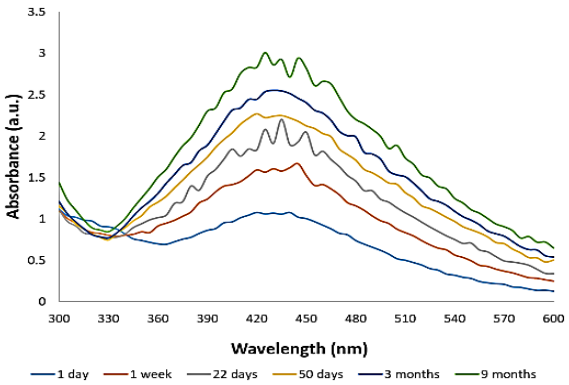

Fig.1 The absorption spectrum of AgNPs.

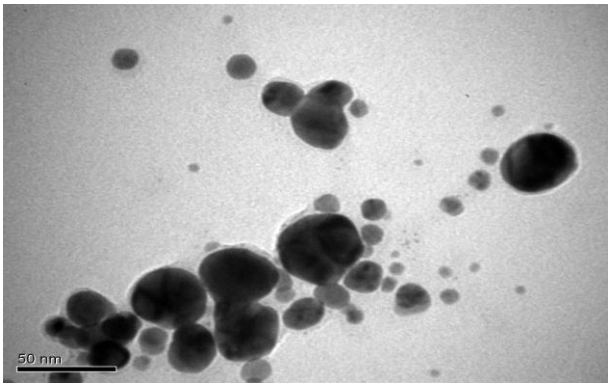

Fig.2. TEM of AgNPs

Keywords: Silver nanoparticles, "green" synthesis, *Artemisia absinthium* L., "hairy" roots.

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Growth and Characterization of CdS Nanoflowers by Chemical Bath Deposition and Effect of Annealing

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Abstract: In this work, we studied on the structural, morphology and optical of chemical bath deposited CdS thin films. The CdS thin films were coated on glass substrates by chemical bath deposition technique. According to the XRD results, the partical size of the as-deposited CdS film was obtained between 8,60 and 17,40 nm. It was observed from the SEM images of the deposited and annealed CdS films that nanoflowers were formed on the film. The UV measurements showed that the optical band gap energies of the annealed CdS nanoflowers decreased from 2.31 to 2.19 eV. Also the conductivity measurements as resistivity and conductivity made by Hall Effect methods for as-deposited and annealed films. Raman spectroscopy was conducted at 785 nm wavelength.

Acknowledge: This study was supported by the Research Fund of Mersin University in Turkey with Project Number: BAP 2020-1-TP3-4032

Keywords: CdS, Nanoflower, Thin Film, Chemical Bath Deposition.

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Growth and Structural Properties of ZnO Materials by Mist CVD Enhanced by Corona Discharge Plasma

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Abstract: Mist-CVD method has been attracted over the last decade. Many oxide-based materials can be grown as transparent oxide materials (TCO) for wide range of optoelectronic applications. In this study, ZnO material which is one of the TCO is grown on different substrates at low growth temperature. The growths are carried out mist CVD method with corona discharge plasma. The carrier gas was turned into O_3 from O_2 using corona discharge plasma generator. The grown ZnO thin films exhibit the polycrystalline wurtzite hexagonal structures. The dominant diffraction peak of ZnO films are found to be (0002). Grown ZnO thin films are shown the hexagonal and triangular shape crystals by atomic force microcopy (AFM) and scanning electron microscopy measurements (SEM). The vibration properties of ZnO thin films are investigated by confocal Raman spectroscopy. The peaks related to wurtzite ZnO cyrstals are shown 437 cm^{-1} and 99 cm^{-1} for $E_2^{(H)}$ and $E_2^{(L)}$, respectively.

Keywords: ZnO, mist-CVD, corona discharge, plasma, hexagonal wurtzite

Acknowledge: This work was supported by TUBITAK under Project No. 116F197. S. B. L was supported in part by the Distinguished Young Scientist Award of Turkish Academy of Sciences (TUBA-GEBIP 2016).

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Illumination-Dependent Electrical Characteristics of Au/(GO:P_3C_4MT)/SiO_2/n-Type Si Structures

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Abstract: Our aim in this study is to investigate electrical characteristics of the Au/SiO_2/n-Si structures with graphene oxide (GO) and poly(3-cyclohexyl-4-methyl-2,5-thiophene) (P_3C_4MT) interface layer under different light intensities. The main electrical parameters such as ideality factors (n), barrier heights (Φ_{bo}), and series resistance (R_S) of the Au/(GO:P_3C_4MT)/SiO_2/n-Si structures were calculated and compared by thermionic emission theory, Cheung and Norde's method in the dark and depending on the light intensity at room temperature. The results obtained from the calculation methods showed that the differences in basic electrical parameters can be due to electron-hole formation of the Au/SiO_2/n-type Si structure with the GO:P_3C_4MT interface layer. Thus, the experimental results shows that Au/(GO:P_3C_4MT)/SiO_2/n-Si structure can be used in optoelectronic applications.

Keywords: Ideality factor, Barrier height, Series resistance, Rectifier ratio, GO:P_3C_4MT, SiO_2

Acknowledge: This work was supported by Kahramanmaras Sütçü Imam University Scientific Research Project Unit (**Project numbers: 2020/9-30 D**). We would like to thank Kahramanmaraş Sütçü İmam University for financial support of the research program

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Illumination-Dependent Photovoltaic Properties of the Al/(GO:PTCDA)/p-Si Structures

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Abstract: The aim of this our study is to produce an Al/*p*-type Si MS structure photodiode based on graphene oxide (GO) and perylenetetracarboxylic dianhydride (PTCDA) interfacial layer for photovoltaic devices, and to determined its basic photovoltaic and electronic properties. The main values such as ideality factors (*n*), rectification ratios (RR), saturation currents (I_0) and barrier heights (Φ_{bo}) were extracted from *I-V* characteristics and discussed in details by thermionic emission (TE) theory in the various illumination conditions. The illumination dependent electrical and photovoltaic properties of Al/(GO:PTCDA)/*p*-type Si structures were investigated using current–voltage (*I–V*) characteristics under dark and in the illumination range of 20–100mW cm^{-2} by increments of 20 mW cm^{-2}at room temperature. Experimental studies shown that GO and PTCDA molecular organic semiconductors can be used as the preferred interfacial layer material in the development of photodiode devices because they are light sensitive materials.

Keywords: Ideality factor, Barrier height, Electrical and photovoltaic properties, GO:PTCDA interface

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Improving the Negative Refractive Index Metamaterials Research via Optical Coherence Theory

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Abstract: Our aim is to introduce the partial coherence theory in metamaterials research. We will be dealing with the partially coherent light beam interaction with negative refractive index materials. As is well known negative index metamaterials is a relatively new topic. And interaction of metamaterials is limited to Gaussian light beams. Therefore, it is necessary to consider all type light beams having different coherence values. We will here show the statistical results of Gaussian Schell-model light beam passing through negative refractive index and positive refractive index material layer. And we will discuss possible further improvements via different types of random light beams. The metamaterial layer we use is also known as perfect lens. It consists of a negative refractive index material stacked into two positive refractive index materials. Our formulation is based on the ABCD-matrix approach and generalized Huygens-Fresnel principle. Therefore, numerical calculations can be shrinked into Gaussian beams. In the analysis, we've found that perfect lens like configuration causes blue/red shifts in the spectrum which is because of the boundary between layers. In conclusion, these types of research are extremely important because these devices are used to manipulate electromagnetic radiation.

Keywords: Optical coherence, negative refractive index, light-material interaction, metamaterials

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Improving the Performance of the Triboelectric Nanogenerator Using Titanium Oxide / Nylon Nanocomposite Materials

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Abstract: A triboelectric nanogenerator (TENG) has been extensively studied as a novel energy harvesting technology since it was introduced by Z. L. Wang. The TENG is based on two physical processes such as contact electrification and electrostatic induction which are caused by reciprocating contact and separation of two films. Electrostatic induction can be enhanced when materials with high dielectric constant are introduced. In this study, the TENG was created by using a nylon-TiO_2 nanocomposite film and a polysiloxane film. The nylon-TiO_2 nanocomposite film was prepared to enhance dielectric property of the nylon film by adding TiO_2 nanoparticles with a large dielectric constant and so electrostatic induction in the TENG. Nylon-TiO_2 nanocomposite films have been obtained by using hot pressing and spray coating methods. As expected, TENGs with nylon-TiO_2 nanocomposite films have shown better dielectric properties than the ordinary nylon film. And enhancement in dielectric properties has lead to an increase in the number of charge carriers on the surface of the film during contact and in the capacitance of the system and in turn, an increase in the electrostatic induction. As a result, TENGs which have been made of nylon-TiO_2 nanocomposite films have demonstrated enhancement in the electric generation.

Keywords: triboelectric nanogenerator, polysiloxane, nylon, dielectric material

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Incorporation of K and Cs into CdS Thin Films during Chemical Bath Deposition as an Alternative Strategy to Post Deposition Treatment of Absorbers

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Abstract: In this study, CdS thin films were coated on FTO substrates by chemical bath deposition method. Alkali metal doped CdS thin films were produced by adding KCl and CsCl salts into the chemical bath solution. Structural, optical and electrical properties of the alkali metal doped CdS thin films were investigated by using FE-SEM, GI-XRD, UV-Vis and HEMS measurements with respect to the type and amount of doped alkali metal. Alkali metal doping into the CdS thin film improved the structural, morphological and optical properties of this film as a first function at certain doping levels. When these thin films with improved properties are used as a buffer layer, they have the potential to increase efficiency by preventing current leakage across the p-n heterojunction and establishing proper electronic band alignment. In addition, if there is alkali metal diffusion from the CdS buffer layer to the absorber, the absorber will be indirectly doped. This new doping strategy, on the other hand, is promising method to increase solar cell efficiencies, as has often been shown in the literature for different alkali treatment methods.

Keywords: Thin film solar cells, CdS buffer, alkali treatment.

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Influence of PEG and PVA Polymers on the Morphological and Photovoltaic Performance of ZnO Photoanodes

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Abstract: In the presence of NH_3, NH_3-PEG and NH_3-PVA, nanostructured ZnO flowers were obtained by hydrothermal method to control the morphological and photovoltaic properties of ZnO photoanodes. The morphological, structural and optical properties of the produced photoanodes were investigated by SEM, EDS, XRD, and UV-Vis. Using these photoanodes of dye sensitized solar cell (DSSC) were obtained with Ruthenium Dye (Z907) dye with two different electrolytes. Photovoltaic (PV) and electrochemical impedance spectroscopy (EIS) characterization of DSSCs were performed. Examining SEM images, different ZnO nanoflowers were obtained. It was observed that the morphological structure changed with the effect of PEG and PVA. ZnO formation and its wurtzite structure also confirmed by the XRD results. Two different electrolytes (AN50 and HI30) were used in DSSCs created by sensitizing these photoanodes with Z907 dye. Here, the photoanode with NH_3-PVA is the lowest series resistance (Rs) and charge transfer resistance (Rct) were obtained for the cell with AN50 electrolyte from the EIS measurements. For this reason, high photovoltaic efficiency was achieved in the NH_3-PVA cell compared to the others.

Keywords: PEG, PVA, ZnO flowers, hydrothermal method

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Investigation and Application of Dislocation and Twist Angel Properties in a GaN/AlN/AlGaN High Electron Mobility Transistor

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Abstract: Gallium nitride has a set of properties that make it possible to develop devices with superior parameters compared to devices based on conventional semiconductors. GaN, as a material for high-temperature, high-voltage, and high-current applications, can significantly expand the operational capabilities of semiconductor technology. The unique combination of physical properties in GaN means that nitride semiconductors may be the most promising materi approaches involve the presence and effective use of an appropriate diagnostic base for high-quality and reliable verification of the resulting structures also for designing new generation devices. The heterostructures of GaN-based high electron mobility transistors (HEMT) occupy leading positions in high-power microwave devices, but the initial presence of a sufficiently large number of various GaN defects leads to the appearance of traps and the so-called effect of current collapse, decreasing frequency and power performance. For this reason, it is especially important to investigate and control both active and buffer layers. When developing solutions to eliminate these negative phenomena and optimize the parameters of heterostructures to increase the subthreshold slope characteristic, operating frequencies, and device power, the most productive.

Keywords: HEMT, GaN, Nitride

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Investigation of Polyvinyl Alcohol (PVA)-Sakacin P Interaction by Molecular Docking

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Abstract: Group IIA bacteriocins, which contain unmodified amino acids and have antimicrobial activity, are a very broad group. Sakacins in this group are bacteriocins produced by Lactobacillus sakei. The most well-known sakacins are sakacin A, G, K, P, and Q. In particular, sakacin A and P are well characterized. In this study, the interaction of a single monomer of PVA polymer, which is among the water-soluble, biocompatible synthetic polymers, and sakacin P bacteriocin, which has a protein structure, was investigated by molecular docking method.

Keywords: Sakacin P, Molecular docking, Polyvinyl alcohol

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Investigation of Structural, Electronic, Optical and Mechanical Properties of $Al_{1-x-y}In_xGa_yN$ Alloys at Constant Temperature and Different Pressure Values by Ab-Initio Method

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Abstract: In this study, III. $Al_{1-x-y}In_xGa_yN$ alloy was obtained by using compounds (AlN, GaN, InN, TiN) made with nitride of elements such as Aluminum (Al), Gallium (Ga), Indium (In) and Titanium (Ti), which are group elements. The amounts of x=In and y=Ga in the $Al_{1-x-y}In_xGa_yN$ alloy at a constant temperature (273 K), depending on different pressure values (0 Pa, 50GPa, 100 GPa, 150 GPa), Structural properties of the alloys, Electronic properties (Band structure, State density curves (DOS)), Optical properties (Dielectric constants, Refraction constant, Damping constant, Absorption coefficient, Loss function, Reflection coefficient), Elastic properties (Bulk modulus (B), Shear modulus (G), Poisson ratio (v) , Compressibility and B/G ratio were calculated by Ab Initio method using CASTEP (Cambridge Sequential Total Energy Package) program. Graphs related to the calculated values were drawn and the properties of the alloy were interpreted.

Keywords: $Al_{1-x-y}In_xGa_yN$ alloy, CASTEP program, Ab Initio method, Structural properties, Electronic properties, Optical properties, Mechanical properties, Band structure, State density curves, Elastic properties

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Investigation of the Efficiencies of the Bi_2O_3-CuO-PVP Interlayer in Au/n-Si (MS) SDs on Electrical Characteristics at Room Temperature by Comparison

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Abstract: Au/n-Si (MS) and Au/Bi_2O_3-CuO-PVP/n-Si (MPS) type SDs were manufactured at identical conditions for investigation of the Bi_2O_3-CuO-PVP organic/polymer interlayer effects on the electrical characteristics using voltage dependent current (I) data and they were compared with each other. The main electrical parameters such as rectifying ratio (RR), ideality factor (n), reverse saturation current (I_o), zero-bias barrier height (Φ_{Bo}) were determined from ln (I)-V plots. Series (R_s) and shunt (R_{sh}) resistances were calculated from the I-V data by using Ohm's law. In addition, the energy and voltage dependent profiles of surface states (N_{ss}) were obtained using the forward bias I-V data by taking into account voltage dependent effective barrier height (Φ_e) and n. While the calculated values of surface states and saturation current for the MPS is lower than Au/n-Si SDs, RR is higher. Obtained results prove the use of a Bi_2O_3-CuO-PVP organic interlayer improved the performance of the Au/n-Si diodes.

Keywords: Current-voltage characteristics; MS and MPS type SDs; Surface states; Series resistance; Polymer interlayer.

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Investigation of Thermal Stability of Boron Carbide Under Shock Compression via Molecular Dynamics Simulations

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Abstract: Boron Carbide[1,2] has been investigated via non-equilibrium molecular dynamics simulations[3] to examine structural changes that occur as a result of high temperatures that are released under shock compression. Simulations are carried out at 10 K initial temperature in different crystallographic directions. Shock compression has been modeled by momentum mirror technique. Dimensions of the structure used in the simulation are 30×30×1200 A^3 and 30×46×2242 A^3. Structural changes caused by high pressure and temperature were observed. It has been observed that the temperature rises above the melting point in the regions where the pressure exceeds the elasticity limit.

Keywords: Boron Carbide, Shock Compression, Molecular Dynamic.

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Investigation of Ti Effect on P2-type $NaMnFeO_2$ Cathode Materials for Sodium-ion Batteries

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Abstract: New battery technologies are needed due to restrictions of lithium metal such as the limited reserves and their high cost. Sodium-ion batteries (SIBs) are regarded as one of the most promising alternative candidates to lithium-ion batteries due to natural abundance and low cost. Thus, finding novel-high-capacity cathode materials for SIBs is highly critical. In this perspective, Ti-substitution $NaMnFeO_2$ cathode materials with different stochiometric ratios were synthesized successfully by modified solid state technique using high purity oxide powders. XRD, SEM and FTIR are used for structural analyses. The cathode materials were fabricated by combining the active material, carbon black and PVdF binder in a weight ratio of 70:20:10 using N-methyl-pyrrolidone as a solvent. Cr2032 type coin cells were assembled by using synthesized cathode materials under inert atmosphere and the electrochemical properties of the cells were investigated. Galvanostatic charge-discharge tests, CV and EIS are applied for electrochemical characterization. In summary, Ti-substitution electrode exhibit a high reversible capacity than pure P2-phase $NaMnFeTiO_2$. The results of the study on Ti effect on Mn-Fe based multi-transition metal layered cathode materials for SIBs will be discussed in details.

Keywords: Energy storage, Sodium-ion batteries, Fe-Mn based Cathode materials, Ti doping.

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Investigations of Methyl Methacrylate Nanocomposite for Optoelectronic Applications

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Abstract: With the emerging of nanotechnology, a lot of thrill in a new area of research in polymer nanocomposites is going on for its application in optoelectronics. Polymer nanocomposites are made up of polymer matrices and nanoparticles of other materials. Mixing of nanomaterial in polymers drastically change the thermal, electrical, optical and mechanical properties witch lead the nanocomposites to vast applications in photonic devices. In this study thin films of Poly (methyl methacrylate) (PMMA) embedded with nanostructured titanium dioxide-rutile phase at various molar concentration were synthesized using solvent casting method. Structural and morphological investigations were carried out with XRD and FESEM. Linear optical parameters, absorption coefficient, band gap energy, extinction coefficient, refractive indices, optical conductivity and dielectric constants at various wavelengths (190-2000 nm) were determined for different amount of nanoparticles in polymer nanocomposites using absorption, transmission and reflection spectra. Nonlinear optical properties, such as nonlinear absorption coefficient, nonlinear refractive indices and third-order nonlinear optical susceptibility of these nanostructured titanium dioxide embedded PMMA thin films using the Z-scan technique were estimated using 532 nm CW laser. The results showed that the thin films have positive nonlinear refractive index and positive nonlinear absorption coefficient. These results are useful for applications in optoelectronics devices.

Keywords: Nanocomposites, linear properties, nonlinear properties, Polymer

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MgZnO Thin Films by Mist-CVD Grown: Structural and Optical Properties

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Abstract: Zinc Oxide (ZnO) is an important semiconductor with a wide bandgap (3.37 eV), high exciton binding energy ~60 meV, and the most stable thermodynamically hexagonal crystal structure. To control the optical properties of ZnO, it can be alloyed with other oxide materials like MgO. The formed MgZnO alloy has crystallized in the hexagonal MgZnO crystal phase up to about 40%<Mg, but with increasing Mg ratio, MgZnO is transforming into the mixing of wurtzite and rock-salt phases. In this study, MgZnO growth was carried out on glass substrate by mist chemical vapor deposition (mist-CVD) method as a low-cost, environmental, and high-productivity film coating method. MgZnO nanostructure has been investigated with X-ray diffraction, Atomic Force Microscope, and Scanning Electron Microscopy (SEM) measurements. The growing MgZnO nanostructures have shown the wurtzite hexagonal crystal phase. There is no other phase related to cubic crystal. The cyrstal shape of MgZnO is found to be hexagonal and triangular-like nanostructures. The calculated optical band gap of MgZnO is increased with increasing Mg mole fraction in MgZnO nanostructures.

Keywords: MgZnO, mist-CVD, optical properties.

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Microwave-Assisted Synthesis of Ion-Doped B-Tri-Calcium Phosphate Powders

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Abstract: Bioceramic materials have become prominent among the other biomaterials due to their exceptional properties such as high biocompatibility, corrosion and wear resistance, aesthetic appearance, etc. β-Tri-calcium phosphate (β-TCP, $Ca_3(PO_4)_2$) is a well-known bioceramic material. It is widely used in coating, powder, or paste/putty form due to its bioresorbable character that enables rapid healing of the damaged hard tissues. Therefore, several methods are developed to obtain β-TCP practically. Nowadays, the microwave-assisted synthesis technique draws attention owing to advantages like producing sub-micron-sized and uniform particles in shorter operation durations than conventional methods, easy control of the process parameters, etc. In this research, β-TCP powders doped with antibacterial ions and ions that promote osteogenesis were fabricated following the microwave-assisted synthesis procedure. Briefly, the preparation of the Ca and P sources, the reaction between them in the modified household-type microwave oven, centrifuging, drying, and heat treatment steps were sequentially applied to achieve the un-doped and ion-doped β-TCP powders. X-Ray Diffraction (XRD) and Scanning Electron Microscope (SEM) were used to analyze the chemical phases and surface features of the powders, respectively. The bioactive behavior of the microwave-assisted synthesized powders was evaluated according to the simulated body fluid (SBF) immersion tests.

Keywords: Bioceramics; microwave-assisted synthesis; β-tri-calcium phosphate; ion doping; powder characterization.

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Molecular Docking Demonstration of the Interaction of AFB1 Aflatoxin and Lactococcin A

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Abstract: Aflatoxins (AF), which cause diseases in humans and animals, are mycotoxins produced by certain types of fungi. Bacteriocins are natural antimicrobial substances synthesized by bacteria. These substances that are in protein structure, generally have short chain and small molecular weight. According to the classification made by Klaenhammer, especially considering Gram (+) bacteria, bacteriocins are divided into 4 different classes. These are Class I (Class IA, Class IB), Class II (Class IIA, Class IIB, Class IIC, Class IID), Class III and Class IV. Enterocin A, Divercin V41, Sakacin A, Lactococcin MMFII, Lactococcin A can be given as examples of Class II bacteriocins. In this study, we examined the interaction of AFB1 aflatoxin and Lactococcin A bacteriocin, which is in Class II, using Molecular Docking.

Keywords: Aflatoxins (AF), Bacteriocins, Molecular docking, Lactocin A

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Molecular Docking Study on Interaction of Polyvinyl Alcohol (PVA) with Group IA Bacteriocin

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Abstract: PVA with the molecular formula $(C_2H_4O)_n$ is a polymer prepared from polyvinyl acetates by replacing acetate groups with hydroxyl groups. It is a synthetic polymer with low surface tension, flexible and soft, water-soluble and cross-linkable thanks to the hydroxyl groups in its structure, biodegradable and non-toxic due to the carbon bonds in its chain. Bacteriocins are compounds of protein nature that are ribosomally synthesized by bacteria. Considering their biochemical properties, they are generally divided into 4 different classes. In this study, Nisin bacteriocin (in Group IA) was chosen as the target, and a single monomer of the PVA polymer was chosen as the ligand. The interaction of PVA and Nisin was simulated and characterized by the molecular docking method. A rational depiction of ligand-protein binding interactions was made. The findings obtained from the analysis results were compared with the experimental data.

Keywords: Polyvinyl alcohol, Molecular docking, Nisin

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Multi-Code, Low-Barrier Python Toolkit For MD/DFT Studies

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Abstract: Nowadays, there are dozens of different software widely used in materials and molecule research. Some of this software are closed-code and needed to pay, and some are open-source and free to use. In general, some codes have come to the fore due to their historical backgrounds and owe their widespread use to the widely known workflows that take place through the research groups. In this presentation, we are reporting our software called 'gpaw-tools' which keeps the simulation process easy and provides familiar workflow methods for the end-user with its UI/GUI. Recently, it uses the ASAP3 and GPAW modules in particular, which are open-source MD and DFT software written in Python, together with ASE, which is used in setting up, running, visualizing, and analyzing atomistic simulations. Thanks to the fact that this software is built on ASE, a Python module that can work with almost all MD and DFT software in the literature, our software can include many MD / DFT software in the future (possible with enough developer work power), therefore the user can focus the work with a generalized workflow and input-output files, not the infrastructure itself.

Keywords: MD, DFT, Python, Software, Development, GPAW, ASAP3, ASE

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Nanocomposite Thin Film Triboelectric Nanogenerator for Self-Powered Contact-Sensor Application

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Abstract: The triboelectric nanogenerator, which converts mechanical energy into electrical energy, is a new generation gadget that can tackle energy demand issues. As a triboelectric layer over friction surfaces, the well-known semiconductor of SnO_2 nanostructured thin films is shown to be more efficient than polymers with lesser performance, resulting in higher nanogenerator output power. SnO_2 is being used as a friction electrode for the poly(methyl-methacrylate) layer in this landmark study, as well as the team like to learn more about the electron transfer process as a consequence of their comprehensive assessments. Higher nanogenerator output power is attributed to tunnelling electrons within SnO_2/Ag nanocomposite thin film layer of triboelectric nanogenerator cause PMMA contact charge at nanoscale. The SnO_2/Ag layer's closeness to the PMMA/ITO surface induces electron field emission and the SnO_2/Ag layer tapping might cause an electron cloud overlap. It's also analogous to a semiconductor/insulator interface, where electron transport is significantly reliant on the Fermi level of the SnO_2. These explanations were accompanied by an examination of the operational condition of the system described above as a contact sensor in commercial computer keyboard that produces its own energy and it was determined to have this efficiency as a consequence.

Keywords: Triboelectric, Nanotechnology, Nano Energy, Triboelectric Nano Generator (TENG), Self-Powered Contact Sensor (SPCS)

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Nickel Oxide and Graphene Oxide Incorporated Molecular Imprinted Coatings for Electrochemical Recognition of Acetylcholine

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Abstract: Herein, we synthesized molecular imprinted polymer (MIP) coatings containing nickel oxide (NiO) nanoparticles and graphene oxide (GO) for enhanced electrochemical recognition of acetylcholine. The preparation of NiO nanoparticles is carried out by polyol's method whereas GO was made by modified Hummer's scheme. Four different sensor coatings i.e., pristine-MIP, NiO-MIP, GO-MIP and NiO-GO-MIP were prepared and integrated with screen printed interdigital capacitors (IDCs), respectively for capacitive sensing of acetylcholine. Among all these sensor devices, NiO-GO-MIP layer coated IDC exhibited highest capacitance shifts for acetylcholine. Additionally, the NiO-GO-MIP coated IDCs showed at least three times higher sensor response for acetylcholine as compared to dopamine and xanthine suggesting high selectivity of receptor layer. It was noticed that the sensor response of two weeks old NiO-GO-MIP coated IDCs was similar to that of freshly coated IDCs which indicates that developed sensor coatings is stable and robust that can be used for extended times without losing recognition performance.

Keywords: molecular imprinted polymer, interdigital capacitor, nickel oxide, graphene oxide.

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On The Illumination Response of The Impedance Characteristics in Al/Gr-PVA/p-Si (MPS) Structure

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Abstract: In this study, both the capacitance-voltage (C-V) and conductance-voltage (G/ω-V) measurements of the fabricated Al/Gr-PVA/p-Si (metal-polymer-semiconductor/MPS) structure have been performed at 500 kHz and room temperature. For the illumination response on the C-V and G/w-V characteristics, these measurements were made both in the dark and under 200 $mW.cm^{-2}$. Moreover, C^{-2}-V characteristics were analyzed under dark and illumination determined from the basic electrical parameters such as the acceptor concentration (N_A), Fermi energy level (E_F), the barrier height (Φ_B) and the depletion-layer width (W_D). In addition, the voltage dependent profile of interface traps (N_{ss}) was extracted from the dark-illumination capacitance method. All of these show that the C-V and G/w-V characteristics or main electric parameters of the structure are very sensitive to the illumination and applied bias voltage.

Keywords: C-V and G/w-V characteristics; Illumination effect; Basic electrical parameters; Series resistance.

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One-Step Synthesis of a Multifunctional MoS_2@g-C_3N_4 Nanomaterial for Adsorption-Based and Photocatalysis Degradation-Based Removal of Rhodamine B and Sildenafil Citrate

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Abstract: Multifunctional materials have gained great attention in water treatment, they can be used as adsorbents and photocatalysts separately or in combination in one step for the removal of organic and inorganic molecules. In this study, a multifunctional MoS_2@g-C_3N_4 nanomaterial was synthesized in one step using different amounts of ammonium molybdate and thiourea. The structure of the synthesized materials and the functional groups present were characterized by X-ray diffractometry (XRD) and Fourier transform infrared spectrometer (FT-IR).The MoS_2@g-C_3N_4 nanomaterials were used as adsorbents and photocatalysts for the removal of rhodamine B (RhB) and sildenafil citrate (SLD), the multifunctional material was obtained at a ratio of 0.3g ammonium molybdate and 10g thiourea, at optimum conditions the adsorption-based removal of RhB and SLD was found 98% and 95% respectively, and the photocatalytic degradation removal was found 100% within 210 min of UV irradiation and 98% within 300min respectively what make the material useful in environmental applications.

Keywords: Photocatalytic degradation, adsorption, removal, multifunctional, nanomaterial

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Optical Properties of ZnAlO Thin Films Produced by One Step Electrochemical Deposition Method

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Abstract: Different electronic components like photovoltaics, displays, transistors, etc. are consisting of metal oxide thin films. Metal oxide thin films exhibit outstanding optic, optoelectronic, electrical and electronic properties and therefore, are vastly researched by researchers from different fields. [1]. Metal oxide thin films have high thermal stability with low electrical resistance while they can be consisting of a single material or multiple materials [2]. The electrochemical deposition method is cost efficient with good thickness control while it does not require expensive equipment such as high vacuum systems, etc. Hence, it is commonly preferred to produce metal oxide films. In this work, we use one step electrodeposition method to produce ZnAlO thin films on ITO. We investigate the optical properties of thin films using a UV-Vis spectrophotometer between 200 nm – 800 nm wavelength. In the absorption spectra of the ZnAlO thin films, an apparent peak at 588nm was seen while the maximum absorption coefficient was found at 372 nm as 9.79×10^5 m^{-1}. Bandgap energy was calculated as 3.57 eV which was found to be coherent with the reports presented in the literature. Transmittance values of ZnAlO films were found to be 80% in the visible region while it can drop up to 37% in the max absorption region. The refractive index of the ZnAlO thin films increased with decreasing wavelength while the extinction coefficient diminished with decreasing wavelength. The maximum n value was found to be 1.26 while the minimum k value was 0.007. Moreover, optical (Єi), dielectric loss(Єi/Єr), optical conductivity (σ) values were found as 1.61, 0.09, 0.06 and 2.92×10^{14}, respectively.

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Organic Field Effect Transistor with Polylinoleic Acid-Graft-Polystyrene-Graft-Polycaprolactone (PLina-g-PSt-g-PCL) Gate Dielectric

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Abstract: Polylinoleic acid-graft-Polystyrene-graft-Polycaprolactone (PLina-g-PSt-g-PCL) three block graft copolymer series were synthesized using a combination of ring-opening polymerization (ROP) and atom transfer radical polymerization (ATRP). -Br polymeric linoleic acid (Plina-Br). The structural characterization of PLina-g-PSt-g-PCL series were carried out (realized) using 1H NMR, GPC methods, thermal properties such as DSC and TGA techniques. After then, monomer concentrations, initiator concentrations and kinetic parameters of novel PLina-g-PSt-g-PCL series synthesized in terms of the specificity of the study were investigated. Organic Field Effect Transistor (OFET) applications of PLina-g-PSt-g-PCL series graft-copolymer were also examined. Regioregular poly(3-hexylthiophene-2,5-diyl) (P3HT) was used as organic semiconductor in PLina-g-PSt-g-PCL insulated OFET devices. The OFET devices obtained using PLina-g-PSt-g-PCL were characterized by determining the output and transfer current-voltage (I-V), and Capacitance-Frequency (C-f). The C-f measurements of OFET devices were performed by forming Al/(PLina-g-PSt-g-PCL) /P3HT Metal/Polymer/Semiconductor (MPS) structure. The calculations of main performance parameters of OFETs such as the threshold voltage (V_{Th}), field-effect mobility (μ_{FET}), and current on/off ratio ($I_{on/off}$) were realized by obtaining the I-V and C–f characterizations. OFET devices were found to exhibit good saturation and minimal leakage current. Results showed that the fabricated OFET device indicated excellent performance including low V_{Th}, remarkable mobility and high $I_{on/off}$.

Keywords: Polymer dielectric, mobility, Organic Field Effect Transistor (OFET),poly(linoleic acid), Atom Transfer Radical Polymerization (ATRP)

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Peptide Amphiphile/Carbon Nanotube Conductive Nanocomposite Hydrogels

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Abstract: Carbon nanotubes (CNTs) show excellent morphological, electrical, and mechanical properties to provide structural reinforcement and electrical conductivity when incorporated into the engineered tissue scaffolds for possible directing neural cell growth [1]. But CNTs cannot be dispersed in aqueous medium directly and have been reported to have cytotoxic effects on cells. Therefore, functionalization with biocompatible materials can be applied to the CNTs to overcome these drawbacks. Peptide amphiphiles are good candidates to add diverse bio-functionality and water dispersibility to CNTs [2]. In this study, to obtain conductive, biocompatible, and extracellular matrix mimicking platforms, CNTs were surface functionalized through non-covalent interactions by positively (Lauryl-VVAGKK-Am, K2-PA) and negatively (Lauryl-VVAGEE-Am, E2-PA) charged peptide amphiphiles which formed hydrogel upon mixing them (Figure 1). The PA/CNT hydrogels were characterized in terms of structural, morphological, and rheological techniques. Morphological analyses revealed homogeneous fibrillar network structures for PA/CNT hydrogels. Slightly differences in viscoelastic properties were observed with the presence of CNTs for PA/CNT hydrogels compared to plain PA hydrogel.

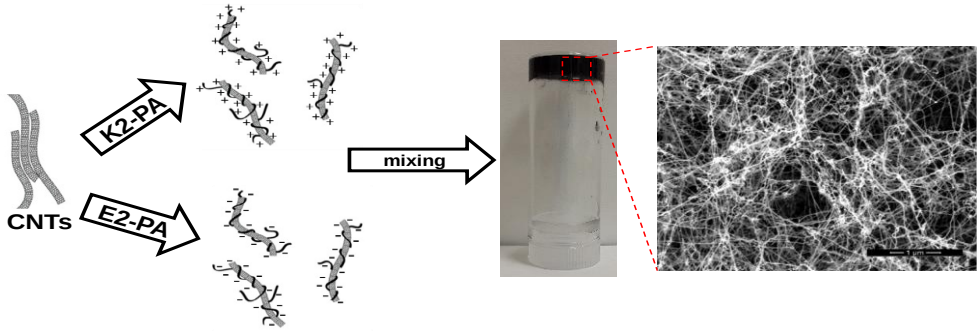

Figure 1. Self-supporting gel behavior and SEM microscope image of PA/CNT hydrogel.

Keywords: Carbon nanotubes, Peptide amphiphiles, Self-assembly, Supramolecular gels

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PHEMA Based Cryogels as 3D Scaffolds for Placental Barrier Studies

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Abstract: Cryogels are advantageous scaffolds for cell adhesion due to their biocompatibility and superporosity. Super-macroporous poly (2-hydroxyethyl methacrylate) (PHEMA) cryogels are hydrophilic, mechanically and chemically stable. In this study, gelatin, fibronectin (FN) or collagen Type IV was added to the structure of cryogels. Folic acid (FA) was also bound to the gels to reflect extracellular matrix (ECM), providing a 3D environment. The swelling states of cryogels have been characterized. Structure analysis by Fourier transform infrared (FTIR), morphological analysis by microtomography (mCT) and scanning electron microscopy (SEM) were performed. Co-culture systems were constituted with human placenta choriocarcinoma cells (BeWo) and human umbilical cord vein cells (HUVEC). *In vitro* release analyses were performed on FA bound cryogels. The cytocompatibility of the synthesized cryogel groups and the viability of the cells for 2, 4 and 7 days were evaluated. Vortioxetine, an antidepressant active ingredient was evaluated in the 3D cryogel co-culture system. The cell viability was investigated by MTT analysis. Human chorionic gonadotropin hormone production and matrix metalloproteinase-2 and matrix metalloproteinase-9 and protein levels were measured. PHEMA+COL Type IV+FA cryogel was the most suitable group for investigating the toxicity of various products exposed during pregnancy, medications that should be used, and food additives.

Keywords: Placental Barrier Model, BeWo, HUVEC, Cryogel, PHEMA, Folic Acid, Fibronectin, Collagen Type IV, Vortioxetine, β-hCG.

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Photosensitivity Enhancement of PVP Thin Films via Exfoliated 2D GaSe Nanoflakes

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Abstract: Two-dimensional (2D) materials can exhibit very different mechanical, optical and electrical properties due to quantum confinement. Researchers who started with graphene are now focused on bringing the 2D properties of different materials to technology. Since the mass production of 2D materials has not become widespread, researchers are producing nanocomposites with cheaper and easier-to-produce materials. In this respect, producing nanocomposites with 2D and polymer materials is a preferred method in terms of using the advantages of both material groups.In the presented study, 2D GaSe nanoflakes were obtained by exfoliating bulk GaSe with sonication. The dimensions of 2D GaSe nanoflakes are measured with AFM. PVP:GaSe nanocomposite thin films were produced by doping 2D GaSe into PVP in different compositions [1]. Undoped PVP thin film was also obtained for comparison. As a result of the Raman and PL analyses of the obtained PVP:GaSe nanocomposite thin films, it was observed that the GaSe nanoflakes significantly increased the photosensitivity. The dark current-voltage characteristics of the photodiodes produced by changing the 2D GaSe nanoflake compositions were investigated. When the photocurrent performance was examined under light with the help of a solar simulator, 5% 2D GaSe nanoflake doping increased the quantum efficiency of the device to 86%.

Keywords: Photosensitivity, Nanocomposite thin films, 2D Materials, GaSe nanoflakes

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Physiochemical Modification of Graphene Nanosheets to Tailor Electrical Properties of Graphene Based PMMA Composites

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Abstract: This research work has been conducted to synthesize modified reduced graphene oxide (m-rGO) based poly methyl methacrylate (PMMA) composite by solution mixing method using chloroform as solvent. Modification of reduced graphene oxide (rGO) was carried out by Friedal craft acylation with 4-bromobenzoic acid that caused introduction of acyl group to the surface of rGO, which may result increase in homogeneity of the synthesized composites of m-rGO and PMMA (m-rGO/PMMA). Series of composites having different wt.% of filler (m-rGO) were prepared. FTIR and UV-Vis spectroscopic techniques were employed for confirmation of modification of the rGO and prepared composites. Significant improvement in electrical properties has been observed because of the surface modification of the rGO. Interesting frequency dependence relationship of conductivity and dielectric constant has been obtained. Lower percolation threshold was observed for these nanocomposites because of enhanced interfacial interaction of m-rGO with PMMA. Above mentioned results encourage the modification of the rGO for its incorporation in PMMA for composite formation.

Keywords: PMMA, modified reduced graphene oxide, nanocomposites, electrical properties

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Preparation of Ag@SiO2 Core-Shell Nanoparticles for Plasmonic Dye-Sensitized Solar Cell Application Using Laser Ablation Liquid Technique

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Abstract: In this work, Ag@SiO2 core-shell nanoparticles were prepared using the laser ablation technique and employed these nanoparticles in Plasmonic Dye-Sensitized Solar Cells (DSSC). Current-voltage (I-V) characteristic curves of DSSCs were preformed both in dark and 100 mW/cm2 and the obtained experimental results were compared each other at room temperature. Ag@SiO2 core-shell NPs were prepared using different laser energies (50 mJ,100mJ,150 mJ) by pulsed laser ablation in silica aqueous solution. The results highly showed the effect of the used laser energy on the structural properties of the prepared nanoparticles, which in turn affect the other properties. The XRD for Ag@SiO2¬ shows that the crystallinity enhanced, and the crystallite size increased with increasing the laser energy (18.8nm for 50 mJ, 24.5nm for 100 mJ, 34.9nm for 150 mJ). The transmission electron microscopy shows an increasing average diameter for both NPs types with the laser energy. The UV-visible absorbance shows significant plasmonic resonance bands around 400 nm for the Ag@SiO2, with a small red shift with increasing the laser energy. Incorporating metal NPs into solar cell layers enhances their efficiency because of increasing the absorption inside the active layer, especially at the plasmonic frequency. The effect of the different NPs was examined and compared with the bare-solar cell without nanoparticles. The DSSC solar cell composed of Ag@SiO2 NPs shows significant enhancement in their characteristics. The results exposed that the Ag@SiO2 can be employed as selective scattering factors which are promising efficient DSSCs.

Keywords: core-shell nanostructure. Laser ablation, plasmon, dye-sensitized solar cell.

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Preperation and Characterization of Functional Graphene Based Dispersions for Wearable Electronics

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Abstract: Graphene has been the focus of attention since it was discovered, due to its superior properties. Graphene has been researching in various application areas for years. The use of various graphene derivatives to obtain functional wearable electronics is one of these issues. Wearable electronics is an emerging concept that is expected to have significant implications for the healthcare, defense and communication industries in the future. For such fields, conductive dispersions that have graphene as an active material have a potential to be obtained as scalable solutions. In this study, we focused on preparation and implementation of stable dispersions to varying substrate. Effects of varying parameters on dispersion properties, factors affecting implementation of conductive dispersions and applicability of outcomes are examined. In addition, characterization techniques such as X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy (SEM), Raman and FT-IR Spectroscopy analyses are examined to develop dispersions. Production parameters, dispersion properties and characterization results are compared.

Keywords: graphene, conductive dispersions, wearable electronics, graphene characterization, dispersion characterization

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Pressure Effects on Mechanical and Electronic Properties of Semiconductor HfPtSn Compound

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Abstract: Half-Heuslers compounds due to their bigger Seebeck coefficient and high electrical conductivity have attracted much attention by researchers. These compounds have also interesting electronic and magnetic properties and spin polarization and can be used for applications in thermoelectricity, data storage devices and spintronics. The objectives of this study is to investigate pressure effects on structural, elastic, electronic properties of semiconductor Half-Heusler compound HfPtSn using first-principles methods based on density- functional methods via the VASP program. We may concluded that this material is stable mechanically and energytically under pressure up to 50 GPa for providing Born stability conditions. The electronic band structure calculations have showed that this material has indirect band gap semiconductors with 0.94 eV. Pressure effects on electronic properties have also studied here. The band gap values increase with pressure up to 50 GPa. Generally obtained results are compatible with other results. These results may provide important informations for experimentalists.

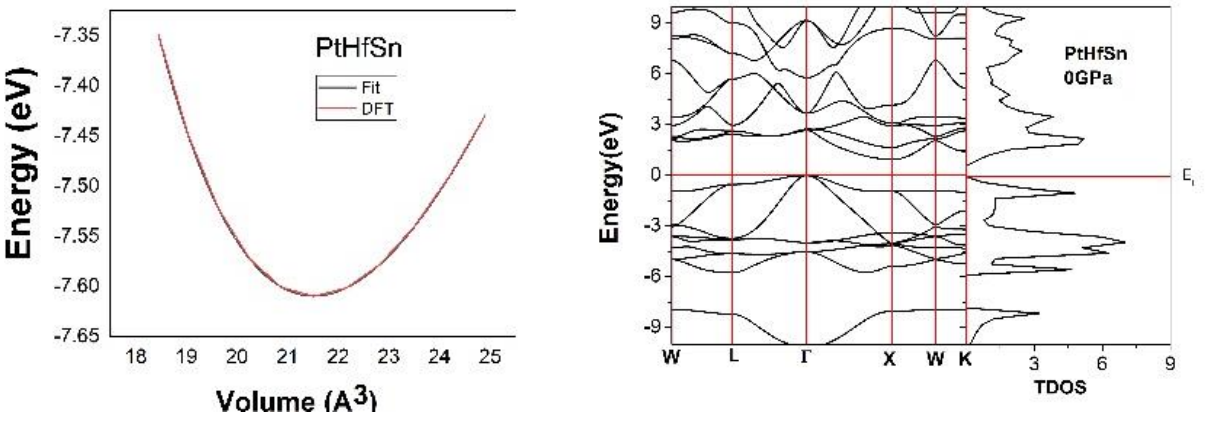

Figure: Energy-volume curves and electronic band strcuture for PtHfSn

Keywords: DFT, Half-Heusler, pressure effects, HfPtSn, electronic properties, mechanic properties

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Production and Characterization of Coenzyme Q10 Loaded Nanofiber Surface

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Abstract: The aim of this study is to produce and characterize coenzyme Q10 loaded polyvinyl alcohol nanofiber mats by the electrospinning method. For this purpose, polyvinyl alcohol and coenzyme Q10 loaded polyvinyl alcohol mats were produced with the specify electrospinning parameters. After that, the produced nanofiber mats were made water resistant by crosslinking process. The morphological characterization of produced mats was done by scanning electron microscopy. At the same time, the contact angle and swelling behavior of the produced mats were investigated.

Keywords: Coenzyme Q10, nanofiber, polyvinyl alcohol, electrospinning

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Revolution of the Electric Field with Darboux Frame

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Abstract: Magnetic field and charged particle relation is researched by many ways in physics and mathematics. After the topological phase was investigated, the geometric phase was also examined. This study, called the Berry's phase, attracts a lot of attention. The Rytow law can be described by the rotation of the polarization plane along an optic fiber. In this study, we research the geometric phase of the polarization plane of a light wave travelling in an optical fiber through Darboux frame in Minkowski 3-space. Next, the direction of the state of the polarized light is studied for three different cases, paying attention the planes on which E lies. After that, we investigate the Fermi Walker parallel transportation law to research the parallel transportation of electric field along an optica fiber in the polarized light with respect to Darboux frame. Finally, we present some motivated examples to observe more easily by mathematical programs.

Keywords: Vector field, magnetic curve, magnetic field, Minkowski 3-space.

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Rytov Curves with Respect to Null Cone Fronts

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Abstract: Investigation of special curves in Minkowski space is especially important for mathematics and physics. These curves give mathematical and physical meaningful descriptions of some problems. In special and general relativity, a cone of light is also of great importance in physics because it is the space-time path of a flash of light emanating from a single event (localized to a single point in space and a single moment in time) and traveling in all directions. In this study, first we introduced to spacelike framed curves and give the Frenet type formulas of the spacelike framed curves. Then, we will investigate space like singular Rytov curves which are trace curves of the tip points of the Electric field on a null cone.

Since our curve are a singular spacelike curves, to examine these curves we will use the spacelike framed curves in Minkowski 3-space. Furtermore, we give some related examples and visualized them with using mathematical programs.

Keywords: null cone, electric field, special curves, Minkowski 3-space, singularities.

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Schiff Base Derived Carbonaceous Material Separator Coating for Li-S Batteries

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Abstract: Battery chemistries involving Lithium-Sulfur (Li-S) are one of the most promising next generation systems. Because theoretical capacity of sulfur (1672 mAh g^{-1}) is order of magnitude higher than conventional battery system $LiCoO_2$ (270 mAh g^{-1}). However, there are some challenges of Li-S batteries including shuttle effect, low conductivity of sulfur and volume expansion. In particular, Li_2S_n ($3 \leq n \leq 6$) generation during discharge leads to diffusion of these species in electrolyte, and when they reach the anode (shuttle effect), they react to form insoluble Li_2S, reducing the Coulombic efficiency and the reversible capacity of the cell. Various strategies have been developed to mitigate shuttle effect. Several additive materials were investigated such as carbonaceous materials, polymers, metals, MOFs etc. Carbons are among the most promising options. Because it is easy to manipulate properties of carbon materials. For instance, presence of nitrogen atoms in the carbon framework endows the material a good sorbent of Li_2S_n, which enables retardation of shuttle effect. Additives can be employed in cells in different configurations.

The most well-known strategy is to use carbon in composite cathode. Rather than using carbons as additives in the cathode, one alternative strategy is coating the separator with a appropriate thin barrier, which can easily be employed by casting methods. In this study, a Schiff base is produced from an aliphatic organic molecule and solvothermally treated to form a carbonaceous material. The material is composed of fluorescent carbon nanoparticles. According to TEM analysis, carbon particles having sizes up to 100 nm are present. XPS analysis revealed that more than 3 at% of the surface contains nitrogen atoms. Separator coating procedure is employed by doctor blade technique. Uncoated separator, conductive carbon coated separator and Schiff base derived carbon coated separator containing cells were prepared. Electrochemical performances were elucidated such as cycling stability tests. In addition, effect of presence of separator coating on electrolyte resistivity and internal resistances were also compared. In summary, Schiff base derived carbon coating enables better capacity retention beyond around 80 cycles compared to only carbon coated separator.

Acknowledge: This work is supported by TÜBİTAK-BİDEB 2219 postdoctoral fellowship programme.

Keywords: battery, Li-S, electrochemical energy storage, separator coating, carbon materials, Schiff base, hydrothermal synthesis

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SILAR Synthesis of $CuCdS_2$ Nanostructures for Photocatalytic Applications

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Abstract: In this study, copper cadmium sulfide ($CuCdS_2$) nanocrystals were synthesized by the successive ionic layer adsorption and reaction (SILAR) method on the base of functionalized nitrile butadiene rubber (FNBR). To obtain ternary sulfides of metals, the sorption of metal ions on the FNBR at different pH was studied, and the initial solutions for the synthesis of nanoparticles were prepared at optimal pH. The optimal pH for the sorption of Cu^{2+} and Cd^{2+} ions in FNBR was pH = 4 (96%) and pH = 6 (94%), respectively. $CuCdS_2$ nanocrystals were synthesized in 5 and 15 cycles. According to the results obtained from X-ray diffraction, the average diameter of the nanoparticles synthesized in periods 5 and 15 was 1.13 and 28 nm, respectively. The band gap energy of the nanoparticles was 2.76 eV. The results of ultraviolet spectroscopy show that the maximum absorbance in the nanoparticles obtained in periods 5 and 15 are in the range of 275 - 300 nm and 230 - 280 nm, respectively. Sorption and photocatalytic degradation of brilliant green dye from aqueous solutions were carried out with the obtained nanocomposites. The photodegradation degree under sunlight increased, reaching 96.25% in 5 cycles and 95% in 15 cycles.

Keywords: $CuCdS_2$, nanocrystals, brilliant green dye, sorption, photocatalytic degradation

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Structural Properties of Vanadium Substituted P2-Type $Na_{0.67}Mn_{0.5}Fe_{0.43}Ti_{0.07}O_2$ Cathodes for Na-Ion Cells

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Abstract: Na-ion cells have seen the future of battery technology and scientists have focused on the development of new electrode materials to improve their properties. It is well known that the cost of the components of the electrode materials is one of the critical parameters for commercialization. Manganese and iron-based metal oxides have a high potential for the commercialization of the cells due to their abundance on the planet, low production cost, and environmentally friendly structure. V-substituted $Na_{0.67}Mn_{0.5}Fe_{0.43}Ti_{0.07}O_2$ cathode materials were synthesized successfully by a modified solid-state technique which processed quenching at high temperature. The structural analyses of the electrode materials were performed by X-ray diffraction technique and FTIR and Raman analysis. We determined the solubility limit of the V-ions in the structure and the lattice parameters were determined by the GSAS-II program. The bond structure of the structure were depending on the ions in the sample were analyzed.

Keywords: Na-ion, V-substitution, battery

Acknowledge: Authors would like to thank both TUBITAK for financial support by the contract number TUBITAK-220N335.

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Structural & Surface Properties of Low Cu Doped ZnO Thin Films

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Abstract: Cu doped ZnO thin films with different doping ratios of 0, 1, 2, and 3 at % are grown by sol-gel dip coating method on microscope glass substrates using a one-day aged solution. The deposition voltage and temperature for 8 cycles of dipping are chosen as 24 V and 500 °C, respectively. The structural properties of ZnO thin films are analyzed by X-ray diffraction (XRD) method. The lattice parameters of the films are determined from XRD patterns. The crystallite size, strain and stress are obtained for all films by applying Williamson-Hall (W-H) [1] method. Surface properties are investigated using scanning electron microscope (SEM) measurement. The elemental composition of the films is confirmed by the energy dispersive X-ray (EDX) analysis.

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Keywords: ZnO, Cu doping, thin film, structural properties, surface properties.

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Structural and Spectroscopic Properties of New Schiff Base (Z)-N'-((5-nitrothiophen-2-yl) methylene) benzohydrazide Compound by Theoretical Methods

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Abstract: Schiff base compounds are used extensively in medicine and medicine production due to their antifungal, antitumor and anti-inflammatory properties. Furthermore, because of non-toxicity, good electrical conductivity, and easy production, schiff base compounds are very promising in optoelectronic devices such as photodiode and photovoltaics. Because of all these fascinating properties, this material is extremely attractive in different fields of application. In this study Schiff base (Z)-N'-((5-nitrothiophen-2-yl) methylene) benzohydrazide compound optimized, and the molecular, vibrational, and electronic properties are investigated using quantum mechanically theoretical methods. As it is known, experimental studies that require a lot of time and cost can be examined theoretically with the development of computers and monitors. Many chemical and physical properties of the molecule can be calculated with computers. Today, many drugs and materials can be produced in medical, optical, electronic, industrial and agricultural fields by modeling using quantum mechanical methods. In this study, theoretical structures, molecular models, stability, geometries, frequencies, electron densities, charge distributions and electronic energies of product, intermediate and transition states will be calculated and obtained by using Hartree Fock (HF) and Density Functional Theory (DFT) methods. In addition, quantum parameters, such as the electronegativity, the chemical potential, the softness and the hardness of the studied complex are calculated and reported.

Keywords: Schiff base; DFT; HF

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Study of Interactions of AFB2 Aflatoxin and Class IB Bacteriocins by Molecular Docking

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Abstract: AFB2, one of the B group aflatoxins, is found in human and animal milk and contains a cyclopentane ring. It, which is produced by *A. flavus* and *A. parasiticus* molds, takes attention among the 18 defined aflatoxin species. Class IB bacteriocins (Mersacidin, Cinnamycin, Ancovenin, Duramycin and Actagardin) are uncharged and negative. These bacteriocins show antimicrobial activity by inhibiting specific enzymes. In this study, the interaction between AFB2 ligand and Cinnamycin bacteriocin in Class IB was investigated using molecular docking.

Keywords: Aflatoxins, Bacteriocins, Molecular docking, Cinnamycin

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Synthesis and Characterization of Fe_3O_4/rGO Nanocomposites

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Abstract: In this study the modified Hummers' method was used to make graphite oxide. GO suspension with 5, 15 and 25 wt% added to Fe_3O_4 suspension. Fe_3O_4/rGO nanocomposites were produced by hydrothermal method. The doping effects of different GO concentrations were examined. The physical characteristics of these nanocomposites were studied using X-ray diffraction (XRD), fourier transform infrared (FTIR) spectroscopy and Raman spectroscopy. The surface morphology of prepared Fe_3O_4/rGO powders was investigated by using field emission scanning electron microscopy (FE-SEM). The reflectance of all nanocomposites was studied as a function of wavelength using UV-Vis-NIR spectrophotometer. Optical band gap of the nanocomposites was determined using the reflectance spectra by means of Kubelka-Munk equation. From optical properties, the band gap energy was estimated for all nanocomposites. The XRD analysis showed the presence of rGO, Fe3O4 diffraction peaks. The FE-SEM analysis confirmed the unification of the compound as a nanocomposite with differences in morphologic structure.

Keywords: Reduced graphene oxide, Iron oxide, Hydrothermal synthesis.

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Synthesis, Characterization, Optical, And Thermal Properties Of P(NVC-Co-BZMA) Copolymer And Its Zno Composites

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Abstract: Researchers have been interested in polymer-nanoparticle composite materials recently because of their electrical, optical, thermal, and several other properties [1-4]. First, the free radical polymerization process was used to create a copolymer of N-vinyl carbazole (NVC) and benzyl methacrylate (BZMA) that is 25-75% by weight each. The polymerization procedure was carried out at 70 ^{o}C with AIBN (Azobisisobutyronitrile) acting as the initiator. Then, nano zinc oxide powders were added to composites in three different ratios. Nano ZnO was added to the composites at a rate of 5, 10, and 15% by weight of the copolymer. In order to better understand the structures of P(NVC-co-BZMA) and its composites, FT-IR, ^{1}H-NMR, and UV spectroscopic techniques were used. Images captured with an AFM (atomic force microscope) were used to inspect the surface topography. Both the pure copolymer and its composites' optical characteristics were examined. The composite with 15% ZnO was found to have the best optical characteristics. Additionally, composites and copolymers' thermal behavior was analyzed in this study.

Keywords: N-vinyl carbazole, benzyl methacrylate (BZMA), zinc oxide, composite, optical properties, thermal analysis.

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The Detection of Pathogens in a Microfluidic Chip System Using Surface-Enhanced Raman Scattering (SERS)

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Abstract: Reliable and consistent bacteria detection in a complex matrix are difficult. This presentation will highlight SERS-based sensitive and selective approaches in microchip system. The main points of this presentation are the new labeled applications of SERS spectroscopy in a complex matrix for detecting pathogens and, especially, the contributions to microfluidics. Optimizing and analyzing SERS-based assays in a microfluidic device will be showed.

Rapid, precise bacteria identification is vital for public health and food safety, but point-of-care testing is limited. Microfluidic chips provide miniaturization, automation, integration, high throughput, and low consumption compared to older technologies. Combining nanomaterials and microfluidics improves pathogen detection with quick, sensitive detection. study. Especially in this study, we synthesized 20 nm iron nanoparticles and. Then, the synthesized iron nanoparticles were functionalized with bacterial (*E. coli*) antibody and made ready for bacterial separation in the microchip system. SERS-based bacteria determination has been successfully applied by moving iron nanoparticles in the chip with the help of a magnet. After observing that the different bacteria do not have an influence on the identification of *E. coli*, the selectivity of the approach was determined to be satisfactory. In the range of 101–105 cfu/mL, it was discovered the calibration curve has a linear relationship.

Keywords: Pathogens, Microfluidic chip system, SERS, MNP, Antibody.

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The Determination of Voltage and Temperature Dependence of Series Resistance of Au/n-GaAs Type M/S Contact

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Abstract: In this study, it is aimed to evaluate the temperature-dependent series resistance (R_s) parameter of the Au/n-GaAs type M/S contact, which can be accepted as the reference sample, to allow comparison with the literature. As it is known, R_s is the resistance of the neutral region outside the semiconductor deposition region to the current flowing through the diode in the M/S contacts. This causes the diode current drop and occurs when high voltage is applied, causing critical inaccuracy in the interface calculations. In this study, temperature dependent R_s effect of the sample was calculated by Ohm's law, Cheung-Cheung and Norde functions using I-V measurements taken in the ±2V range and compared with each other. It was observed that the Rs values derived using Ohm's law, Cheung-Cheung, and Norde functions tended to decrease with rising temperature as expected, in accordance with the results. It is obtained that the temperature dependence of R_s for all calculation methods are compatible with each other with minor differences. As a result, it is concluded that the series resistance (R_s) parameter of the Au/n-GaAs type M/S contact is the strong function of temperature and applied voltage.

Keywords: M/S contacts, serial resistance, Ohm's Law, Cheung-Cheung functions, Norde function.

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The Effect of Series Resistance on Current-Voltage (I-V) Characteristics of Ag/Perylene/n-Si Schottky Barrier Diode in Various Methods

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Abstract: In aim of this work is to experimentally investigate the effect of series resistance (Rs) on current-voltage (I-V) characteristics in Ag/Perylene/n-Si Schottky Barrier Diode (SBD). The parameter Rs is determined by performing different plots from the experimental forward bias I-V measurements. The current-voltage (I-V) characteristics of Ag/Perylene/n-Si Schottky Barrier Diode was measured at room temperature. We determined the values of Rs using the Ohm's law, Cheung's methods and Norde's function. We contrasted the series resistance values acquired using this various techniques. Cheung's methods are only applied to the nonlinear region in high voltage section of the forward bias ln I–V characteristics, while Norde's functions are applied to the whole forward bias region of the ln I–V characteristics of the junctions. The series resistance values obtained from Norde, Cheung and Ohm's law are different and are given in the table. In our study, the cause of this discrepancy is revealed. It is clearly seen that there is a good agreement between the values of the Rs obtained from these methods. Among them the most simplest, accurate and reliable one is the Ohm's law from the sufficient high forward voltages. The I-V characteristics confirmed that the distribution of Rs is important parameters that influence the electrical characteristics of diodes.

Keywords: Ag/Perylene/n-Si, Series resistance, Ohm's law, Norde's function, Cheung's methods

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The Effect on Electrical Parameters and the Use of ($NaYF_4$:Yb, Er) as an Interface Layer in Schottky Diode Application

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Abstract: Ytterbium And Erbium Doped Sodium Yttrium Fluoride ($NaYF_4$:Yb, Er) is a luminescent phosphor material for use in solar energy and alternative energy applications. In the present study, the rare earth element doped material was coated on p-Si as an interface layer by a thermal evaporation method. The electrical properties of the fabricated Al/($NaYF_4$:Yb, Er)/p-Si were analyzed under various physical conditions. The various electrical parameters such as ideality factor, the saturation current, barrier height, series resistance, and rectifier rate were obtained using Current-Voltage measurements. The photo-conductive behavior of the diode was investigated under various light intensities. The diffusion potential, Fermi Level, barrier height, and acceptor concentration were obtained using Capacitance-Voltage and Conductance-Voltage. Experimental results showed that this structure can be used in semiconductor technology.

Acknowledge: This work was supported by Bingöl University (BÜBAP, Grant no. BAP-SHMYO.2021.002).

Keywords: Rare earth element; Main electrical parameters; I-V, C-V, and G/ω-V measurements; Photovoltaic

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The Efficiency Comparison of Fully Sprayed $MASnI_3$ and $MASnIBr_2$ Perovskite Solar Cells

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Abstract: The perovskite solar cells (PSCs), which have $MASnI_3$ and $MASnIBr_2$ absorber layers, were fabricated by the fully ultrasonic spray pyrolysis (USP) method. The FTO/TiO_2/Perovskite/P3HT/Ag architecture was preferred. $MASnIBr_2$ based PSCs have shown better performance than $MASnI_3$ based PSCs. This case mainly stems from the better wettability of $MASnIBr_2$ perovskite. While the power conversion efficiency of $MASnI_3$ based PSCs for the champion cell was obtained as 0.03%, it was determined as 0.29% for $MASnIBr_2$.

Keywords: Perovskite Solar Cells, Sn Based, Pb Free, Fully Ultrasonic Spray Pyrolysis

Acknowledge: This study was supported by The Scientific and Technological Research Council of Turkey (TUBITAK) under ARDEB 3501 Career Development Program (Grant No: 117F417).

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The Electrical Properties of the Al/CuO:Ni/p-Si Photodiodes

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Abstract: The interface of the Schottky type photodiode is important to improve performance of that devices. We used 5% Ni doped CuO thin film as interfacial layer between Al and p type Si by homemade spray pyrolysis technique. Thus, we fabricated Al/CuO:Ni/p-Si device by thermal evaporation of Al on the back and front surfaces of p-Si and 5% Ni doped CuO thin film as ohmic and metallic contacts, respectively. *I-V* measurements were performed on the Al/CuO:Ni/p-Si device under dark and various light power illumination intensities. The device exhibited good photodiode behavior. Various diode parameters such as ideality factor, barrier height and series resistance values were extracted and discussed in details. The device can be improved for optoelectronic applications.

Keywords: Schottky diodes, CuO:Ni thin film, photodiodes, Al/CuO:Ni/p-Si

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The Half-metallic and Magnetic Properties of $CrAl_2F_4$ Spinel: A Density Functional Theory Study

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Abstract: Half-metallic materials are one of the most frequently used material groups in spintronic applications with their high spin polarization. Since the materials show both metallic and semiconducting nature depending on the spin orientations, half-metallic materials have been frequently studied both experimentally and theoretically. First, the ferromagnetic phase of $CrAl_2F_4$ spinel was more stable energetically than the non-magnetic phase. In the ground state, the equilibrium lattice parameter was obtained as 9.80 Å. Second, the electronic properties were examined, and the majority of spins showed metallic character while the minority of spins showed semiconducting character. In minority electrons, the valence band maximum was located at -0.252 eV, while the conduction band minimum was placed at 0.979 eV. The total band gap was obtained as 1.231 eV. This band gap provided 100% spin polarization and $CrAl_2F_4$ spinel is a true half-metallic ferromagnetic material. Then the total magnetic moment in the cell was obtained as 8.00 μ_B, while the magnetic moment value per unit formula was 4.00 μ_B/f.u. The main contribution to the total magnetic moment came from Cr atom with a value of 3.521 μ_B. Finally, $CrAl_2F_4$ spinel was obtained as a suitable new material that can be used in spintronic applications.

Keywords: Half-metallic, DFT, $CrAl_2F_4$, Ferromagnetic, Spinel, GGA.

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The Investigation of $CuBO_2$ Thin Films Produced by the Spray Pyrolysis Method

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Abstract: The transparent copper boron oxide ($CuBO_2$) thin films were coated on quartz glass substrates by the spray pyrolysis method. The produced films were annealed at three different temperatures (600, 700, and 800 °C). While the crystallographic properties of the as-grown and annealed films were analyzed by X-ray diffraction (XRD), their surfaces were examined by scanning electron microscopy (SEM). In XRD analysis, the peak intensity was not observed in thin films as-grown and 600 °C annealed conditions. The peaks were observed at ~36° and ~39° in the XRD analyses for other films. It was seen from the SEM images that the films had smooth surfaces. The optical properties of the thin films were investigated by means of UV-Vis measurements.

Keywords: $CuBO_2$ thin film, electronic materials, advanced materials, energy materials

Acknowledge: This work was supported by the 2211-C Domestic Doctorate Scholarship Program for Priority Fields and the YOK 100/2000 PhD Scholarship.

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The Investigation of Temperature-Dependent Current-Transport Mechanisms of the Au/n-GaAs Type M/S Contact

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Abstract: Au/n-GaAs type M/S contact is considered a reference sample to enable comparison with the literature, and therefore, its temperature-dependent electrical properties were investigated in this study. Although recent studies have shown that the deposition of an interface material between the metal and semiconductor is beneficial in preventing diffusion at the M/S interface and controlling charge transitions in metal-semiconductor contacts, it is important to examine a reference sample without an interfacial layer to understand the quality of the produced materials. The temperature-dependent current-voltage (*I-V*) measurements of the M/S contact were taken in the temperature range of 80-360 K with 20 K steps to investigate its current-transport mechanisms (CTMs). Two linear regions with different slopes, also called the 2-parallel diode model, were obtained from the *I-V* characteristics of the M/S reference contact. The essential parameters of the contact, such as ideality factor (n), potential barrier height (Φ_{Bo}), and reverse saturation current (I_o), were also calculated for both regions. When critical plots (n, Φ_{Bo} *vs T,* n *vs* Φ_{Bo}, nkT/q *vs* kT/q) were examined, a deviation from the classical Thermionic emission theory can be considered to be observed. As a result, the Double Gaussian Distribution could explain the temperature-dependent CTMs of Au/n-GaAs contact.

Keywords: M/S contacts, current-conduction mechanisms, the double Gaussian distribution.

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The Production of Hollow Nanofibers from PBS / TPU Blends for Biomedical Applications

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Abstract: In this study, the production of hollow Polybutylene Succinate (PBS)/Thermoplastic Polyurethane (TPU) nanofibers as biodegradable nanomaterials with improved mechanical properties was carried out by coaxial electrospinning method. The polymer solutions of pure PBS, pure TPU, PBS/TPU blends (60/40, 40/60, 20/80 w/w) (as shell), and pure PVP (as core) were prepared for bi-component nanofibers production. The core structure of nanofiber was dissolved in distilled water. Thus, hollow nanofibers were obtained with the removal of PVP from the structure. Characterization studies (SEM, FTIR, and Tensile tests) of hollow nanofibers were performed. The morphological properties of PBS/TPU blends in ratios of 60/40 and 20/80 were observed as homogeneous and non-adhered fiber structures. It was determined that the hollow PBS/TPU (60/40) mat has the thinnest nanofibers. New bond formations in the chemical structures of blended nanofibers were investigated with FTIR analysis. Therewithal, this test showed the removal of PVP in core of all nanofibers. It was observed that the adhered fibers increased the tensile stress and decreased the tensile strain at mechanical test results, which was supported also by SEM images. It is suggested that the hollow nanofibers produced by this study can be used in biomedical field as biodegradable and breathable wound dressing.

Keywords: coaxial electrospinning, hollow, biodegradable, polymeric nanofiber, bi-component, wound dressing

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The Sonochemical Synthesis and Characterization of Ni-Cr-LDH Nanocomposite Film Based On PVA

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Abstract: The development of bifunctional and stable non-noble metal electrocatalysts for high-performance hydrogen evolution reaction and oxygen evolution reaction is very important and challenging for renewable energy. Nanocomposites of polyvinyl alcohol (PVA) with Ni-Cr- layered double hydroxide (LDH) were prepared with different weight of LDH, by sonochemical method at room temperature. This work is focused on investigating the mechanical properties, gas barrier properties, and reduced flammability, increased heat distortion temperature, reduced solvent uptake, and lower flammability properties of PVA/Ni-Cr-LDH nanocomposites. Bath type ultrasonicator (VCX500) was used for the synthesis of PVA/Ni-Cr-LDH nanocomposite film. The properties of the PVA/Ni-Cr-LDH nanocomposites films were investigated using X-ray powder diffraction analysis (XRD), Ultraviolet-visible (UV-Vis) spectroscope, Scanning electron microscope (SEM), Energy-dispersive X-ray (EDX) spectroscope and Fourier transform infrared (FT-IR) spectroscope. The optical band gap of Ni-Cr-LDH was estimated to be 2.5 eV and 4.4 eV, respectively. Ni-Cr-LDH compound describes high-value band gap energy than nanocomposite, which attributed to the presence of organic anions in LDH galleries.

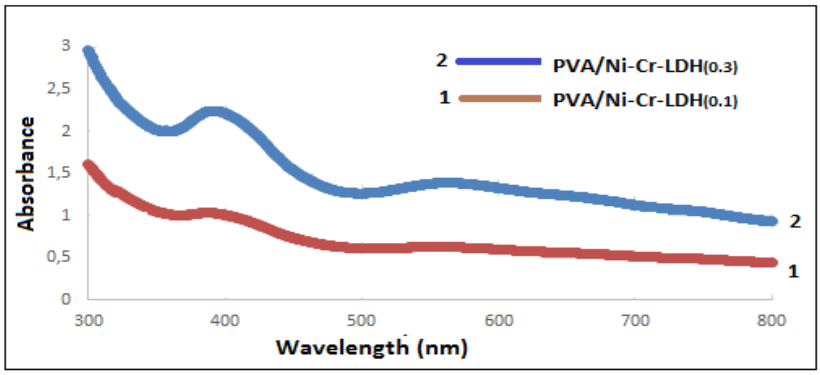

Figure 1. UV-Vis absorption spectra of 1) PVA/Ni-Cr-LDH$_{(0.1)}$; 2) PVA/Ni-Cr-LDH$_{(0.3)}$;

Keywords: nanocomposite film, sonochemical synthesis, polyvinyl alcohol, layered double hydroxide

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Thermodynamic Properties of PtZrSn: Ab-initio Study

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Abstract: A suitable semiconductor due to the fact that better, available, and tunable materials is insatiable provide a significant advantage to the technology and industry. Between the various materials in use as semiconductor devices, the half-Heusler alloys have proved to be promising contribution on the possibilities of tuning the various properties to meet the desired demand. Half-Heuslers (HH) alloys are ternary compounds and have cubic MgAgAs structure. These kind of compounds have extraordinary electronic, elastic, optical, thermodynamical and thermoelectric properties. The structural properties of various novel Heusler alloys are investigated for the precise understanding of the physics behind these alloys. Under the extreme conditions of temperature and pressure the fundamental properties of the various properties of materials may change as compared to the ambient condition. Therefore, the knowledge of thermodynamical properties under the variation of temperature and pressure acts as an extremely helpful tool for their technological applications in extreme conditions. The temperature- and pressure- dependent thermodynamical functions such as specific heat at constant volume, entropy, volume, thermal expansion coefficient, Debye temperature, Gruniesen parameters have been investigated using quasi-harmonic Debye approximation The thermodynamic parameters are determined in the pressure range from 0 to 100 GPa and temperature range from 0 to 2000 K.

Keywords: DFT, Half-Heusler, thermodynamic properties, PtZrSn, electronic properties, mechanic properties

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Tuning SO_2 Capture Capability of Oxygen Substituted MnN_4 Graphene Layer

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Abstract: Sulphur Dioxide (SO_2) is one of the harmful gases in the atmosphere that should be eliminated through capturing or converting to other useful chemicals[1]. For conversion, activation of intramolecular S-O bonds is indispensable after capturing with an acceptable adsorption energy. In this work, activation of S-O bonds in SO_2 molecule have been investigated by Density Functional Theory (DFT) calculations. On MnN_4 layer, nitrogen atoms have been changed with oxygen atoms to create different MnN_mO_n/G ($m+n=4$ and $1<m\leq 4$) layers. As more oxygen atoms incorporated in porphyrin units for bare layers, bond types between Mn and neighboring atoms switched to have more ionic character. Oxygen incorporation also change the bond strength between oxygen and neighboring carbon atoms. Moreover, as the bond strength decrease in all oxygen containing bonds, formation energies of the corresponding layers follow the same trend. For SO_2 adsorption configurations on all MnN_mO_n/G layers, S-O bonds are weakened by populating/depopulating antibonding/bonding orbitals, respectively. The bond type classification and weakening mechanism has been elucidated by AIM-Bader Topological analysis, ICOHP (integrated crystal orbital Hamiltonian population) and ICOBI (integrated crystal orbital bond index) parameters[2-4].

Keywords: Sulphur dioxide, DFT, Graphene, COHP, COBI, Bader Topological Analysis.

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Utilization of Textile Substrate Materials Towards Photocatalytic Applications via Atomic Layer Deposition

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Abstract: Photocatalytic wastewater treatment is a promising way to deal with the wastewater problem of the planet. The process degrades the toxic organic pollutants and therefore minimizes the effects on the ecosystem. The heterogeneous photocatalytic mechanism is surface driven; therefore, a higher surface area of the catalyst material is desired for higher photocatalytic activity. The surface area of the photocatalyst materials can be increased by reducing the material sizes to nanometer dimensions. However, using particle materials requires additional processing to remove the photocatalytic materials from the treated water. Immobilization of the photocatalytic species can overcome the problem. An ideal immobilization substrate should have a high surface area and thus maintain a high surface area. Due to their fibrous structure, textile materials can provide a relatively higher surface area. They are also highly accessible and inexpensive materials used in a wide variety of applications. Atomic layer deposition (ALD) is a thin film deposition method that can form highly conformal films even on high aspect ratio materials. In this study, ZnO and TiO_2 materials were deposited onto fiberglass substrates with and without Al doping to investigate the photocatalytic activities. The photocatalytic performance of the materials was explained with structural characterizations.

Keywords: photocatalysis, atomic layer deposition, textiles, ZnO, TiO_2

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Poster Presentations

A Comparative Basic Electrical Parameters Al/(Cd:Zno)/P-Si Structures By Using Forward And Reverse Bias Current-Voltage (I-V) Characteristics At Room Temperature

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Abstract: In this study, the basic electrical parameters of the fabricated Al/($Cd_xZn_{1-x}O$)/p-Si (x = 0.10, 0.20 and 0.30) structures were calculated from the forward and reverse bias current-voltage (I-V) measurements and compared each other at room temperature. Thin ($Cd_xZn_{1-x}O$) film was grown onto p-Si wafer by using sol-gel method. The values of ideality factor (n), barrier-height Φ_B(IV), series-resistance (R_s), shunt-resistance (R_{sh}) and rectifier-ratio ($RR=I_{for.}/I_{rev.}$ at ±5V) were obtained as 5.293, 0.597 eV, 34.12 Ω, 0.196 MΩ, and $5.74x10^3$ for 0.1 Cd-doped interlayer, 5.115, 0.607 eV, 51.71 Ω, 31.3 MΩ, and $56.06x10^5$ for 0.1 Cd-doped interlayer, and 4.347, 0.582 eV, 10.69 Ω, 30.2 MΩ, and $2.83x10^6$ for 0.3 Cd-doped interlayer, respectively. All these experimental results show that the best one doping-rate of Cd into ZnO is 10 % in respect of low R_s, n; high R_{sh}, RR, and good reverse saturation current. It is clear that the Cd doped into ZnO thin film can be successfully used an interfacial layer between metal and semiconductor instead of conventional insulators such as SiO_2 and SnO_2 in the electronic device applications, but the Cd and Zn additive ratios should be well adjusted to get improve the performance of them.

Keywords: Thin ($Cd_xZn_{1-x}O$) film, forward and reverse bias current-voltage characteristics

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Changes in the Energy Spectrum of Ge–Si⟨Ga,Ni⟩ Crystals Heat-Treated at 1020–1050 K

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Abstract: Based on experimental data on the temperature dependences of the free carrier concentration in complex doped $Ge_{1-x}Si_x$ ⟨Ga,Ni⟩ crystals ($0 \le x \le 0.25$), it is established that sample quenching at 1020–1050 K leads to the formation of additional acceptor centers in them. The activation energy of these centers increases with an increase in silicon content in the matrix and is described by ratio= E_v+(75+420x) meV. Crystal annealing at 550–570 K leads to the disappearance of additional acceptor levels. An analysis of the data shows that the most likely model for these deep acceptors is a complex composed of substituent nickel and gallium atoms (Ni_sGa_s) or an interstitial nickel atom and a substituent gallium atom (Ni_iGa_s). It is established that the generation of additional electroactive centers in $Ge_{1-x}Si_x$ ⟨Ga,Ni⟩ must be taken into account in precisely controlling the electronic properties of crystal via the decomposition of supersaturated solution of nickel impurity in the matrix.

Keywords: Doping, Impurities, Solid solutions, Bridgman technique, Growth from melt, Semiconducting materials.

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Computational Prediction of Electronic, Elastic, and Optical Properties of $LiNb_3Ir_4Sb_4$ and $LiNb_3Rh_4Sb_4$ Quadruple Half-Heusler Compounds

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Abstract: Based on the density functional theory (DFT), the electronic, elastic and optical properties of $LiNb_3Ir_4Sb_4$ and $LiNb_3Rh_4Sb_4$ quadruple half-Heusler compounds are calculated. Then exchange-correlation potentials are treated within the generalized-gradient approximation of Perdew-Burke and Ernzerhof (GGA-PBE). The analysis of band gap shows that these two compounds are semiconducting materials. The band gaps are found to be 0.403 and 0.364 eV for $LiNb_3Ir_4Sb_4$ and $LiNb_3Rh_4Sb_4$, respectively. The calculated elastic constants for these compounds indicate that they are mechanically stable structures. The optical properties of $LiNb_3Ir_4Sb_4$ and $LiNb_3Rh_4Sb_4$ are studied for the first time with different photon polarizations.

Keywords: Density Functional Theory, Semi-Conductors, Heusler Alloys,

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Density Functional Theory Investigation of the Interaction of CO molecule with CuO Nanolayer Defect Centers

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Abstract: Nowadays, the most used semiconductors in gas detection are oxide materials. Copper oxides differ from other oxides by their naturally p-type behavior. Defect centers in two-dimensional materials are known to manipulate drastically the electronic properties of the 2D materials. In this study, possible two defect types, substitutional N-doped (N_O^0) and Oxygen vacancy (V_O^0) of CuO nanolayer will be examined and how the CO molecule adsorbed by these defect centers will be investigated. For geometry optimizations, DFT calculations, and user interaction-I/O, ASE, GPAW and gpaw-tools software are used, respectively. In DFT calculations, LCAO mode is chosen and as XC, GGA+U is used. A surface unit cell of 4 × 4 × 1 is employed for the free-standing CuO nanolayer. A vacuum of nearly 20 Å was introduced between the layers to avoid the interactions between the periodic cells. The forces were converged until they were as low as 0.05 eV/Å. A 7 × 7 × 1 Monkhorst-Pack k-points grid was used to sample the Brillouin zone. It is thought that our study may be a step towards designing a new generation oxide gas sensor.

Keywords: copper oxide, DFT, gas detector, two-dimensional oxide, GPAW, ASE, Python

Acknowledge: S. B. L was supported in part by the Distinguished Young Scientist Award of the Turkish Academy of Sciences (TUBA-GEBIP 2016).

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DFT Study of Thermodynamic and Vibrational Properties of PtTiSn Half-Heusler Compound

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Abstract: Due to the development of spintronics, quantum computing, optoelectronic applications, Half-Heusler (HH) alloys have important technological and scientific interest for many researchers. The elastic, mechanical stability, high melting point, low value of lattice thermal conductivity, piezoelectric properties which make them incredible candidates for several applications in electromechanical resonators, microbalances, and scanning probe microscopes of high precision. The knowledge of thermodynamical properties under the variation of temperature and pressure is important for technological application due to fact that the materials properties under high pressure and temperature can change as compared ambient conditions. In this study we have studied thermodynamic and lattice dynamics properties of PtTiSn which is Half-Heusler cubic semiconductors material based on the Perdew–Burke–Ernzerhof–generalized gradient approximation density functional theory. Thermodynamic properties have been obtained using Gibbs program based on Quasi-harmonic Debye approximation. We have employed the total energy values E(V) as a function of volume for numerous primitive cells in classic thermodynamic equations to get the macroscopic thermal characteristics at different sets of temperature and pressure in the pressure range from 0 to 100 GPa and temperature range from 0 to 2000 K. Obtained equilibrium lattice parameter are in good agreement with available literature. Our results for phonon frequencies show that this material is stable dynamically. Also, we can conclude that from the tone of the mode-Grüneisen parameter, specific heat capacity at constant pressure and volume, and thermal expansion PtTiSn is favorable material for thermal conductivity at high temperature.

Keywords: DFT, Half-Heusler, thermodynamic properties, PtTiSn, vibrational properties

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Dielectric Behavior of 5CB Nematic Liquid Crystal Doped With MDC/DDC

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Abstract: In the present work, the dielectric properties of liquid crystal composites (doped with two liquid crystal molecules **MDC** and **DDC** with different chain lengths at 2 and 5 wt%) were investigated. Dielectric properties of **5CB** (4-cyano-4'-pentylbiphenyl)**, 5CB**:**MDC** ((S)-4-(2-Methylbutoxy)phenyl 6-(4-dodecyloxyphenyl)pyridine-3-carboxylate) and **5CB:DDC** ((S)-4-(3,7-Dimethyloctyloxy)phenyl 6-(4-dodecyloxyphenyl)pyridine-3-carboxylate) have been investigated. In this respect, dielectric properties of **5CB+(2wt.%)MDC, 5CB+(5wt. %)MDC, 5CB+(2wt.%)DDC, 5CB+(5wt.%)DDC** have been compared with **5CB**. The real and imaginary components (ε', ε'') of dielectric constant have been calculated by capacitance method. Dielectric strengths ($\Delta\varepsilon_s$), ε''_{max}, conductivity mechanisms dependence of frequency have been calculated for all composites. It has been also determined that adding **MDC and DDC** to **5CB**, increases the dielectric strength.

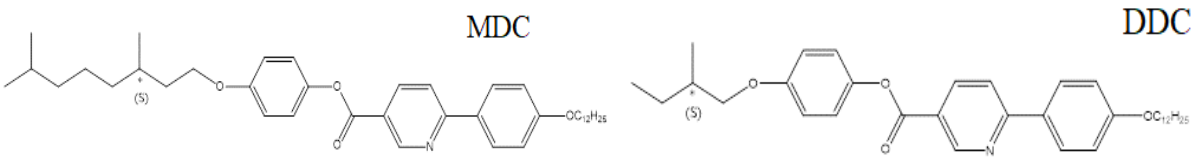

Fig.1. Molecular structure of **MDC** and **DDC**.

Keywords: Liquid crystal, Dielectric Spectroscopy (DS), Dielectric strength, 5CB (4-cyano-4'- pentylbiphenyl), Conductivity mechanisms.

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Doped Tin Carbide (Snc) Based Nanostructure for Applications In Nanoelectronics

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Abstract: In the present era of emerging electronics, the need of robust material is flourishing profoundly. A robust material possesses great structural and electronic properties. In this context, we have modelled a SnC monolayer and assess the effect of doping on its structural and electronic properties. The analysis was done in the light of density functional theory (DFT) implemented via a computational software Quantum ATK v.2017.2. The doping embraces the replacing of both C and Sn atom of SnC lattice by Si as dopant atom Since doping intercalates defects, the structure morphology in SnC sheet is changed only when Sn atom got replaced with the dopant Si atom. Besides this, the modelled doped SnC sheet exhibits good structural stability and profound an indirect bandgap semiconducting nature. Furthermore, replacing Sn atom with Si induces more stability additionally, the shorter bond length, larger formation energy. The pristine SnC monolayer also found to exhibits bandgap tuning feature that extend its applicability for useful electronic operations such as fast switching, logic etc.

Keywords: Hexagonal Tin Carbide monolayer sheet (SnC), Density functional theory (DFT), LCAO

Acknowledge: S. B. L was supported in part by the Distinguished Young Scientist Award of the Turkish Academy of Sciences (TUBA-GEBIP 2016).

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Effect of Bioactivity of *Artemisia Vulgaris* L. "Hairy" Root Extracts on the Synthesis of Silver Nanoparticles

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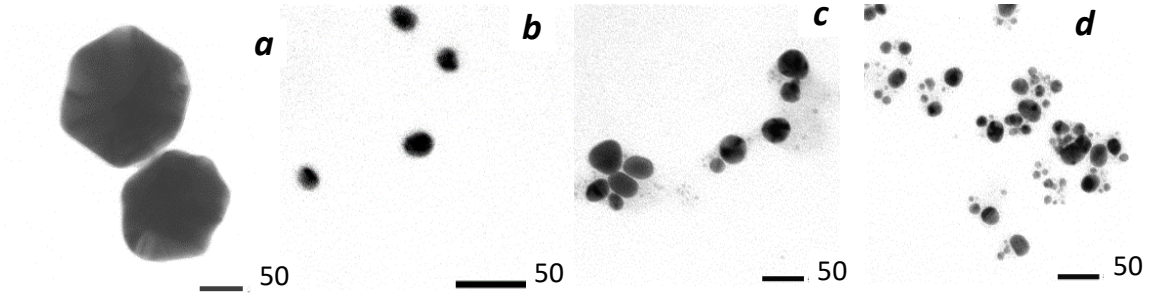
Abstract: "Green" synthesis of silver nanoparticles (AgNPs) is possible due to the presence in plant extracts components with reducing and stabilizing activity. "Hairy" roots can be used for this purpose. We studied the synthesis of AgNPs using aqueous and ethanol (70%) *Artemisia vulgaris* "hairy" root extracts and roots of the control plants. Aqueous and ethanol control roots extracts allow to obtaine nanoparticles with an average size of 71.02 (235.01 nm maximal, ***a***) and 14.26 nm (33.58 nm maximal, ***b***). Nanoparticles obtained using aqueous and ethanol extracts from "hairy" roots had an average size of 34.80 (***c***) and 8.57 (***d***) nm with a maximal size of 62.63 and 31.26 nm, respectively.



The total content of flavonoids and the reducing activity of the extracts were determined. Aqueous extract from the roots of the control plant had the lower content of flavonoids and reducing activity (0.24±0.002 mg/ml and $EC_{0.5}$=1.818) compared to the ethanol one (0.58±0.007 mg/ml and $EC_{0.5}$=0.836). Content of flavonoids in "hairy" root extract was 0.71±0.01 and 0.68±0.01 mg/ml in the water and ethanol extracts, respectively.

Hereby, the results suggest the participation of flavonoids in AgNPs formation. Concentration of flavonoids and related reducing activity are the factors influencing AgNPs formation process.

Keywords: AgNPs, "green" synthesis, "hairy" roots, *Artemisia vulgaris*, flavonoids, reducing activity

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Effect of Reaction Time and Reduction Condition on Physicochemical Properties of Graphene Oxide

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Abstract: Within the scope of the study, GO was prepared by the Modified Hummers method at different reaction times (6h, 24h, 48h), and RGO was prepared by thermal (H_2, 450°C, 1 h) and chemical reduction method by ascorbic acid (AA) agent. In the FTIR analysis of GO samples, it was understood that the increased reaction time influenced the oxygen-containing functional groups. In addition, it was determined that the highest oxygen-containing functional group was obtained with a reaction time of 48 hours in synthesis. Then, RGOs were prepared by using the 48-hour sample with high oxygen level to different reduction methods. FTIR, Raman, XRD and XPS analyses of the RGO materials were performed. As a result of characterization studies, GO and RGO samples were successfully synthesized. In the XRD analysis of the RGO samples, characteristic peaks of graphene (2θ: 26°) and graphene oxide (2θ: 8°) were observed in the bulk phase. Raman analysis indicated that RGOs with multi-layered structure have been obtained in RGO-AA and RGO-T. The XPS analysis of the RGO materials showed that the highest C/O ratio was obtained using the chemical reduction method.

Acknowledge: Gazi University Research Fund (FYL-2021-7137) grant is gratefully acknowledged.

Keywords: Graphene oxide, reduced graphene oxide, C/O ratio

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Effect of the Thickness of Dielectric Layer on Electrical Performance of SnO_2 Based-Phototransistor

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Abstract: In this study, SnO_2-based thin film transistors (TFTs) were fabricated by using sol-gel spin coating method which is known its low-cost and simplicity. SnO_2 semiconductor films used as active layer were coated on Si substrates with 100 nm, 150 nm, 200 nm, 250 nm and 300 nm thick SiO_2 layers. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) was used to analyze the surface morphology of the tin oxide active layer. The presence of the elements expected to be present in the films was confirmed by Energy Dispersive Spectrometer (EDS) analysis. TFTs are designed as gate electrode at the bottom and source-drain electrodes at the top (TC/BG). The output and transfer properties of SnO_2-TFT have been investigated. Basic parameters demonstrating the electrical performance of a transistor such as mobility, threshold voltage and subthreshold voltage have been determined depending on the thickness of the dielectric layer. The SnO_2 thin film transistors have been worked in an n-channel operational mode because the drain current increases with the positive gate voltages. The thickness of the dielectric layer played an important role on the device performance. The result obtained from the measurements performed at different light intensities is that the SnO_2 thin film transistor can be used in visible photo-detecting device applications.

Keywords: SnO_2, TFT, sol-gel, Phototransistor

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Electrochemical and Spectroelectrochemical Properties of Double-Decker Lanthanides Phthalocyanine Complexes

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Abstract: Phthalocyanines (Pcs) are aromatic compounds with an 18 π-electron arrangement that exhibit multiple and reversible electron transfer properties. Pcs containing different metals and substituted groups are designed by researchers for these goals. In addition, different molecular structures of Pcs can be designed up to the metal that centered in the ring such as, mononuclear, ball type and double-decker. Interest in double-decker phthalocyanines of lanthanide group elements is absolutely increasing because of providing exceptionally new opportunities with the high intrinsic conductivity and electrochromism when compared to most other compounds. It is clear that determining the electrochemical features of Pcs required for technological applications is very important in defining the preference potential of these complexes.

In this study, electrochemical and *in-situ* spectroelectrochemical characterization of the features of double-decker lanthanides Pcs have been elucidated by voltammetric techniques such as cyclic voltammetry (CV) and square wave voltammetry (SWV) in DCM/TBAP and DMSO/TBAP non-aqueous electrolyte solution. During the *in-situ* spectroelectrochemical and *in-situ* electrocolorimetric analyses, when Pcs have reduction and oxidation processes under the constant potentials, their absorbance spectrums and colors. These measurements provided supplementary information in addition to electrochemical analyses to illuminate the redox processes.

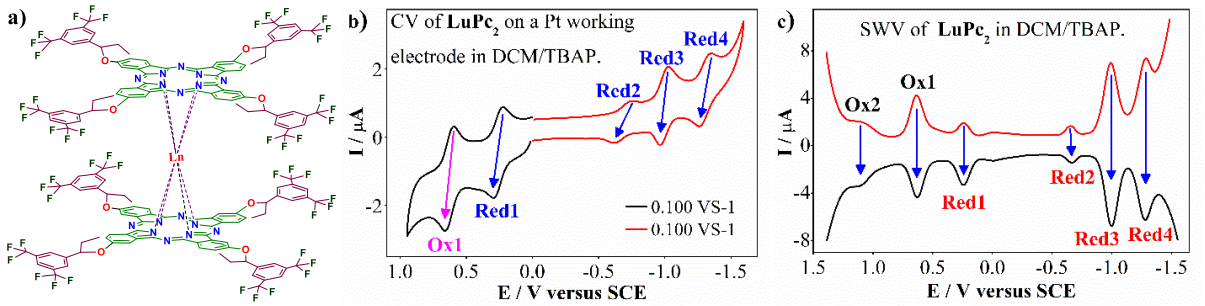

Figure:

a) Phthalocyanine Complexes (**Ln**:**Gd**, **Lu**, **Nd**)

b) Cyclic and

c) Square Wave Voltammograms of **LuPc2** in DCM/TBAP.

Keywords: Phthalocyanine, Double-decker Phthalocyanines, Electrochemistry, *in-situ* Spectroelectrochemistry

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Electrochemical and Spectroelectrochemical Properties of Novel Metallophthalocyanine Complexes Involving Azo and Oxo Bridging Groups

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Abstract: Phthalocyanines (Pcs) have exclusive chemical, biological and physical properties including extensive π-electron delocalization with their 18 π-electron macrocyclic system. A considerable number of distinctive properties arise from this electronic delocalization which makes these compounds precious in different fields of technology. They can be easily modified with different substituents and metals that can be centered in the ring of Pc complexes. Pcs that modified in different ways have different redox properties. Because there is a strong relation between the molecular structure of Pc complexes and the electrochemical redox features.

The aim of this project is to show the effects of azo and oxo substitutions on the electrochemical properties. In order to achieve this goal, two different group of substituents that have azo and oxo bridges were attached to Pcs. By using voltammetric measurements such as Cyclic Voltammetry (CV) and Squarewave Voltammetry (SWV) techniques, electrochemical redox behaviors of azo and oxo substituted Pcs were analyzed. Furthermore, *in-situ* UV-vis spectral and associated color changes of Pc complexes were displayed during the controlled potential electrolysis of complexes at suitable constant potentials corresponding to the relevant redox processes.

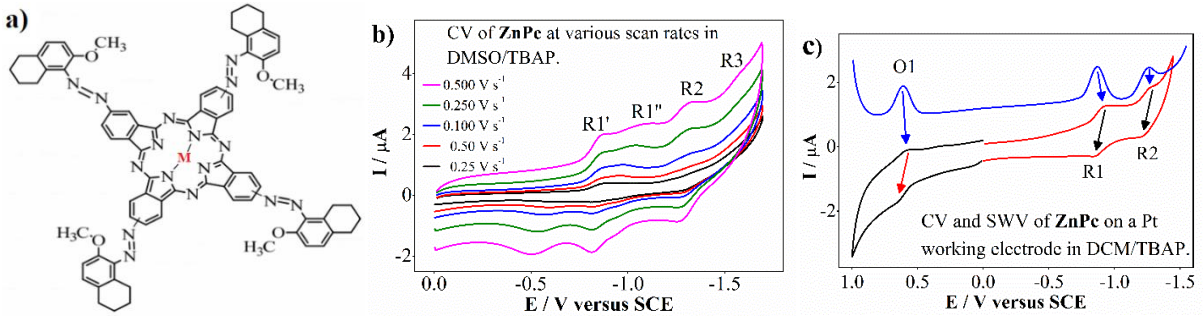

Fig.1 a) Azo Bridged Phthalocyanine Complexes (**M**: **H_2**, **Cu**, **Zn**). Cyclic Voltammograms of azo Bridged **ZnPc b)** in DMSO/TBAP, **c)** in DCM/TBAP.

Keywords: Phthalocyanine, Electrochemistry, *in-situ* Spectroelectrochemistry, *in situ* Electrocolorimetry

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Electrochemical And Spectroelectrochemical Properties of Novel Phthalocyanine Complexes Involving Thio Bridging Groups

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Abstract: Phthalocyanines (Pcs) are aromatic macromolecules which having 18 π-electrons and multiple and reversible electron transfer properties. The core of PCs is capable of coordinating almost all metal ions and this in turn enables the macrocycle to have a broad spectrum of properties. Pcs can be modified by changing synthetic procedures, the central metal and nature/number/attachment type of substituents. In that way, Pcs can be easily designed to use in different applications. These materials are important because of their interesting physical and chemical properties. The determination of the electrochemical properties of the newly synthesized phthalocyanine complexes is very important in determining their usability in different technological fields. In addition, spectroelectrochemical techniques have enabled us to detect color changes associated with redox processes of compounds. *In-situ* spectroelectrochemical and electrocolorimetric measurements help to determine easily whether these reactions are on the ring of phthalocyanine and on the redox active central metal. In this study, redox behaviours of Pcs carrying different metal centers were determined by voltammetric techniques such as; cyclic voltammetry (CV) and square wave voltammetry (SWV) in an appropriate organic solvent medium on the Pt working electrode.

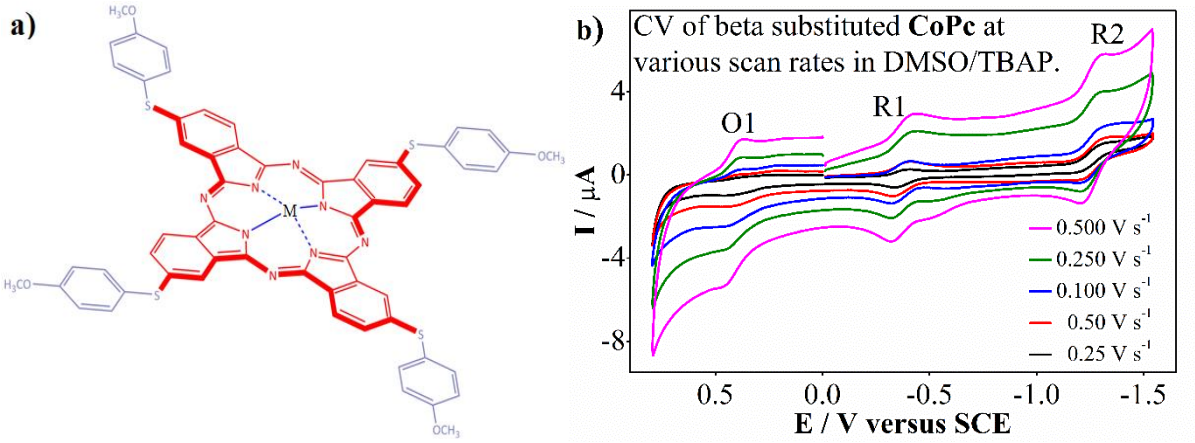

Fig.1 a) Beta Substituted Phthalocyanine Complexes (**M**: **Fe**, **Co**, **Mn, H2**, **Ni**). **b)** Cyclic Voltammograms of Beta Substituted **CoPc** in DMSO/TBAP.

Keywords: Phthalocyanine, Electrochemistry, *in-situ* Spectroelectrochemistry, *in situ* electrocolorimetry

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Electrochemical Properties of Hydroxyphenyl Coumarin Substituted Novel Metallophthalocyanine Complexes

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Abstract: It is crucial to describe characteristic redox properties of novel phthalocyanine complexes which include redox active and inactive metal centers. The behaviors of redox inactive metal centered complexes are quite similar to each other and redox active metal centered complexes have similar redox properties among themselves. The attachment of different functional groups to the phthalocyanine ring extremely changes the properties of phthalocyanines (Pcs), such as electronic, chemical and solubility properties. In order to improve solubility of phthalocyanines, coumarin groups can be attached to this ring from different positions. Research on environmentally friendly and sustainable energy systems is particularly focused on finding alternative catalysts to replace noble metals especially in the oxygen reduction reaction (ORR) and developing efficient, active and cheaper catalyst. In this context, electrochemical, *in-situ* spectroelectrochemical and electrocatalytic features of coumarin substituted phthalocyanine complexes which have been modified on electrode surfaces by carbon electrode have been intensely investigated. Therefore, the redox properties of hydroxyphenyl coumarin substituted Pcs were identified by voltammetric and *in-situ* spectroelectrochemical measurements as given Fig. 1. In addition, the catalytic performances of the compounds for ORR were tested by dynamic voltammetry measurements in the mediums similar to working conditions of fuel-cell and metal-air battery systems.

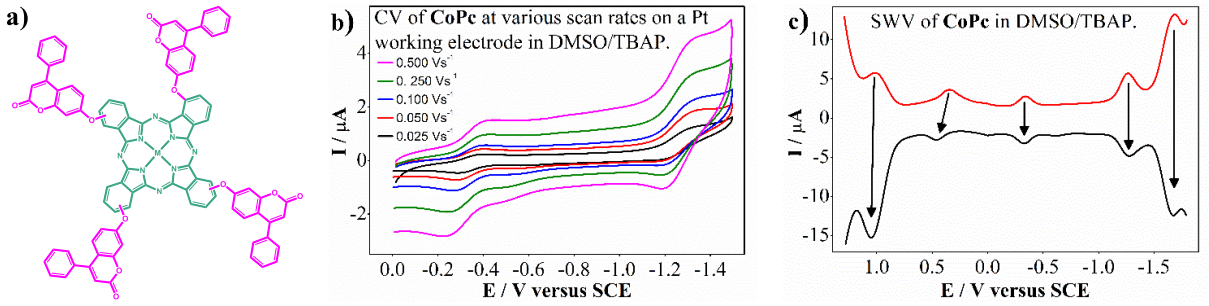

Fig.1 a) Phthalocyanine Complexes (**M: Fe, Co, Cu, Zn**) **b)** Cyclic and **c)** Square Wave Voltammograms of **CoPc** in DMSO/TBAP.

Keywords: Phthalocyanine, Coumarin, Electrochemistry, *in-situ* Spectroelectrochemistry, *in situ* Electrocolorimetry, Electrocatalytic, Vulcan, Nanomaterial, Oxygen Reduction

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Electrochemical Properties of Novel Mononuclear Metallophthalocyanine Complexes Including Tertiary Butyl and Bis (Oxy)Bis (Ethylene)Bis(Oxy) Bridging Groups

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Abstract: The redox electron transfer processes of the newly synthesized complexes should be clarified due to the strong relationship between the electrochemical responses and technological usage of these compounds in various areas. Especially, fuel cells (FC) have also been receiving great attraction to come into widespread commercial use in portable power generation for decades. However, reducing high overvoltage with cost-effective catalysts is still an unsolved problem in many battery systems. Although precious metals can effectively reduce oxygen overvoltage, alternative catalysts are sought instead of precious metals to reduce material cost.

The phthalocyanines (Pcs) have been known great candidate catalyst material as a result of their high π-electron transfer abilities, makes it an attractive alternative. Pcs can be modified by changing the central metal and attachment type of substituents on the periphery, and Pc derivatives having different properties can be easily designed in that way. The reason for the selection of Pc compounds is the rich redox properties of their metal complexes, different substituents and their advantages for the preparation of targeted materials. Thus, electrochemical measurements were performed in order to understand their possibility of the usage in technological applications.

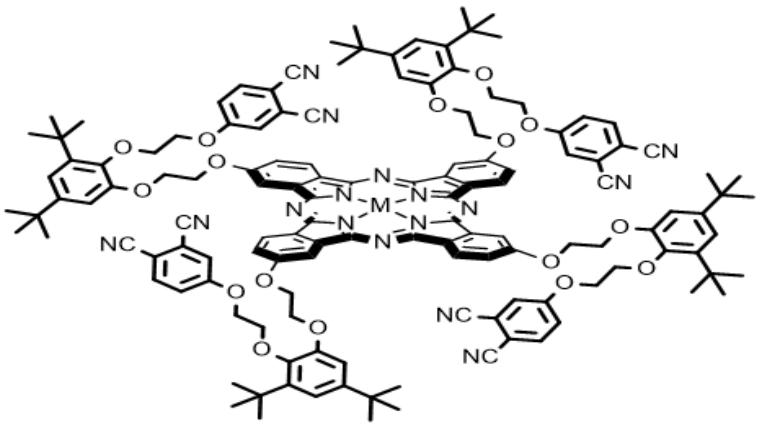

Fig. Beta Substituted Phthalocyanine Complexes (**M**:**Co**, **Zn**).

Keywords: Phthalocyanine, Electrochemistry, Redox Properties

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Electrochemical, Spectroelectrochemical and Electrocatalytic Properties of Ball-Type Thiobis Naphthalen Bridged Metallophthalocyanine Complexes

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Abstract: Although oxygen reduction reaction (ORR) lies in the hearth of many important energy systems including fuel cells and metal-air batteries, due to its sluggish kinetics, applicability of these systems requires alternative electrocatalysts to replace precious Pt-based materials.

Transition metal N_4-macrocycle complexes have long been known to be highly active for the catalytic reduction of molecular oxygen. Among various electrocatalyst in this family, phthalocyanine (Pc) complexes, especially ones that having redox-active metal centers with highly reversible and rich electron transfer abilities are the promising candidates with their high activity and low-cost. Their 18-Π electronic systems show great compatibility with carbon materials which supports essential porosity for reactive oxygen to diffuse and ensures high conductivity for the cathode of above-mentioned systems. Thus Pc-carbon binary composites regarded as promising cathode materials.

In this project, four 1,1`-Tiyobis(naphthalen-2-oxy) bridged ball-type metallophthalocyanine complexes were selected due to their dual metal centers that expected to show higher catalytic activities than mononuclear counterparts. Their electrochemical and spectroelectrochemical properties identified via electrochemical techniques such as cyclic voltammetry (CV) and square wave voltammetry (SWV). After this stage binary composites prepared with carbon materials for electrode modification and their catalytic activities towards ORR were investigated with hydrodynamic electroanalytical methods.

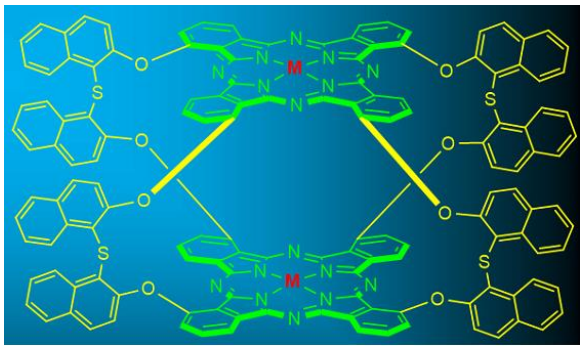

Fig. Phthalocyanine Complexes (**M:Mn, Cu, Ni**)

Keywords: Phthalocyanines, Nanomaterial, Electrode Modification, Oxygen Reduction, Electrocatalysis, Nanoparticle, Vulcan

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Electrochemical, Spectroelectrochemical and Electrocatalytic Properties of Novel Hybrid Coumarin-Phthalocyanine Compounds

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Abstract: Phthalocyanines (Pcs) are aromatic macrocyclic compounds having unique conductive, catalytic, chemical, physical and biological properties including extensive π electron delocalization. By attaching different substituents to phthalocyanines from the peripheral and non-peripheral ends, the physical and chemical properties of the complexes can be changed. Coumarins belonging to a group of compounds known as benzopyrans, have important photophysical and photochemical properties and increase the solubility of the phthalocyanine complexes to which they are binded. Pcs used in this project were obtained by binding the active group oxyphenyl coumarin to the phthalocyanine ring from the peripheral ends.

Electrochemical, spectroelectrochemical and electrocatalytic properties of these hybrid coumarin-phthalocyanine compounds were examined. The electrochemical redox properties of the novel Pc compounds involving coumarin groups have been identified by the electrochemical techniques such as cyclic voltammetry (CV) and square wave voltammetry (SWV). The color changes associated with the redox processes were also identified by *in-situ* spectroelectrochemistry and *in-situ* electrocolorimetry. The Electrochemical properties allow the determination of the compounds which have the ability to show high catalytic activity and thus, suitable for preparing electrocatalyst for oxygen reduction reaction (ORR). Electrocatalytic measurements have been made with linear sweep voltammetry and hydrodinamic rotating disc and rotating ring-disc voltammetry techniques.

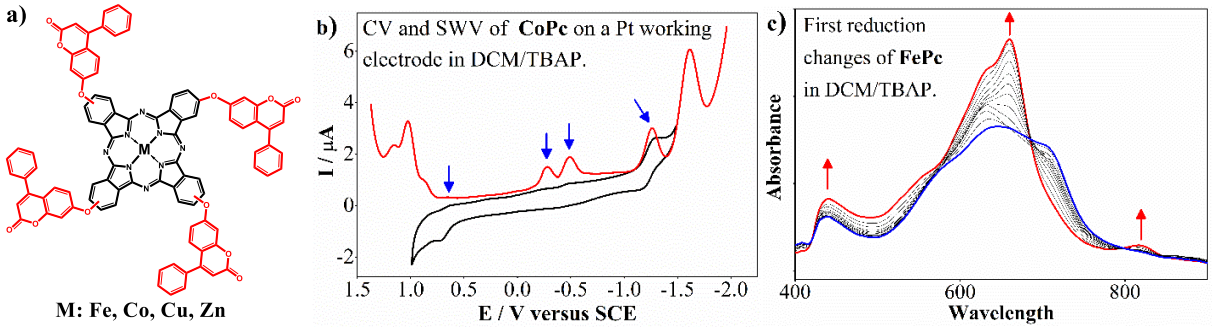

Figure:

a) Phthalocyanine Complexes

b) Cyclic and Square Wave Voltammograms of **CoPc** in DCM/TBAP and

c) Spectral Changes of **FePc** in DCM/TBAP.

Keywords: Phthalocyanine, Coumarin, Electrochemical Methods, *in-situ* Spectroelectrochemistry Electrocatalytic, Vulcan, Nanomaterial

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Electrochemical, Spectroelectrochemical and Electrocatalytic Properties of Thiobis-Napthol Substituted Metallophthalocyanine Complexes

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Abstract: Environment-friendly and sustainable energy systems are needed due to the possible energy shortage in the near future. Fuel cells have arisen great attention due to their high specific energy density, energy conversion efficiency, low to zero emissions, and high safety, which are promising for sustainable and clean energy. In addition, the metal-air batteries, especially the Zn-air battery with a theoretical energy density is much higher than that of the current Li-ion batteries, while being much cheaper and safer, are also promising systems. Oxygen reduction reaction (ORR) electrocatalysts dominates the overall performance and efficiency of these systems. As a result, developing cost-effective ORR electrocatalysts alternative to precious Pt-based materials is important for the applicability of these systems.

Phthalocyanine (Pc) complexes are one of the promising candidates that frequently investigated due to their high redox activity, chemical and thermal stability, and also their high compatibility with carbon materials. Their composites with carbon materials are highly active and valuable for the cathodes of the above-mentioned systems.

In this work, redox behaviors of 1,1`-thiobis(naphthalen-2-oxy) substituted Pc complexes were investigated by voltammetric and *in-situ* spectroelectrochemical measurements and glassy carbon electrodes (GCE) modified afterwards with MPc-carbon composites to evaluate their catalytic activities towards ORR.

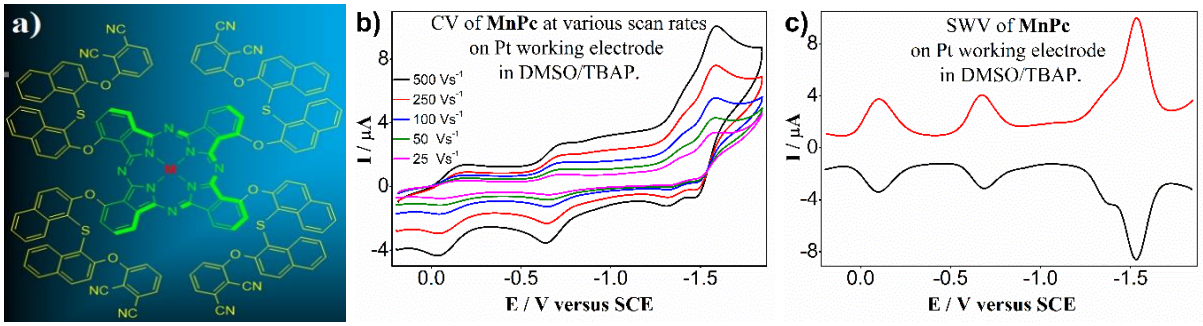

Figure:

a) Phthalocyanine Complexes (**M:Mn, Cu, Ni**)

b) Representative Cyclic and

c) Square Wave Voltammograms of **MnPc** in DMSO/TBAP.

Keywords: Phthalocyanines, Nanomaterial, Electrode Modification, Oxygen Reduction, Electrocatalysis, Nanoparticle, Vulcan

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Electrochemical, Spectroelectrochemical and Electrochromic Properties of Novel Dimethyl Coumarin-Phthalocyanine Compounds

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Abstract: Phthalocyanines (Pcs) are aromatic macromolecules with 18 π-electrons showing multiple and reversible electron transfer properties. Pc's are used in LEDs, solar cells and electrochromic display technologies due to their ability to make coordination compounds with various optical, electronic, structural and various metals. While designing redox active Pcs, they can be modified with functional groups according to the technological use target. Hybrid compounds formed by modification show rich redox properties. In this project, it is aimed to increase the solubility of Pc's, which are known to have solubility problems and whose targeted technological applications are restricted due to this problem, by adding coumarin groups to the structure. Coumarins are used in various applications thanks to increasing the solubility of the complexes they form with Pc compounds. For this purpose, unique hybrid coumarin-Pc molecules were synthesized.

In this work, electrochemical redox behaviors of hybrid coumarin-Pc molecules were analyzed via Cyclic Voltammetry (CV), Squarewave Voltammetry (SWV) techniques. In addition, color changes associated with the redox processes under constant potentials were also monitored by *in-situ* spectroelectrochemical and *in-situ* electrocolorimetric techniques with the aim of identifying the possibility of the usage of the compounds as electrochromic materials.

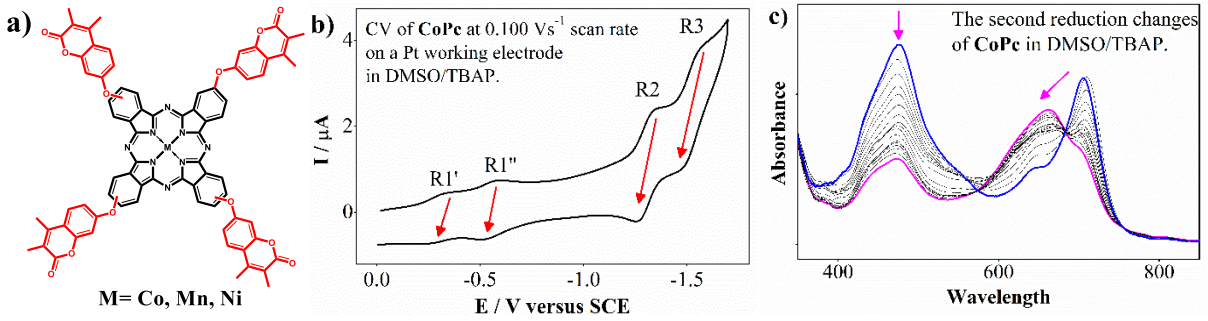

Figure:

a) Phthalocyanine Complexes

b) Cyclic Voltammogram and

c) Spectral Changes of **CoPc** in DMSO/TBAP.

Keywords: Phthalocyanine, Coumarin, Electrochemistry, *in-situ* Spectroelectrochemistry, Electrochromic

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Electrochemical, Spectroelectrochemical Properties of Non-Peripheral Tetra-3-(2,4,6-Trimethoxyphenoxy) Substituted Iron, Manganese, And Zinc Phthalocyanines

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Abstract: Phthalocyanine compounds are aromatic macrocyclic compounds with 18 π-electron system. They have been received greater interest in recent decades due to unique optical, electronic, catalytic, and structural properties. Pcs usually have known possessing well-defined subsequent reversible or quasi-reversible reduction and oxidation processes. Pcs also have wide usage areas due to their spectral properties in the visible region of the light spectrum. In addition, spectroelectrochemical techniques are also important to detect the color changes associated with the redox processes of the compounds in terms of determining the characteristic behaviors. Determination of the electrochemical properties of newly synthesized Pc complexes is important in terms of determining their usability in different technological areas.

In this study, the electrochemical redox behaviors and spectroelectrochemical properties of the 3-(2,4,6-trimethoxyphenoxy) substituted iron, manganese, and zinc phthalocyanines characterized by cyclic voltammetry (CV) and square wave voltammetry (SWV) techniques (Fig. 1). *In-situ* spectroelectrochemical and electrocolorimetric measurements support to determine whether redox behaviors are belongs to the ring of phthalocyanine and the redox active central metal.

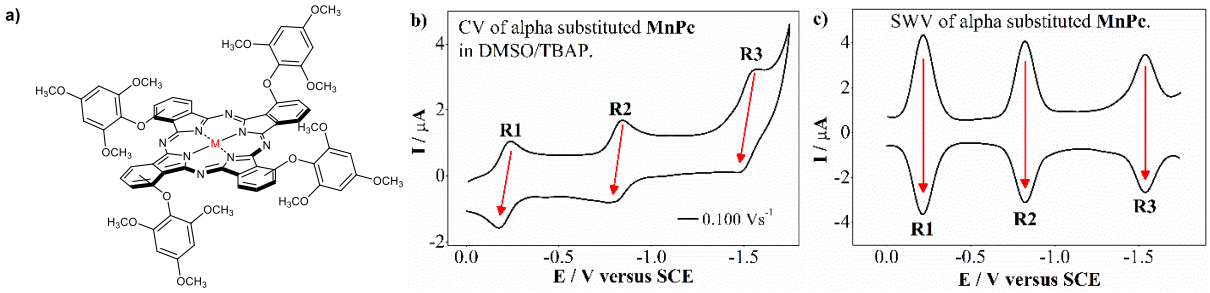

Figure:
a) Phthalocyanine Complexes (**M:**Fe, Mn, Zn)
b) Cyclic and
c) Square Wave Voltammograms of alpha substituted **MnPc** in DMSO/TBAP.

Keywords: Phthalocyanine, Electrochemistry, *in-situ* Spectroelectrochemistry

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Fabrication and Characterization of Hydroxyapatite (HAP) Doped-Biocompatible Membranes

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Abstract: Hydroxyapatite is an inorganic/ceramic material for medical, dental, and biomedical applications, because of its similar composition to the mineral phase of the human bone. The PVA is water-soluble, has high chemical and thermal stability, and has faster biodegradation properties.[1] Herein, the fabrication of membranes was carried out with hydroxyapatite (HAP) doped monolayer or bilayer ingredients including the hydrophobic and hydrophilic properties. The transparent materials of PVA/Hap/Col and PVA/PVA/Hap/Col@PVA membranes by the doctor blade method were produced, and then, the lyophilization procedures were applied for the final products.

Figure 1. Hydroxyapatite (HAP) doped membrane.

Also, the PVA/Hap/Col, PVA/ PVA/Hap/Col@PVA membranes were characterized by Infrared Spectroscopy (FT-IR), Powder X-ray Diffraction (XRD), Field Emission Scanning Electron Microscope (FESEM), Energy Dispersive X-Ray Analysis (EDX) and Mapping analyses. Thus, the newly hydroxyapatite (HAP) doped membranes will be able to be used in different applications such as medical, dental, etc. in the future.

Keywords: Membrane, Hydroxyapatite, PVA

References:

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Germanene: DFT investigation of Electronic and Optical Properties changing with Au and Cu doping

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Abstract: Germanene, is 2D allotrope of germanium and a structure like graphene, has been a remarkable material in recent years due to its unique properties such as high carrier mobility, spin-orbit coupling (23.9 eV), sp^3 hybridization, quantum spin Hall effect. Furthermore, its honeycomb lattice parameter is stable when it is possessed of low buckled in the researches. The investigation of natural impurities in the germanene structure, which was synthesized on different substrates by a wide variety method experimentally, is only one of the important problems in this material. In our study, the change in the electronic and optical properties of germanene material with gold and copper doping was investigated using Density Functional Theory (DFT). In the structure selected for the 4x4 supercell and buckled form, all calculations were calculated using Atomistix Toolkit-Virtual Nano Lab(ATK-VNL) software based on DFT. In the calculation, it was taken 9x9x1 for the k-point and 100 Hartree for the cutoff energy. Band structure, Density of State (DOS) and optical spectrum of the pristine and Au, Cu doped states of structure were investigated using the SGGA-PBE approach.

Keywords: Germanene, Density Functional Theory, doping, honeycomb

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Green Synthesis and Characterization of Tea Waste Based Silver Nanoparticles

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Abstract: The increase in the amount of waste has revealed the concepts of food safety, sustainability and environmental protection. It is important to develop new high valued products with the usage areas of wastes in the cosmetics, energy, and pharmaceutical industries. Nanotechnology is a multidisciplinary science that includes the use of nanoparticles sized between 1-100 nm in different applications. Black tea is an important beverage that is heavily consumed by people. In this study, silver nanoparticles were synthesized with green synthesis technique by using the extract obtained from the waste black tea pulp by re-extracting. The synthesized nanoparticles were characterized. Electrochemical property of the particles was also determined. It was determined that the obtained nanoparticles had absorbance at 450 nm. Then, a modified carbon paste electrode (MCPE) was prepared with synthesized silver nanoparticles and it was determined that MCPE was sensitive to hydrogen peroxide formed as a result of many enzymatic reactions by amperometric measurements. The sensitivity of the prepared MCPE to hydrogen peroxide was found to be the best at +0.4 V. The compatibility of the nanoparticles obtained with the studies to be carried out for the glucose biosensor design will be determined.

Keywords: Green synthesis, glucose biosensor, silver nanoparticles, food waste

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Investigation of Binding Interactions Between Novel Pyrazole Derivatives and Bovine Hemoglobin by Spectroscopic and Molecular Docking Studies

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Abstract: Hemoglobin is a tetramer, because of its quaternary structure, it contains grids into which small molecules such as drugs can bind. Recent findings imply that hemoglobin can serve as "super-carrier" of drugs and imaging probes by altering their pharmacokinetics through prolonging their circulation or engineering their biodistribution.

Pyrazole and its derivatives which have been proven to be effective pharmacophores for the treatment of various metabolic disorders. They are the active ingredients of a number of well-known different categories of drugs. The main method used for synthesis of substituted pyrazoles is a cyclocondensation reaction by nucleophilic addition of hydrazine to chalcone compounds containing α,β-unsaturated ketone structures.

In our study, novel pyrazole derivatives with well pharmacokinetic and pharmacodynamic features were synthesized according to their appropriate; "Absorption, Distribution, Metabolism and Excretion" properties. The compounds were synthesized according to main synthesis method, characterized by IR and NMR analysis. Binding interactions between pyrazole derivatives and hemoglobin were investigated by molecular docking and multi-spectroscopic methods. In silico and in vitro studies were evaluated; binding energies and constant, stoichiometry of pyrazoles, their conformations and interactions with hemoglobin and changes in hemoglobin's secondary structure, quenching mechanisms were determined.

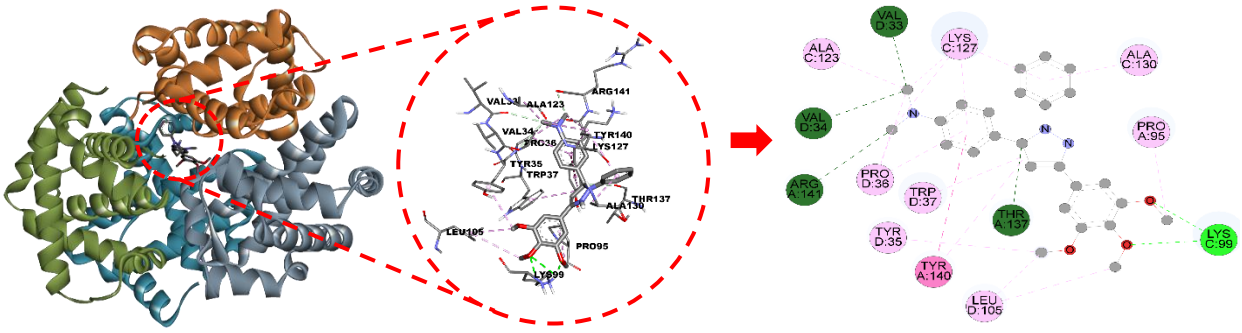

Fig: Interaction of pyrazole derivative with amino acid residues of hemoglobin active site (α1: A, α2: B and β2: D)

Keywords: drug delivery, hemoglobin, pyrazole, multi-spectroscopic measurements, molecular docking

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Investigation of Dielectric Properties of 5CB With Liquid Crystal and Crystal Doping

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Abstract: Nematic liquid crystals are widely used in imaging technologies. In this new research area nematic liquid crystals are doped with different materials to obtain new LC properties [1-3]. In this study, the dielectric properties of liquid crystal and crystal doped liquid crystal composites were compared. Dielectric properties of **5CB** (4-cyano-4'-pentylbiphenyl)**, 5CB**:**LC** and **5CB:Cr** have been investigated at room temperature. In this respect, dielectric properties of composites have been compared with **5CB**. The real and imaginary components of dielectric constant have been calculated by impedance spectroscopy measurements. The conductivity mechanisms dependence of frequency have also been calculated for all composites.

Fig. 1. Molecular structure of doping materials.

Keywords: Liquid crystal (LC), Dielectric Spectroscopy (DS), Conductivity mechanisms.

References:

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Investigation on Water Adsorption Properties of Aluminum Hydrolysis Mechanism: A DFT Study

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Abstract: Due to its high energy efficiency and environmentally friendly characteristics, hydrogen is known as one of the most ideal energy carriers and fuels [1]. In recent years, the reaction of aluminum materials with water to produce hydrogen has received significant attention owing to efficient and cheaper hydrogen generation from aluminum compared to other metals [2].

This work is a density functional theory (DFT) investigation of the detailed reaction mechanisms of the hydrolysis of water on the oxidized Al (111). We first explore the adsorption properties of all species involved as both reactants and products. We then proceed to carefully construct and calculate the energy barriers of a multiple-step reaction mechanism.

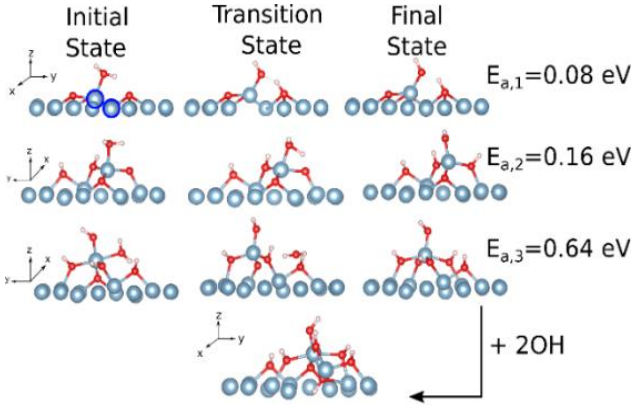

Figure 1. The reaction steps of Al hydrolysis

Water splitting potential energy profiles for each hydrolysis process and hydrogen generation on both O pre-adsorbed Al (111) and clean Al (111) surfaces are mapped out via the Nudged Elastic Band (NEB) method calculations. All calculations were conducted using the Vienna Ab-Initio Simulation Package (VASP) [3]. The activation barriers of an eight-step surface reaction mechanism (0.16 eV-0.65 eV) are compared with the experimentally estimated barrier and yield very good agreement. These results validate the proposed reaction mechanism involving the mixture of dissociated water molecules and direct surface adsorption of free OH^- radicals from the solution.

Keywords: Hydrogen Energy, Hydrolysis, Aluminum, DFT

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Liposomal Amphotericin B and Their Nanoformulations

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Abstract : Liposomal amphotericin B (LAmB) is an antifungal drug used in visceral leishmaniasis and invasive fungal infections [1]. Amphotericin B has a lipid-based structure developed from deoxycholate (DAmB), and the DAmB is also called traditional Amphotericin B. The main reason for its development is the excessive toxicity of conventional Amphotericin B [2]. Therefore, when ingested into the body, it is manifested by effects such as high fever, chills, hypertension, anorexia, nausea, vomiting, headache, and shortness of breath [3]. The LAmB is in a more advanced state of toxicity than DAmB and is more suitable for medical use. Therefore, it is to try to develop formulations with different lipid structures, and *in vitro* and *in vivo* studies are carried out by researchers [4]. These researchers also help us to understand the pharmacokinetics and pharmacodynamics of LAmB and to create more different usage areas. When combined with therapeutic doses of LamB, it can minimize damage to the kidneys, liver, and other organs, primarily using methods such as aggregation regulation and drug release to reduce toxicity further. [5]. The necessary research on this issue has not been done enough, and it continues.

Keywords: Amphotericin B, Liposomal amphotericin B, Drug

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Obtaining Physical Parameters Using BME280 Sensor and Arduino

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Abstract: In this study, the operation of sensors made of semiconductor materials with microcontroller control and obtaining physical parameters were examined. For this purpose, Arduino Uno was used as a microcontroller. The BME280 Sensor, which was developed for simultaneous reading of the pressure, temperature, altitude and humidity information of the environment, was used. Special codes were created to process the data obtained from the sensor and save it to the computer. In addition, JHD204A 20X4 LCD screen was used to display the data obtained from the system instantly. By changing environmental parameters, how they affect each other wasmeasured by the system we prepared.

Keywords: Arduino Uno, BME280 Sensor, JHD204A 20X4 LCD, Pressure, humidity, temperature

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Polyurethane Based Flexible Gel Polymer Electrolyte for Lithium-Ion Batteries

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Abstract: Lithium-ion batteries have dominated the consumer electronics market as a power source for decades, thanks to their advantageous features such as high energy density, high efficiency, light weight, portability and safety. In the application of lithium-ion batteries with liquid electrolytes, it has been reported that some serious problems such as leakage, flames and explosions occur due to the presence of highly flammable organic liquid electrolytes. The use of solvent-free solid electrolytes is the ideal way to solve the current safety issue of liquid electrolytes, but this advantage comes with significantly reduced conductivity. In order to combine the positive properties of liquid and solid polymer electrolytes, respectively gel polymer electrolytes with higher ionic conductivity and greater stability have been introduced. Polyurethane acrylate (PUA) based polymer electrolytes have been investigated for use in electrochemical energy storage applications due to their. high ionic conductivity, excellent mechanical strength, and easily controllable physical properties and high curing rate. Aliphatic Polyurethane acrylate and polyurethane methacrylate based films were prepared using ionic monomers such as Pentaerythritol tetrakis (3-mercaptopropionate) and 3-mercaptopropyl trimethoxysilane using photoinitiator and thiol-ene with solgel method. The preparation step of the bendable flexible polymer electrolytes was carried out with UV curing technology. UV curing technology, which has been used as a method in gel film preparation, has received great attention due to its various advantages such as high efficiency, light curing conditions, low capital expenditure, low energy consumption.

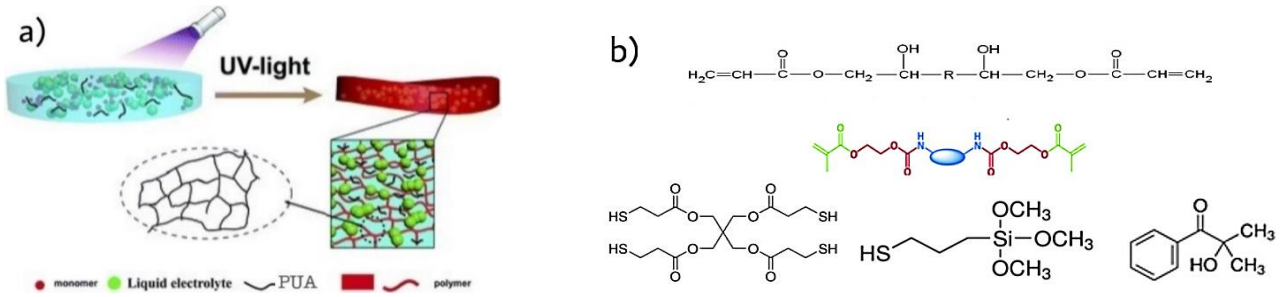

Figure:

a) Schematic representation of the preparation process of PUA-PUMA electrolyte films

b) Open structures of the chemicals used

Keywords: Lithium-ion battery, Gel Polymer Electrolyte, Energy Storage Systems, Polyurethane Acrylate, Polyurethane Methacrylate

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Preparation and Characterization of Hypericin-Loaded Chitosan Nanoparticles

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Abstract: The development of nanomaterials has cleared the door for their application as carriers in biological systems. Due to the size of the NPs and the advantages they provide, many different types of studies are being conducted in cancer biology systems. Alternative methods are being sought to alleviate the problem of lung cancer.

The goal of the study was to create nanoparticles from materials that would cause the minimum amount of harm to the body by utilizing the least number of chemicals. Chitosan is a coherent option because it is a natural and easily obtained biopolymer. Because of its anticancer effects, Hypericin (HY) was chosen as a photosensitizer. Hypericin-loaded chitosan nanoparticles (HY-CH-NPs) in A549 lung cancer cells has been evaluated.

Characterization analyses were made with dynamic light scattering (DLS), scanning electron microscopy (SEM) and The Fourier transform infrared (FTIR). According to DLS analysis, NPs were found in the expected size range (150 nm-300 nm). The SEM analysis provided confirmation of the NP's morphology. By FTIR analysis, it was shown that HY was successfully loaded. With this method, HY was loaded to chitosan NPs for the first time and a natural-based NP was demonstrated that could be used in anti-cancer studies.

Keywords: Nanoparticles, Chitosan, Hypericin, Lung cancer

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Preparation of Polybenzoxazine-Based Hydrophobic Nanocomposite Materials

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Abstract: The aim of this study is the preparation of hydrophobic nanocomposites with Polybenzoxazine (PBZ) and ethylene-propylene-diene-monomer rubber (EPDM) reinforced by nano TiO_2 and Teflon. We were prepared the polymer nanocomposite with PBZ (40%) - EPDM (40%) - nano TiO_2 (10%) - Teflon (10%) weigh ratios. Two different PBZ-EPDM polymer nanocomposites with and without sulphur have been investigated. The samples were treated at 25 °C, 100 °C, 150 °C and 180 °C curing temperatures, respectively. The samples were characterized with FTIR, UV and drop shape analyzer. The requirement of the hydrophobicity is the contact angle between the surface and water should be higher than 90°. The contact angle was measured as 101.1° for the sample with sulphur cured at 180 °C. Regarding the UV results, it was observed that the samples with sulphur heated at 150 °C showed more absorption compared to the other samples. According to the test results, relatively high contact angle measurements were observed indicating the preparation of hydrophobic polymer nanocomposites. Especially, the PBZ-EPDM polymer nanocomposite sample with sulphur, vulcanized over 150 °C exhibited better hydrophobic surface properties.

Keywords: Polybenzoxazine, nano TiO_2, Teflon, hydrophobic nanocomposite.

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Preparation of Vegetable Oil-Based Composite Coatings by UV Induced Thiol- Ene Click Chemistry and Investigation of Their Properties

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Abstract: UV-curable coatings are gaining a lot of attention due to their low energy consumption, low volatile organic chemical (VOC) emissions, low capital investments and very fast cure rates even at ambient temperature. Most of the raw materials cured with UV in previous years were prepared by petrochemicals. Since petrochemical products are non-renewable resources, they also have negative effects on environmental control. For this reason, it has gained importance in recent years to use vegetable oils in coatings cured by UV, since they are biologically renewable, have low toxicity, high usability and triglyceride structures are converted into the components of the coating in a suitable way. In this study, vegetable oil-based UV curable composite coatings will be prepared and their properties will be examined. The environmentally friendly vegetable oils, cardanol and linseed oil will be used in the coating. First of all, epoxy functional groups will be attached to linseed oil by epoxidation process. Then, these epoxy groups will be acrylated through the ring-opening reaction by acrylic acid (AELO). The functional monomer containing both thiol groups and carboxylic acid groups will be synthesized from 1,6-hexanedithiol with maleic anhydride. Oil-based formulations will be prepared by adding thiol-en/thiol-acrylate from acrylated linseed oil, cardanol and thiol components at different ratios under UV irradiation. At the same time, nanosilica (SiO2) and/or titanium dioxide (TiO2) will be added at various amounts (1%, 5% and 10%) to the formulations. The chemical, thermal and mechanical properties of the prepared materials will be examined. At the same time, coating performance tests will be carried out.

Keywords: Cardanol, Acrylated Epoxidized Linseed Oil (AELO), SiO2/TiO2 nanoparticle, UV curing composite

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Production of Carbon Quantum Dots and Their Flexible Sensor Applications

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Abstract: Diagnosing the disease from biological samples such as blood, sweat and urine plays a critical role in the treatment of the disease and the monitoring of the process. Different types of biosensor systems have been developed for accurate and sensitive detection of small marker molecules in a biological sample. Biosensor systems are analytical devices that detect target molecules using biological materials and provide the opportunity to detect different types of electrochemical, optical, mass, magnetic signals that occur during detection. Integration of biosensors, developed for the purpose of analyzing various marker molecules in vivo and in vitro, with flexible, wearable, body-embedded systems emerges as a preferred system in clinical applications.

Semiconductor quantum dots have been investigated for their tunable strong fluorescent emission properties, which enables them to be used in biosensing and bioimaging. Compared with conventional quantum dots, chemical composition, tunable fluorescent emissions, easy functionalization, physicochemical and photochemical stability makes carbon quantum dots attractive to use in technical applications.

Ways to produce inks contain carbon quantum dots and using it to print electrochemical sensors investigated. Carbon quantum dot production methods and printing parameters researched.

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Redox Properties and Oxygen Electrocatalysis of Novel Dinuclear Ball-Type Phthalocyanine Complexes Involving Tertiary Butyl and Bis(Oxy)Bis(Ethylene)Bis(Oxy) Bridging Groups

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Abstract: Metal Air Batteries achieve the highest energy densities and can also be used as rechargeable batteries with high efficiencies. However, effective catalysts are required for the reduction of oxygen from the ambient air. It is known that in addition to platinum, nanomaterials with additives such as various metals or nitrogen significantly increase the electrocatalytic effect in fuel cells and metal air batteries. To effectively use and commercialize these battery systems, alternatives to platinum must be investigated. In order to achieve this goal, various composite materials are prepared and their electrocatalytic properties are characterized. Phthalocyanines (Pcs) with the attachment of different functional groups to the phthalocyanine ring extremely changes the properties such as electronic, chemical and solubility. Recent studies showed that ball-type Pc involving redox-active metal centers display high catalytic activity for dioxygen reduction.

These works focus on the suggesting new oxygen electrocatalysts that containing ball-type Pcs. So as to suggest new electrocatalysts, electrochemical and *in-situ* spectroelectrochemical properties of Pcs were investigated by voltammetric techniques. Also, the electrocatalytic features of carbon-based ball-type Pcs being modified on electrode surfaces were explored by dynamic voltammetry measurements in the mediums similar to working conditions of Fuel Cell and Metal Air Battery Systems.

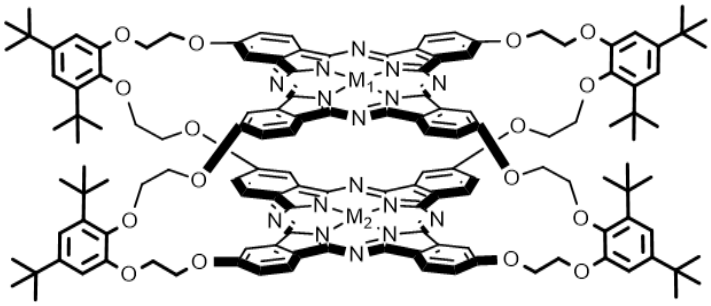

Fig.1 Beta Substituted Ball-Type Phthalocyanine Complexes (**M**: **Co**, **Zn**).

Keywords: Phthalocyanine, Ball-Type Phthalocyanine, Electrochemistry, Electrocatalyst, *in-situ* Spectroelectrochemistry, *in-situ* electrocolorimetry, Vulcan, Nanomaterial, Oxygen Reduction

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Redox Properties of New Manganese Phthalocyanine Complexes Including Methoxy and Thio Bridging Groups

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Abstract: Phthalocyanines (Pcs) have electronic, electrical, electrochemical and optical properties that are very interesting and vary widely on the scale due to their conjugated 18-π electron systems. They are also physically and chemically stable compounds. Because of their specific properties, these compounds find many applications in the technological fields. Those compounds can be used for high-technological applications owing to their redox and spectral properties in the visible part of the light spectrum. Altering the metal center and substituents of those type complexes easily affects their physicochemical, optical, electrocatalytic and electrochemical properties. Thus, it is important to determine the electrochemical responses of the newly synthesized complexes to decide their possible application in different technologies.

In this research, in order to understand and to show substituents effects on the redox and specrochemical properties, manganese metal centered Pcs with different substituents analyzed. Their electrochemical and spectrochemical properties were identified by voltammetry, *in-situ* spectroelectrochemistry and *in-situ* electrocolorimetry. Electrochemical redox behaviors of Pcs were analyzed by using cyclic voltammetry (CV) and square wave voltammetry (SWV). Furthermore, *in-situ* spectroelectrochemistry and *in-situ* electrocolorimetry measurements were carried out to determine whether the reduction and oxidation reactions of the compounds occur on the phthalocyanine ring or in metal center.

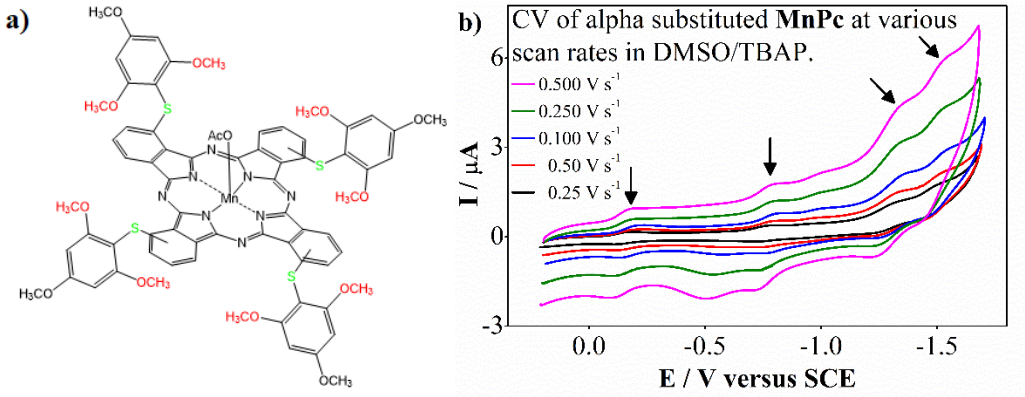

Figure:

a) Alpha Substituted Manganese Phthalocyanine Complex.

b) Cyclic Voltammograms of Alpha Substituted **MnPc** in DMSO/TBAP.

Keywords: Phthalocyanine, Electrochemistry, *in-situ* Spectroelectrochemistry

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Redox Properties of New Metallophthalocyanine Complexes Including Methoxy and Azo Bridging Groups

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Abstract: Phthalocyanine is a planar and fully aromatic macrocycle having 18-π electronic system. The central part of the molecule consists of four nitrogens directly involving complexation, and two imino hydrogens. The core is capable of coordinating almost all metal ions and this in turn enables the macrocycle to have a broad spectrum of properties. If it is considered that electrophilic and nucleophilic substitution reactions can easily be applied to aromatic systems, phthalocyanines (Pcs) also have a great range of substitution opportunities. Addition of several substituents to the peripheral and/or non-peripheral positions of Pcs, along with inclusion of several metals into the core, specially designed macrocycles are possible upon application. Pcs are stable molecules; therefore, their terminal functional groups can be utilized in several functional group conversion reactions. Reactivity of terminal groups is another factor increasing the functionality of phthalocyanine molecules. In this study, by using electrochemical and in-situ spectroelectrochemical measurements in non-aqueous media, electron transfer properties of azo substituted Pcs were analysed. *In-situ* spectroelectrochemical analyses were utilized to support electrochemical measurements. Metals based and phthalocyanine ring-based reduction and oxidation electron transfer processes were observed via voltammetric techniques.

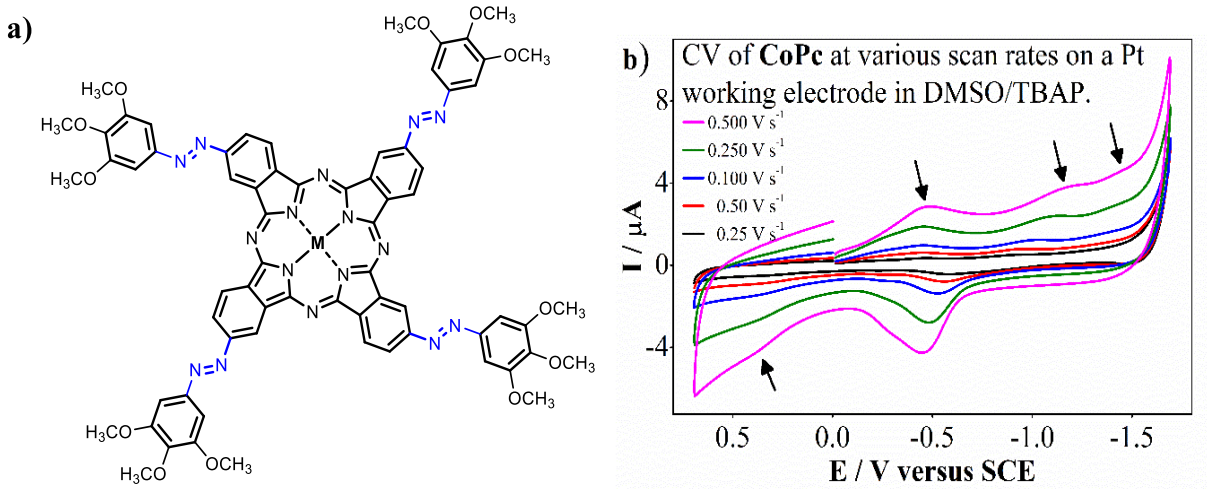

Figure:

a) Scheme of Phthalocyanine Complexes (**M**:**Fe**, **Co**, **Mn, H2**, **Ni**, **Zn**).

b) Cyclic Voltammograms of **CoPc** in DMSO/TBAP.

Keywords: Phthalocyanine, Electrochemistry, in-situ Spectroelectrochemistry, in situ Electrocolorimetry

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Redox Properties of Peripheral Tetra-3-(2,4,6-Trimethoxyphenoxy) Substituted Iron, Manganese, and Zinc Phthalocyanines

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Abstract: Phthalocyanines (Pcs) are complexes that have macro aromatic molecule structure that was used as a by-product in the early 20th century. Pcs have extensive π-electron delocalization with their 18 π-electron macrocyclic system. A considerable number of distinctive properties arise from this electronic delocalization which makes these compounds precious in different fields of technology such as electrochromic materials and displays, electrochemical energy conversion and storage systems. They can form coordination complexes with almost all metals in the periodic table. Pcs complexes are among the most versatile and functional dyes for supramolecular structures displaying characteristic high absorptions properties and well-defined subsequent electron transfer processes as the prerequisite for optoelectronic thin film devices. Changing the substituents attached to the rings and/or the central metal often causes a significant change in the electrochemical and physicochemical properties of phthalocyanines.

The aim of this study is to investigate the redox behavior of newly synthesized Pcs. Therefore, 3-(2,4,6-trimethoxyphenoxy) substituted newly synthesized metallo Pcs at peripheral position have been investigated by cyclic voltametry (CV) and square wave voltametry techniques (Fig. 1). In addition, *in-situ* spectroelectrochemical and *in-situ* electrocolorimetric measurements are discussed. These analyses support the determination of the redox properties of the Pcs.

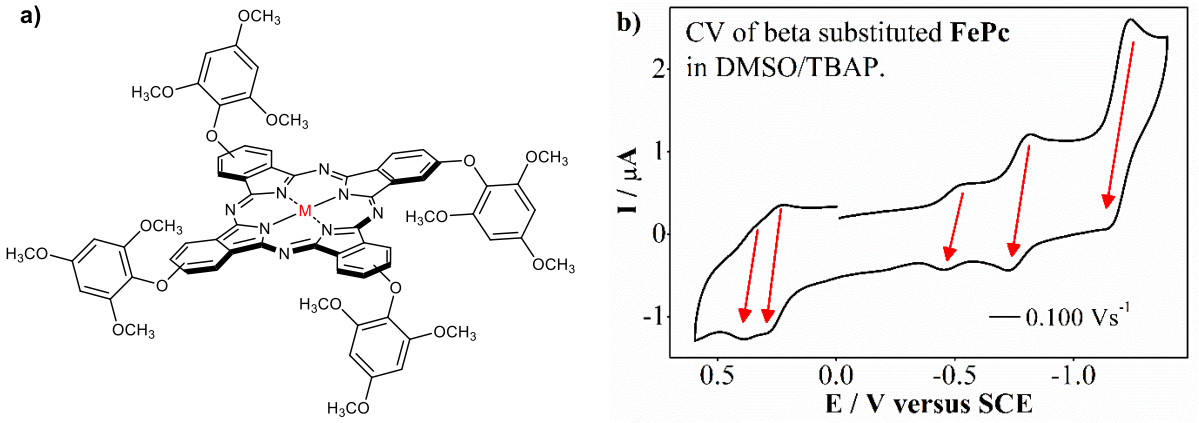

Figure:
a) Phthalocyanine Complexes (**M:** Fe, Mn, Zn)
b) Cyclic Voltammogram of beta substituted **FePc** in DMSO/TBAP.

Keywords: Phthalocyanine, Electrochemistry, in-situ Spectroelectrochemistry

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Regulation of Biosynthetic Activity of *Inonotus Obliqus* (Ach.:Pers.) Pilát Using Colloidal Solutions of Biogenic Metal Nanoparticles and Low-Intensity Laser Radiation.

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Abstract: In our earlier studies we demonstrated the biological effects of low-intensity laser radiation and colloidal solutions of Ag (AgNPs), Fe (FeNPs), and Mg (MgNPs) nanoparticles on the growth and biosynthetic activity of the medicinal macromycete *Inonotus obliquus*, which is a source of antioxidant, hepato-, chemo-, and radioprotective and antitumor components. In this work, we have studied the complex effect of colloidal nanoparticles Ag (AgNPs), Fe (FeNPs) and Mg (MgNPs) and low-intensity laser radiation of a long wavelength of 488.0 nm at a dose of 230 mJ/cm^2 on the growth characteristics and biosynthetic activity of *I. obliquus*. Irradiation of mycelium in the medium with NPs reduced the growth activity of mycelium induced by NPs in all variants of the experiment by 14.0-45.5%.Irradiation of mycelium with FeNPs in the indicated regime inhibited the synthesis of endopolysaccharides by 1.7 times and increased exopolysaccharides twice. In general, the use of low-intensity laser radiation for the treatment of seed mycelium with FeNPs is impractical to produce polysaccharides. Irradiation of mycelium with MgNPs induced a sharp increase in polysaccharides in the culture liquid (20 times).

Irradiation of the seed mycelium of *I. obliquus* on the medium with AgNPs increased the synthesis of flavonoids by 3.14 times. High yield of melanin was detected with the combined use of MgNPs and irradiation (26%).

Keywords: Inonotus obliquus, metal colloidal nanoparticles, low-intensity laser radiation, biosynthetic activity

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RGO and Pd(II) Immobilization on Oxidized Copper Foil for Biosensor Applications

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Abstract: A biosensor is often defined as an analytical device that converts a biological response into a processable and measurable signal [1]. Electrochemical biosensors such as glucose biosensors have many advantages over other types of biosensors in terms of cost, sensitivity, and real-time sampling capability [2]. In this study, the reduced graphene oxide (RGO) and palladium(II) acetate (Pd(II)) compounds were immobilized by sonication methodology on oxidized copper foil (CFS). And, the fabricated RGO/Pd@CFS material was characterized by Powder X-ray Diffraction (XRD), Fourier-Transform Infrared Spectroscopy (FT-IR) and Field Emission Scanning Electron Microscope (FESEM), Energy Dispersive X-Ray Analysis (EDX) analyses. Moreover, the electrochemical performance of the RGO/Pd@CFS working electrode was carried out in the glucose/gluconolactone reaction as a biosensor application. There is a potential for the fabrication of this type of working electrodes in the future and their use as biosensors.

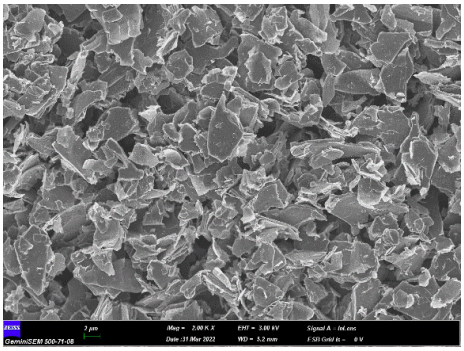

Figure-1. FESEM image of RGO/Pd@CFS working electrode

Keywords: Glucose, Biosensor, Working Electrode.

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Solar Cell Apparatus Without Profile

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Abstract: Nowadays, Usage of the renewable energy sources by people has accelerated due to their orientation to clean energy. Solar panels are one of the clean energy sources that convert solar energy into electrical energy. Currently, solar energy system projects on sandwich panel type roofs are carried out using classical methods. Considering the labor operations and material costs, these methods are not the only solution to obtain clean energy. As the number of parts in the assembly process increases, the probability of a problem also increases. Another issue is that the solar energy system to be installed on the roofs carries the wind load. The load-bearing value of the fasteners is found with the tensile test kit after the apparatus is mounted on the pitch of the roof panel. By determining the wind load, the safety factor of each apparatus can be calculated.

As a result of a double-lock development that obtained as a result of this project comparing with the standards, both ease of assembly and more durable systems has been obtained.

Our project aimed to increase the output of more durable products, decrease the costs and increase the environment-friendly buildings.

Keywords: solar compatible, solar energy system installation, wind load

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Solvatochromism of Nanomaterials

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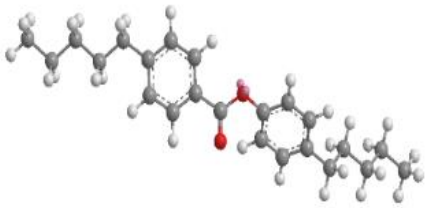
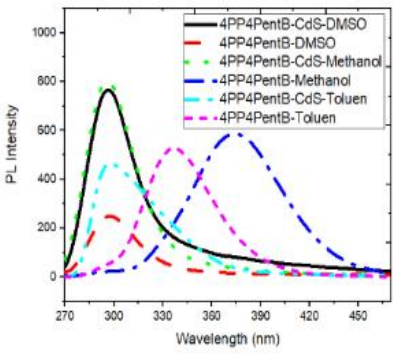
Abstract: Liquid crystals are unique materials because their molecules flow in a long-range order can self-organize, and are anisotropic in optical, electrical, and magnetic properties. While experimental studies show that nanoparticles can improve the properties of liquid crystals, they can also cause negative effects such as increased dielectric losses. In addition, factors affecting the properties of nanoparticle liquid crystals such as dipole-dipole interactions and photochemical reactions were investigated. So, the optical properties of materials called semiconductor nanoparticles, which are nanometer in size, vary depending on their size. Nanoparticles can change the order parameters of liquid crystals. Depending on the structure and properties of liquid crystal molecules, they can interact with nanoparticles and cause their fluorescence to change. [1-3] In this study, we have been studied fluorescence spectra of nanomaterials to be composed of 4-Pentylphenyl 4-Methoxybenzoate (4PP4MetoxB), 4-Pentylphenyl 4-Pentylbenzote (4PP4PentB), and 4-Pentylphenyl 4-(Octyloxy)Benzoate (4PP4OctoxB) with ZnS, CdS and CdSe nanoparticles in solvents having different properties.





In the figure, the 4PP4PentB molecule is seen and the fluorescence bands of this molecule in the solvent medium are given in the graph on the right. Solvatochromic shifts were observed in nanomaterials in our study.

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Syhthesis of Platinum Nanotubes for Hydrogen Sensor Applications

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Abstract: In this report, hydrogen sensing properties of platinum (Pt) nanotubes that synthesized by using ZnO nanorod template are investigated depending on temperature and gas concentration. Firstly, ZnO nanorods were produced by hydrothermal method on ZnO seed layer coated glass substrates using equimolar (0.01 M) zinc nitrate hexahydrate and methenamine at 90 °C for 3 hours. Then, Pt thin film with approximately 50nm are coated on ZnO nanorods by using magnetron-sputtering method. In order to obtain Pt nanotubes, ZnO nanorods are removed in a 5 % hydrochloric acid solution at room temperature for 5 hours, and then the obtained Pt nanotubes are rinsed with distilled water and dried at 50 °C for one hour. The structural properties of Pt nanotubes are characterized by XRD, SEM, EDS and XPS techniques. It is observed that Pt nanotubes with pore diameter of about 30nm are obtained on all over the surface. Resistive hydrogen gas sensing properties of Pt nanotubes are measured with two silver contacts in the temperature range from room temperature to 100 °C. The sensitivity of Pt nanotubes for 1% hydrogen is observed as 3 at room temperature and the hydrogen sensing mechanism of the nanotubes could be explained with surface scattering phenomenon. The detailed hydrogen gas sensing properties of Pt nanotubes will be discussed depending on temperature, and gas concentration.

Keywords: Platinum, Nanotubes, Hydrogen sensor, Resistive sensor, ZnO nanorod template.

Acknowledge: This study was partially supported by The Scientific and Technological Research Council of Türkiye (TUBITAK) with a project number of 121M681 and Inonu University with a project number of FYL-2022-2851.

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Synthesis and Characterization of $Cu_2Mo_6Se_8$ and $Fe_2Mo_6Se_8$particles

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Abstract: The field of ternary molybdenum chalcogenides $M_xMo_6T_8$ (M being the cation and T the chalcogen) - also known as Chevrel phases has experienced a recent surge in interest owing to the new revelations about their contributions as low-cost alternatives to conventional energy conversion materials. Since last few decades, these Chevrel phases have continued to captivate the research community with a wide range of outstanding physical and chemical properties [1-2].

In this study, selenium-based $Cu_2Mo_6Se_8$ and $Fe_2Mo_6Se_8$Chevrel phases were obtained by a facile solid-phase synthesis at 1000 °C (depending on composition), in vacuum oven. The produced chevrel phases were characterized by X-ray diffractometer (XRD), Scanning electron microscopy (SEM), and UV-vis-NIR spectrophotometer. Our results showed that single phase $Cu_2Mo_6Se_8$ and $Fe_2Mo_6Se_8$particles have Rhombohedral crystal structure. The band gaps of nanocrystals were calculated to be around 1.92 ($Cu_2Mo_6Se_8$) and 2.02 ($Fe_2Mo_6Se_8$) eV from UV-vis-NIR spectra. This is the first time that earth abundant elements have been used to control the composition dependence optical properties of $M_xMo_6T_8$ particles for efficient energy conversion.

Keywords: Chevrel Phase, $Cu_2Mo_6Se_8$ and $Fe_2Mo_6Se_8$

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Synthesis and Characterization of New Alpha-Substituted Cobalt Phthalocyanines with Phenoxy Groups Containing Electron Withdrawing or Electron-Releasing Groups

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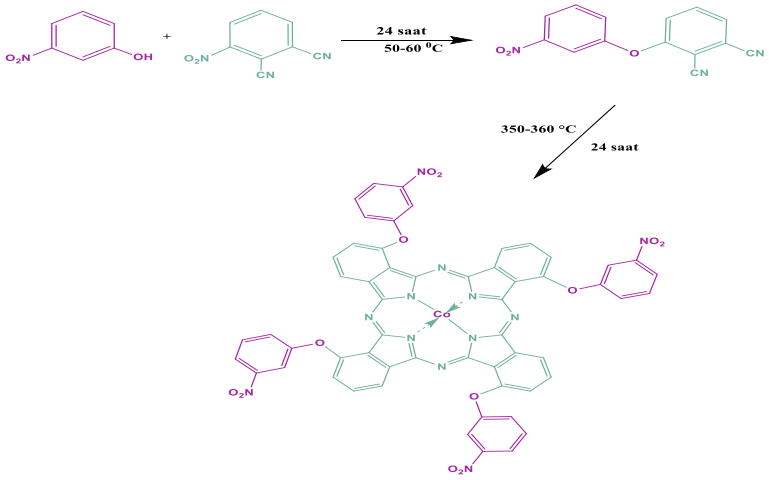
Abstract: Phthalocyanines (Pcs) are a class of macrocyclic compounds possessing a highly conjugated − 18 π electron system, intensely blue-green-colored. Phthalocyanines (Pcs) display a number of unique properties, when modified by substituent or metal change. Due to their remarkable chemical, mechanical, and thermal stability MPcs have become popular for a multitude of scientific and technological applications. Pcs have been used in various fields such as electrocatalyst, Langmuir–Blodgett films, liquid crystals, nonlinear optics, electrochromism in display devices, chemical sensors, optic keys, photovoltaic solar cells, light emitting devices, organic field-effect transistors, and photodynamic cancer therapy.



Scheme: Phthalocyanine Synthesis

In this study, the effect of electron withdrawing or electron releasing groups on the spectral, physical and chemical properties of CoPc were investigated in Pc compounds that have electron withdrawing or electron releasing groups as distant substituents. Alpha substituted phthalonitrile derivative was obtained by using meta-nitrophenol and 3-Nitrophthalonitrile, and CoPc has been achieved by using the starting compounds. After the phthalocyanine compound were purified and characterized by classical methods, their solubility, UV–Vis and FT-IR spectroscopy studies were performed, and it was revealed how the effects of electron withdrawing and releasing groups changed the spectroscopic properties of phthalocyanines.

Keywords: Phthalocyanine, Alpha Pc, Synthesis, Nitrophenoxy, Characterization

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Synthesis and Characterization of New Type Zn, Co Containing Homo Mono Nuclear Phthalocyanines, Investigation of Electrochemical and Spectroelectrochemical Properties of Metal Difference

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Abstract: Phthalocyanines and their metal complexes have extremely stable and interesting electronic, electrical, electrochemical and optical properties because they have a conjugated 18-electron system. Due to their specific properties, these compounds are used in many applications in technological fields such as dyestuffs, conductive materials, optical/electronic/optoelectronic materials and devices, sensors, photodynamic therapy, electrocatalysis, electrochromism, photovoltaic devices, and electrochemical cell/battery systems [1-3]. They attract attention due to their wide usage area.

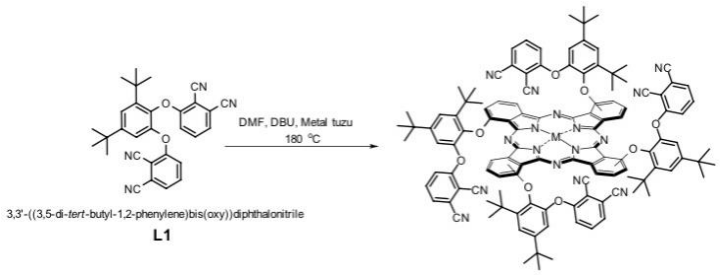

Fig.1 Alpha Substituted Phthalocyanine Complexes (**M**:**Co**, **Zn**).

Phthalocyanines are used as catalysts due to their high π-electron transfer properties, and Pcs with different properties can be obtained by changing their substituents and central metals. In this study, using 3,3'-((3,5-di-tert-butyl-1,2-phenylene) bis(oxy))diphthalonitrile with different core metals (Co (II), Zn (II)) and mononuclear (MPc type) complexes were synthesized and characterized. At the same time, its electro-spectro and catalytic properties were measured. Thus, electrochemical measurements were made to understand the possibilities of use in technological applications.

Keywords: Phthalocyanine, mono nuclear, synthesis, characterization, Electrochemistry, Redox Properties

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Synthesis and Characterization of PEO/$Li_{1+X}Al_xTi_{2-X}(PO_4)_3$ Flexible Composite Solid Electrolyte for Solid-State Li Batteries.

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Abstract: As it is increasingly seen that lithium-based batteries are dangerous, expensive and insufficient for the growing power needs in the future, lithium solid-state batteries that use solid electrolytes instead of liquids have begun to be studied as a result of the search for low-cost, lightweight, safe, high-energy density solid batteries. Solid state batteries are formed by replacing the liquid electrolyte (and separator) in the lithium-ion battery with a solid with high ionic conductivity, which does not contain a liquid component.

In this study, it was aimed to increase the ionic conductivity of solid-state electrolytes obtained by making composites with PEO polymer electrolyte and LATP solid electrolyte to produce flexible NASICON type $Li_{1+x}Al_xTi_{2-x}(PO_4)_3$ (LATP) material. In this way, it is intended to prevent dendrite formation at the electrolyte-electrode interface in a solid-state battery. The crystal structure, morphological properties and Li^+ ion conductivity of the synthesized flexible composite electrolyte was investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM), electrochemical impedance spectroscopy (EIS) techniques, respectively.

Keywords: Flexible Solid Electrolytes, Solid-State Lithium Batteries, LATP electrolyte, PEO polymer

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Synthesis and Characterization of Polydimethylsiloxane Nanocomposites

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Abstract: In this study, basic pumice and scoria volcanic rocks, the effects of which have not been studied before, and nano silver and multi-walled carbon nanotubes, which are frequently added filling materials, are added to the polydimethylsiloxane elastomer, which has many uses due to its flexibility, non-reactivity, durability and transparency. The effects of elastomer materials on these materials were investigated. In addition, the same materials were added to the oil form of PDMS without elastomer and compared with the elastomerized form. While basic pumice and scoria slightly increased the thermal properties of PDMS, they did not affect its electrical properties (insulation) at all and completely eliminated its transparent property. MWCNT has increased the thermal and electrical properties of the elastomer, made the thermally and electrically insulating elastomer conductive. The nano-sized silver had no electrical effect on the elastomer. Its inertness was proven only by the fact that the FTIR spectra were similar to the peaks of pure PDMS. It has been observed that the use of PDMS polymer in the form of silicone oil improves the electrical properties of the polymer compared to the elastomer form, and the filling materials basic pumice and scoria further improve this feature. As a result, it has been seen that basic pumice and scoria can be added to the inert PDMS, which has no harm in terms of health, instead of dyestuffs, and it can increase the usage areas of silicone oil in the form of pastes that will not be deformed over time and can be applied to all kinds of surfaces, since it can be mixed with silicone oil at very high percentages.

Keywords: pumice, scoria, polydimethylsiloxane, transmittance, SEM-EDX.

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Synthesis and Spectroscopy of New Anthraquinone Sciff Base Dye

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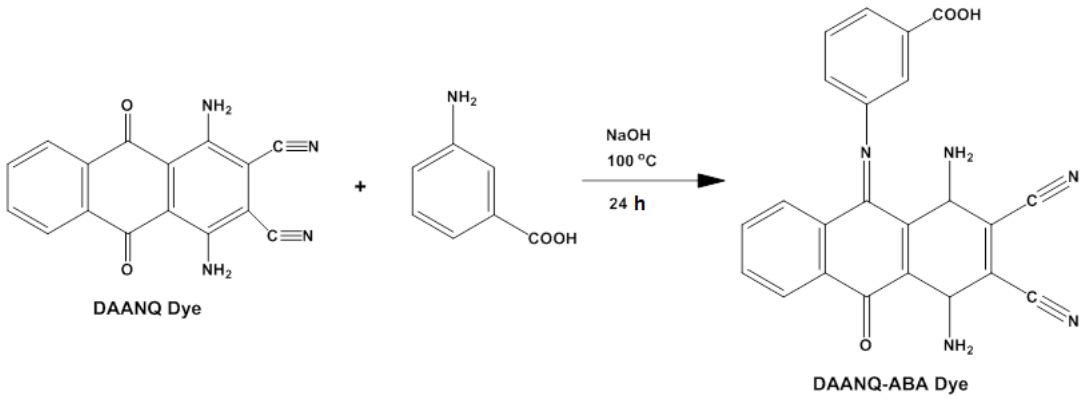
Abstract: In order to prepare a new Schiff base anthraquinone compound, 1,4-diamino-2,3-dicyano-9,10-anthraquinone (DAANQ) was reacted with 3-amino benzoic acid under basic conditions at 100 ºC for 24 hours. A red color solid dye product (DAANQ-ABA) was isolated after the reaction. The product was characterized by using MS, UV-Vis. absorption, FT-IR and fluorescence spectroscopy. The DAANQ-ABA Schiff base dye solution in methanol showed two absorption peaks at 523 nm and 556 nm wavelengths. The methanol solutions of prepared new anthraquinone dye also exhibited strong red color emissions. It was seen that the band gap energy of the aromatic anthraquinone dye has been increased after the formation of a Schiff base structure.

Keywords: Schiff base, anthraquinone, fluorescence dye, spectroscopy



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Synthesis of Chevrel Phase Catalysts and Investigation of Their Electrocatalytic Effects on Alcohol Oxidation

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Abstract: Fuel cells are one of the most important energy conversion technologies of the future. Fuel cells are electrochemical devices that convert chemical energy directly into electrical energy through electrochemical reactions. Alcohols are an alternative fuel for fuel cells that can be used in atmospheric conditions. Alcohols such as methanol and ethanol, which stand out with their low molecular weights and high energy densities, have many advantages over other fuels with these properties.

Pt or platinum alloy is a popular catalyst for fuel cells, so the catalyst layer is a significant fraction of the cost for a fuel cell. In addition to its high cost, the use of platinum catalysts causes various problems such as being extremely sensitive to impurities and decreasing its strength in the presence of water.

In this study, it is aimed to synthesize alternative, more economical and more effective catalysts to the platinum catalyst, which directly constitutes a large part of the cost of the alcohol fuel cell and has activation problems in the alcohol oxidation reaction. For this purpose, environmental phases ($Cu_2Mo_6S_8$, $Fe_2Mo_6S_8$, $Mn_2Mo_6S_8$), which are predicted to exhibit remarkable electrocatalytic activities in alcohol oxidation, were synthesized and their electrocatalytic properties were investigated.

Keywords: Energy, Chevrel Phase, Catalysts, Electrocatalytic Properties

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Synthesis, Characterization and Electrochemical Properties of New Ball-Type Phthalocyanine Compounds

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Abstract: Phthalocyanines have heterocyclic biaromatic systems containing 18 pi electrons, consisting of four iminoisoindoline units in which pyrrole groups are conjugated to benzene rings and bridged by azanitrogens [1]. Metal-free and metallic phthalocyanines are used in many applications in modern technological fields with their interesting properties such as high thermal and chemical stability, effective light absorption in the near infrared region, and both semiconductor and photoconductive properties [1-3].

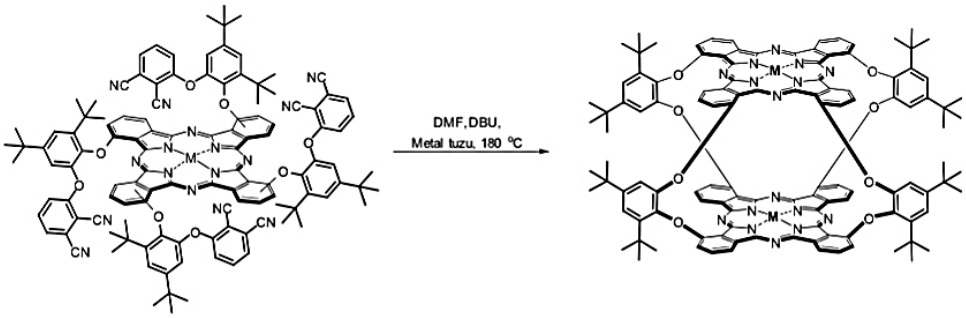

Fig.1 Alpha Substituted Phthalocyanine Complexes (**M**:**Co**, **Zn**).

In this study, firstly, 3,3'-((3,5-di-tert-butyl-1,2-phenylene)bis(oxy))diphthalonitrile compound was synthesized by nucleophilic aromatic substitution, and the metal dinuclear ball was adjusted by adjusting the conditions and the ligand/salt ratio. type (M2Pc2 type) phthalocyanine complexes were synthesized and characterized, their electro-spectro and catalytic properties were investigated.

Keywords: Phthalocyanine, di nuclear, synthesis, characterization, Electrochemistry, Redox Properties

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The Effect of Expanded Perlite as an Alternative Reinforcing Mineral Filler on EPDM Rubber Vulcanizates

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Abstract: Incorporation of mineral fillers into polymeric matrices is one of the common ways to improve physical and mechanical properties of polymers. Using expanded perlite (EP), which is naturally occurring inexpensive mineral, as a sustainable filler in rubber compounds is promising regarding its low environmental impact as well as relatively low price. In this study, ethylene-propylene- diene-monomer rubber (EPDM) based rubber compounds were prepared with various amounts (5, 10 and 15 phr) of EP. Effect of EP concentration on rheological properties and cure characteristics of EPDM rubber compounds were investigated. Vulcanizates obtained from EP containing EPDM compounds were also tested in terms of crosslink density, physical and mechanical properties. Results showed that EP incorporation could provide considerably higher crosslink density, tensile strength, and elongation at break whereas slight changes were measured for the other indicative properties. This improvement was more pronounced in the case of 10 phr and above EP incorporation.

Keywords: Expanded perlite, EPDM rubber, Crosslink density, Mechanical properties, Mineral filler

Acknowledge: Authors gratefully acknowledge the financial support of TÜBİTAK under the framework of TUBITAK-2244 Industrial PhD Scholarship program and project number 119C120.

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The Effect of Natural Hemp Fiber on Rubber Compounds

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Abstract: In recent years there has been an increasing interest in searching for environment-friendly alternatives to fossil fuel-based reinforcement material. Natural fibers are widely used as reinforcement materials, especially in polymeric materials, due to their renewable and sustainable production, eco-friendly, easy to process, good mechanical properties, and low density. In this study, natural rubber (NR) based rubber compounds were prepared with various amounts (0, 5, and 10 phr) of ground hemp fiber from Black Sea region in Türkiye. Moreover, an alkali treatment was applied to the fiber to investigate the effect of the surface modification of the fiber. The prepared compounds were tested rheologically and mechanically. The test results showed that the NR compound containing alkaline treated fiber (10 phr) had better mechanical properties than the others.

Keywords: Natural rubber (NR), hemp fiber, alkali treatment

Acknowledge: Authors gratefully acknowledge the financial support of TUBITAK under the framework of TUBITAK-2244 Industrial PhD Scholarship program and project number 119C120.

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The Effects of Thermal Annealing at Different Temperatures on Some Electrical Characteristics of Mo/n-Si Schottky Diodes

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Abstract: The Mo-n-Si Schottky diode manufactured using the magnetic scattering method was subjected to annealing at 300°C, 400°C, 500°C. Diode parameters were calculated separately from the I-V and C-V characteristics for the non-annealed and heat-treated state of the structure. As a result of the measurements, the ideality factor (n), barrier height (Φb) and series resistance (Rs) values were calculated. n and Φb were calculated as 2.36 and 0.69 eV for the non-annealed sample. After annealed at 300ºC, 400ºC, and 500ºC, n and Φb were found as 2.20 and 0.70 eV, 1.63 and 0.73 eV and 1.49 and 0.74 eV, respectively. In addition, the energy density distribution profiles of the interface states for different annealing temperatures were investigated. Thus, the changes made by the heat treatment in the diode parameters were determined.

Keywords: Termal annealing, Schottky Barrier Diode, n-type Si.

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The Investigation of Complex Dielectric, Complex Electric-Modulus, Loss-Tangent, and ac Conductivity (Σ) at Different Frequency of Au/n-Si Structures with Different Doping-Level Graphene into PVA Interfacial Layer

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Abstract: In this study; the real/imaginary components of complex-dielectric (ε′, ε”), complex electric-modulus (M’, M”), loss-tangent (tanδ), and ac-conductivity (σ) of the Au/n-Si (MS) structure with pure, %3, and %5 graphene-doped PVA interlayer for various-frequencies (1,10,100, and 1000 kHz) were extracted from the impedance-measurements (Z-V) in voltage range of ±6V and compared each other. Experimental results are indicated that all these parameters are strong function of frequency as well as electric field. The changes in these parameters are quite large at small-frequencies due to the existence of interface/surface traps (N_{ss}), surface or dipole polarization. The observed peak in the ε’-V and ε”-V curves and shift its position is the result of reordering/restructuring of charges at traps under electric-field. Therefore, both an excess dielectric-constant/dielectric-loss may be supplied to the real-value of them at low frequencies. But, at high-frequencies, N_{ss} and dipoles have not enough-time to follow the alternating-signal and to rotate themselves, respectively. While N_{ss} were found effective in depletion-region, but series-resistance and interlayer at accumulation region. All these-parameters are strong function of doping-ratio of graphene into PVA. These result show that (Gr:PVA) interlayer can be successfully used instead of conventional-oxides/insulators due to its low-cost/weight, flexibility, and high-charges/energy storage capacity. The maximum number of words is 200, 12 points, font: Times New R.

Keywords: Complex dielectric and electric modulus; Frequency and doping ratio effects; Loss-tangent and ac electrical conductivity; Polarization and relaxation processess

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Use of PVDF 275000-Graphene Nanocomposites in Gasoline-Water Separation

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Abstract: Polyvinylidene fluoride (PVDF) has received great attention as a membrane material due to its superior properties such as high mechanical strength, thermal stability, chemical resistance and high hydrophobicity compared to other commercial polymeric materials [1]. Graphene can be incorporated into polymeric materials to form graphene-polymer composite materials. Since many polymeric materials have strength-related issues, the addition of graphene can improve the electrical properties as well as help increase the tensile strength and shelf life of polymeric materials in commercial applications.

In this study, PVDF and PVDF/HNO_3 modified graphene reinforced composite nanofiber mats with different compositions were produced using PVDF with a molecular weight of 275000 by electrospinning method. In addition, PVDF and composite films were prepared by solvent evaporation method in order to compare the gasoline-water separation efficiency. Hydrophobic graphene has been given hydrophilic properties by applying HNO_3 modification in order to increase mixing and interaction. Surface, structure and thermal characterizations of composite nanofibers and films were performed using SEM, XRD, FT-IR and TGA-DSC methods.

When the separation performances of PVDF/HNO_3 modified graphene nanofibers and films in the same composition were compared, it was found that the separation with nanofibers was more successful (67% separation was obtained for the film, while this value was found to be 85% for nanofibers).

Keywords: Electrospinning, nanofiber, Polyvinylidene fluoride, graphene.

References:

[1] Ji, J., Liu, F., Hashim, N. A., Abed, M. M., & Li, K. (2015). Poly (vinylidene fluoride)(PVDF) membranes for fluid separation. *Reactive and Functional Polymers, 86*, 134-153.

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Zirconium Doped Tungsten Oxide Thin Films Coated by Magnetron Sputtering Method and Their Detailed Electrochromic Performance

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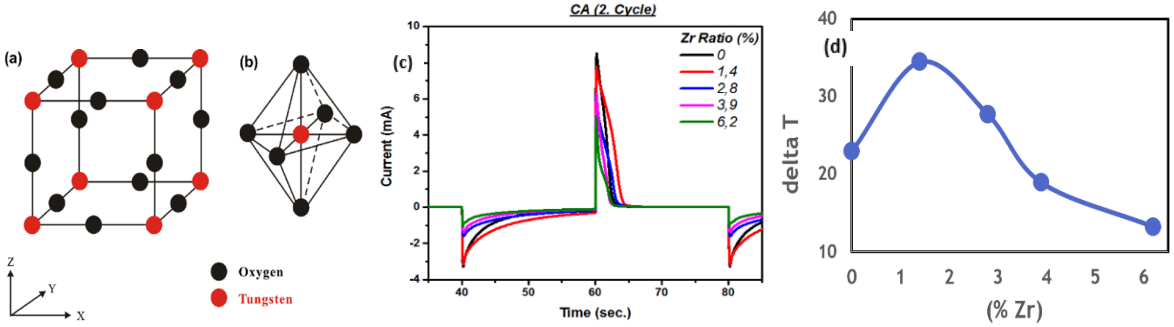
Abstract: Electrochromic technology has an increasing usage area day by day. Rear-view mirrors, which provide more comfortable vision day and night, are among the most common electrochromic products commercially to date. However, it is also very common in exterior cladding and window applications (smart glass) in architecture. The nature of electrochromic smart glasses is transparent and does not need potential difference feeding to maintain its optical position. Thanks to this feature, it is more advantageous. The biggest advantage of electrochromic glass systems is that they provide heat insulation in summer by blocking the infrared (IR) region of sun rays, and they provide heat gain in winter with transparency control. There are studies in the literature in which the energy gains of buildings with electrochromic glass cladding are modeled according to different climatic zones.

The aim of this study is to maximize the number of cycles of the formed thin film and to examine the effect of the film formed by doping WO_3 at different rates on the coloration mechanism. In this way, it is aimed to increase the life of electrochromic devices.

In this study, the cathode layer of colored smart devices will be carried out. Zr:WO_3 coating will be applied with magnetron sputtering method in different parameters as an electrochromic layer on ITO coated glasses used as TCO (transparent conductive oxide). WO_3 target and Zr metal target will be used. Electrochromic properties will be measured using CV (Cyclic voltammetry), CA (Chronoamperometry) and simultaneous spectrometry. Measurements will be made using 0.3 M $LiClO_4$-propylene carbonate solution as the liquid electrolyte. Surface and particle properties will be examined using SEM, AFM, XRD methods. The characterization, electrochromic measurements and calculations of these samples will be completed and the results will be compared. It will be investigated according to which conditions the life cycle of the films and the coloration efficiency change.



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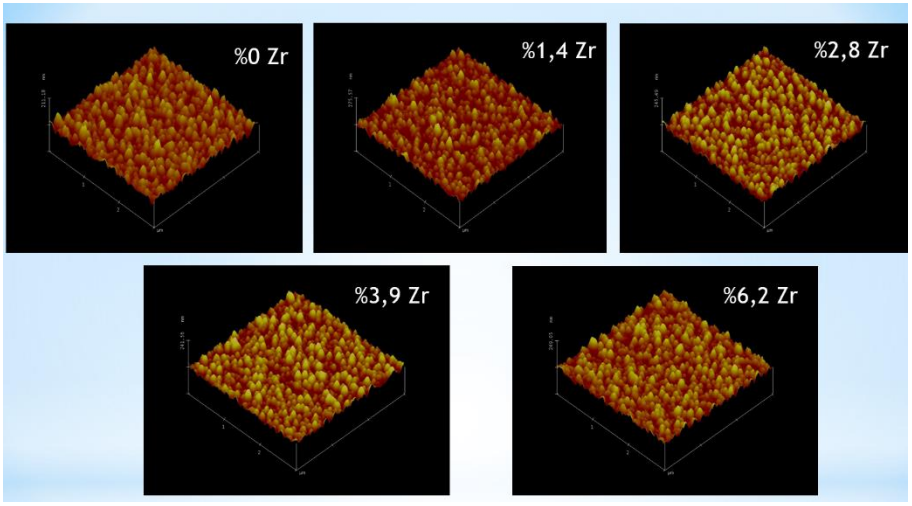

Figure:

a-b) WO_3 Structure

c) Chronoamperometric measurements of thin films

d)The transmittance difference bleach and colored state of thin films

e) SEM images of thin films

Keywords: Tungsten oxide, Electrochromic, Thin films, Doping, Magnetron Sputttering, Zirconium doped

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