

Special Issue  
BSW2019  
**Eighth Bozok Science Workshop**

Bozok Science Workshop 2019, Yozgat, July 25-27, 2019.

**Preface to the Special Issue BSW2019**

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*Editor-in-chief*

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This special issue of Electronic Letters on Science & Engineering (e-LSE), An International open Access Journal, includes the abstracts of the presentations at the workshop, BSW2019 (Eighth Bozok Science Workshop) held during July 25-27, 2019 at Yozgat Bozok University, Yozgat, Turkey.

At the workshop the discussions were based on active researches from basic to several applied fields. The fundamental scientific philosophy behind the meeting, Bozok Science Workshops, is the stimulation of cross-disciplinary flow of knowledge and expertise from both the experimental and theoretical standpoints. At the first, second, third, fourth, fifth, sixth and seventh workshops the main topics were chosen as "Boron studies in nano-scale" for BSW2010, "Computational Chemical Physics" for BSW2011, "Computational Studies on Structure and Dynamics from Nuclei to Biological Molecules" for BSW2012, "Studies on Structure and Dynamics from Nuclei to Clusters" for BSW2013, "Nano Carbon Materials and Their Applications" for BSW2016, "Studies from Nuclei to Nanomaterials with Applications" for BSW2017 and "Boron and Boron Containing Nanomaterials with Applications" for BSW2017, respectively. However, any special topic was not chosen for BSW2019. We believe that the meeting is well-known and mainly similar studies can be come together by means of this platform. The studies on boron, computational chemical physics, atomic/molecular and cluster systems were still welcome again to BSW2019.

As for the workshop planned to be held as BSW2019; the abstracts are prepared as a special issue of e-LSE. All referees have been selected from the Scientific Committee of BSW2019, consisting with national and international experts. In order to take part at the above-mentioned special issue; presenting the selected abstract by applicant is the main principle. By means of the workshop and this

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special issue of e-LSE, we hope to give opportunity to the authors to improve the quality of their works also give the same opportunity to the referees to make critics and to be aware of the active studies submitted to the meeting.

This e-LSE issue may be a good reference material and be a great source for the experts who are interested in the discussed topics. I am pleased to be Editor of this special issue of e-LSE. I would like to thank to the Scientific Committee for the generous support for recommending invited lectures, subjects and sharing their opinion to improve the workshop. Especially, I would like to thank to the members accepting my invitations to be referee for selecting the abstracts for this volume, and to the members of the Organizing Committee for their help. Finally, I would like to thank to Founding Editor Dr. Feyzullah Temurtaş for giving me this opportunity and helping me in managing this issue.

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**NUMERICAL INVESTION OF SIZE-BASED SEPARATION OF  
BIOLOGICAL NANOMATERIALS BY PIEZOELECTRIC PHONONIC  
CRYSTALS**

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**Abstract:** A piezoelectric phononic crystal (PhC) with a square array of annular holes in a YX-128° lithium niobate substrate [1] is utilized for size-based separation of biological nanoparticles with diameters on the order of 100 nm. Surface acoustic wave (SAW) microfluidics has been extensively utilized in size-based fractionation of bacteria [2], circulating tumor cells [3] and exosomes [4], etc, from blood cells. Especially exosomes, nanovesicles that mediate cell-to-cell communication, are valuable tools for early cancer diagnosis. In SAW microfluidics, SAWs are generated via interdigital transducers (IDTs), where the induced standing [5], travelling [6] or focused [7] acoustic field in a microchannel facilitates size-based fractionation. PhCs are artificial periodic structures for controlling acoustic/elastic waves [8]. Although they have found numerous applications, their use in microfluidic systems is very limited. In this work, a piezoelectric PhC is employed to obtain standing SAWs for size-based separation. Band structure calculations via the Finite-Element Method (FEM) reveal that the PhC possesses a band gap around 50 MHz for Rayleigh SAWs on the substrate. For an IDT-PhC pair with a distance equal to an integer multiple of wavelength, standing SAWs are obtained in between. Time-dependent FEM simulations are employed to demonstrate nanoparticle separation with 200 nm threshold diameter in a microchannel in a polydimethylsiloxane mold above the substrate. Radio frequency (RF) signals with small amplitudes, such as 10 V, would be sufficient for efficient separation of nanoparticles. The introduced method can be employed in efficient purification of nanosized biological materials.

**Keywords:** Biological nanomaterial, piezoelectric phononic crystal

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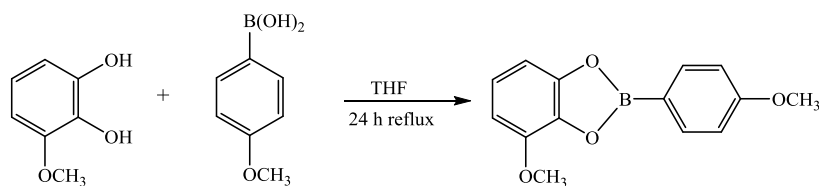
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BIOLOGICAL ACTIVITIES AND COSMETIC APPLICATIONS OF NEW  
BORON COMPOUNDSHamdi TEMEL<sup>1,\*</sup>, Metin ATLAN<sup>1</sup>, Abdulselam ERTAŞ<sup>2</sup><sup>1</sup> Dicle University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Diyarbakır, Turkey<sup>2</sup> Dicle University, Faculty of Pharmacy, Department of Pharmacognosy, Diyarbakır, Turkey

**Abstract:** The use of boron minerals and products that are used commercially in a wide and diverse field is increasing. Examples of industries where boron minerals and products can be used are glass industry, ceramic industry, cleaning and bleaching industry, fire prevention (retardant) materials, agriculture, metallurgy, nuclear applications. However, many studies on boron have been reported to show strong antioxidant properties [1]. Due to its strong hydroxyl ion receptor, it forms complexes with organic compounds containing this group and therefore interacts with biological materials [2].

*Synthesis of Boron compound:* 1 mmol of 3-Methoxy catechol was dissolved in 30 mL of THF. Then 1 mmol of 4-methoxy phenyl boronic acid was dissolved in 10 mL of THF. The reaction was maintained at 120 ° C for 24 hours.



A new boron compound was synthesized and characterized by FT-IR, Mass Spectra, UV, <sup>1</sup>H NMR and <sup>13</sup>C NMR. The antioxidant activities of obtained boron compound were determined by CUPRAC, DPPH free radical and ABTS cation radical removal methods. Anticholinesterases, antiurease and antityrosinase activities were also examined. In addition, this boron compound has been used to make cream. The microbiological and dermatological suitability of the cream has been tested and approved by the Cosming Laboratory.

**Keywords:** 3-methoxy catechol, boronic acid, biological activities, cream.

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**INTRODUCING NATEN: RARE EARTH ELEMENTS RESEARCH  
INSTITUTE**

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## CHEMICAL SENSORS BASED ON ELECTROSPUN NANOFIBERS

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**Abstract:** Volatile organic compounds (VOCs) are used in both domestic and industrial applications, including transport, household chemicals, paints and adhesives. Air quality contamination by many kinds of VOC vapor has become a serious problem for human life [1]. Because of their widespread use and irritation effects, the detection of low-level VOC vapors plays important role in various fields including medicine, agriculture and food industries. Most of the studies on sensing element for VOC vapor sensing are focused on the thin films of metal-oxide semiconductors including SnO<sub>2</sub>, W/TiO<sub>2</sub>, and SmFe<sub>3</sub> [2]. The main drawback in the use of metal-oxide semiconductor thin film as sensing element is their high operating temperature [3].

Nano structured metal oxide semiconductors with high surface area to volume ratio are well known as multifunction materials and gas sensing application [4]. Among the inorganic materials, nanostructured zinc oxide is a promising material for the development of gas sensing device because of its large surface-to-volume ratio, which improve its response. Electrospinning is an efficient, relatively simple and low-cost way to produce nano fibers with diameters ranging from several nanometers to a few micrometers by applying a high voltage to a polymer solution or melt ejected from a micro-syringe pump.

In this study, zinc oxide (ZnO) nanofibers were successfully synthesized by electrospinning method. The structure and the surface morphology analysis of the nanofibers was made through X-ray diffractometry and scanning electron microscopy technique, respectively. Room temperature VOC vapor sensing performance of the nanofibers were then characterized in methanol, ethanol, and propanol atmosphere at different concentration levels between 50 and 300 ppm of the target molecules. Nanofibers presented the highest sensitivity to methanol vapors at room temperature. The results obtained in this work show that the use of electrospun ZnO nanofiber produce excellent sensitivity for sensing VOC vapors.

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**Keywords:** VOC sensing, Adsorption kinetics, Elovich

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## ELECTRICAL PROPERTIES OF NITINOL DOPED LIQUID CRYSTALS

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**Abstract:** Liquid crystals (LC) are non-linear optical materials, and actually they exhibit unique electro-optic, magneto-optic properties and display applications [1]. Nitinol, which is a Ni-Ti alloy, is a well-known shape memory alloy (SMA) with high flexibility. It is possible to control its memory shape via temperature with very good repeatability. It also has high strength, high toughness and low hardness, high corrosion resistance and good biocompatibility [2]. In this study; Nitinol particles were prepared and doped to the liquid crystals and their electrical characterization were performed to acquire interesting results by dielectric measurements.

**Keywords:** Liquid crystals, Nitinol

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**THE EFFECTS OF SURFACE STATES, SERIES RESISTANCE AND  
INTERFACIAL  
(Ca<sub>3</sub>CO<sub>4</sub>Ga<sub>0.001</sub>O<sub>x</sub>) LAYER ON CAPACITANCE AND CONDUCTANCE  
MEASUREMENTS AT 7 kHz AND 500 kHz**

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**Abstract:** In this study, we focused on the effects of surface states ( $N_{ss}$ ), series resistance ( $R_s$ ) and interfacial ( $\text{Ca}_3\text{CO}_4\text{Ga}_{0.001}\text{O}_x$ ) layer on the capacitance/conductance impedance characteristics for 7 kHz and 500 kHz at room temperature. For this aim,  $\text{Au}/(\text{Ca}_3\text{CO}_4\text{Ga}_{0.001}\text{O}_x)/\text{n-Si}$  capacitors were fabricated, and their capacitance/conductance-voltage (C/G-V) measurements were performed between -3.5V and 5V. Their some main electrical parameters such as doping concentration atoms ( $N_D$ ), Fermi energy level ( $E_F$ ), barrier height ( $\Phi_{C-V}$ ), both voltage dependent series resistance ( $R_s$ ) and surface states profile ( $N_{ss}$ ) were obtained from these data. The values of  $N_D$ ,  $E_F$ , and  $\Phi_{C-V}$  obtained from the reverse bias  $C^{-2}$ -V plot. Voltage dependent profile of  $R_s$ -V and  $N_{ss}$ -V plots were also drawn by using Nicollian -Brews and high-low frequency capacitance method, respectively [1-4], and these plots show a peak behavior due to a special density distribution of interface traps or states between interfacial layer and semiconductor with energies located in the forbidden band gap of semiconductor [1,5]. Experimental results show that such a polymer interfacial layer can be used instead of traditional  $\text{SiO}_2$  due to its low cost, high dielectric, high charges or energy storage and easy processing [6-7].

**Keywords:** Interfacial layer, surface states, series resistance profiles

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**THE INHIBITION EFFECT OF THE MAIN MEDICAL PLANT'S ACTIVE COMPOUNDS ON BREAST CANCER**

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**Abstract:** The anti-cancer capacity of piperine was identified in breast cancer rats and breast cancer cell lines [1]. Garlic has been used for centuries for its flavor and health promoting properties that include protection against cancer [2]. Diallyl trisulfide in garlic induces apoptosis in cultured human breast cancer cells through activation of c-jun N-terminal kinase [3]. Anticancer activity of thymoquinone in black seed for breast cancer cells is possible [4]. Origanum syriacum including carvacrol and thymol, origanum vulgare, and salvia triloba against human breast adenocarcinoma cells [5]. Cucurbitacin E and I in Ecballium elaterium are plant derived metabolites that inhibit cancer cells [6]. In this study, the inhibitory effect of the active substances obtained from the main medical plants (Ecballium elaterium, garlic, black seed and origanum syriacum) will be compared by using docking [7] and it will be tried to find out what kind of interactions may occur. These theoretical studies are very important in terms of guiding the experimental studies and preventing loss of time and substances.

**Keywords:** Piperine, Garlic, Origanum syriacum, Ecballium elaterium, docking.

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**TOXIC ELEMENT ANALYZES WITH ICP-OES AND LIBS METHODS IN  
RECENT MARINE SEDIMENTS BETWEEN SILIVRI (ISTANBUL) AND  
ÇANAKKALE STRAIT**

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**Abstract:** In this work, the LIBS (Laser Induced Breakdown Spectroscopy) and ICP-OES technique has been applied to the determination of total contents of heavy metals (Fe, Zn, Al, Mn, Co, Cr, Cu, Ni, Na, Mg, K, Ca) in soil samples of Marmara Sea. In order to validate the technique, LIBS data were compared with data obtained on the same soil samples by application of conventional Inductively Coupled Plasma ICP spectroscopy. The partial agreement obtained between the two sets of data suggested the potential applicability of the LIBS technique to the measurement of heavy metals in soils.

According to the results, it was seen that the elements determined by ICP-OES analysis were also determined by LIBS method. The LIBS method is an important and practical technique for determining the elements that are enriched with anthropogenic factors as well as the elements resulting from natural processes. The presence of the elements present in the sample by the LIBS method is determined by a probability defined by%. In contrast, the analysis does not provide the amounts of elements in the sample. Although this is seen as a disadvantage, this method gives very useful results for practical and preliminary investigations.

**Keywords:** LIBS, ICP-OES, Toxic Element, Marmara Sea, Çanakkale Strait

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**CERN-ATLAS EXPERIMENT STUDIES AND ADCoS SHIFT DUTIES ON  
DATA DISTRIBUTION AT INSTITUTE OF ACCELERATOR  
TECHNOLOGIES**

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**Abstract:** CERN-Large Hadron Collider (LHC) project was approved by the CERN council in December 1994. Then the commissioning with the beam collision process started in the second half of 2009. LHC at CERN has been built to lead the field of particle physics, having unprecedented high energy and luminosity. The goal of LHC is that  $10^{11}$  number of protons collide 40 million times per second to provide 14 TeV proton-proton collision energy at a design luminosity of  $10^{34} \text{ cm}^{-2}\text{s}^{-1}$ . A general-purpose detector, ATLAS (A Toroidal LHC ApparatuS) has been built for probing p-p collisions in addition to CMS (Compact Muon Solenoid) Detector. The ATLAS detector represents the large collaboration work including many physicists, engineers, technician, and etc. I am a member of CERN experiments collaboration since 1999. During this period, I have focused on studying Higgs boson productions and decays, fourth family existence, and isosinglet quarks. After experiment started at CERN, especially last ten years, I contributed the shift duties on Class1 and Class2 shifts at CERN-ATLAS experiment. Class2 shift includes data transferring all over the world depending on Tier Centers while Class1 focuses on run control. In this presentation, I summarize simulation studies with various collision energy and shift duties by using DDM Dashboard, transfer and deletion issues.

**Keywords:** Design luminosity, Higgs boson, Isosinglet quarks, DDM Dashboard

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## INVESTIGATION OF THORIA BASED INERT MATRIX FUELS

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**Abstract:** RepU products plutonium and Minor Actinides, MA can be managed, within specific fuel cycle scenarios, by thorium-based or inert matrix fuels. These fuels show very high plutonium consumption rates, and can therefore be effectively used to reduce or stabilize plutonium stockpiles. A lot of research has been done on thorium fuels and their irradiation behavior. Good results have been obtained for Th/Pu fuels under PWR conditions. Thorium, is a candidate nuclear fuel in near future. There has been interest in utilizing thorium as a nuclear fuel since it is more abundant in the Earth than uranium. All of the mined thorium is potentially useable in a reactor, compared with the natural uranium. Nuclear energy to be environmentalist and sustainable needs to resolve the concern that contains the proliferation risk of plutonium and minor actinides. The thorium fuel cycle and thoria based nuclear fuel types are the candidate that resolving this problem. Thoria (ThO<sub>2</sub>) based inert matrix fuel (IMF) is a candidate in last years that has a new concept to annihilate plutonium and minor actinides. At the same time inert matrix fuel is appropriate to direct disposal in repository. There are many studies on inert matrix fuel concept in recent years. In this study inert matrix fuel production was examined by powder metallurgical and sol-gel route. The powder metallurgical route includes: Powder synthesis, blending, pressing and sintering steps. Sol gel route steps are: Sol preparation, gelation, drying, calcination-reduction, pressing and sintering. In this study thoria based IMF are prepared by powder metallurgy and sol-gel routes. In this study magnesia, alumina and ceria are used with thoria. (Cerium is used as a simulation of plutonium). The densities of sintered pellets were measured by immersion method. Microstructure of powders, sol-gel products and sintered pellets characteristics were determined by scanning electron microscopy. Solid state investigations are carried out by x-ray diffraction. Homogeneity in sintered bodies are controlled by energy dispersive x-ray analysis and results discussed with ecological benefits and nuclear safety.

**Keywords:** Inert matrix, thorium, plutonium, nuclear fuel

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**CHARACTERIZATION OF Fe- AND Ni- BASED MAGNETIC ALLOYS  
PRODUCED BY RAPID SOLIDIFICATION METHOD**

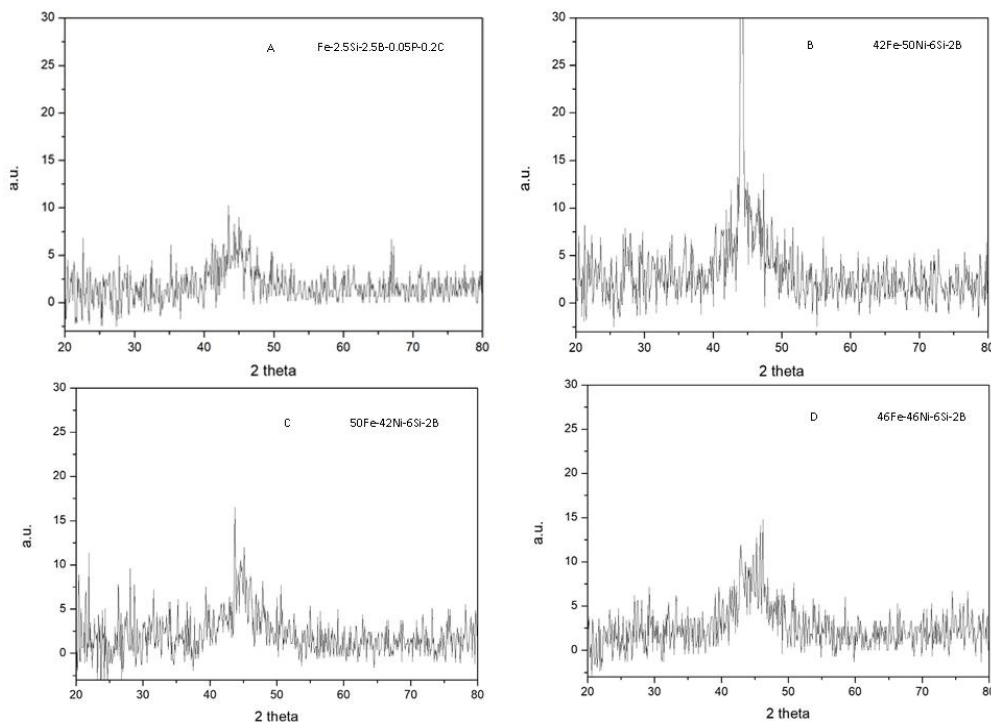
Hakan KARATAS<sup>1</sup>, Can Dogan VURDU<sup>2</sup> and Muhammed Fatih KILICARSLAN<sup>3,\*</sup>

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**Abstract:** In this study, Fe-2.5Si-2.5B-0.05P-0.2C, 50Ni-42Fe-6Si-2B, 50Fe-42Ni-6Si-2B and 46Ni-46Fe-6Si-2B (% by weight) alloy strips were produced by using rapid solidification method. The microstructure and mechanical properties of the alloys have been investigated. In addition, microstructural properties of the produced alloys were examined by X-ray diffraction (XRD). The results of this analysis showed that the strips produced by melt spinning, the rapid solidification technique, were amorphous. When the patterns are examined, it is seen that an amorphous structure with a small number of crystal peaks emerges in all samples (as shown in Figure).



**Keywords:** Fe-Ni based alloys, rapid solidification, amorphous materials

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**HYPERSPHERICAL HARMONICS METHOD FOR THE SOLUTION OF  
QUANTUM MECHANICAL THREE BODY PROBLEMS**

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**Abstract:** Hyperspherical coordinates and hyperspherical harmonics method are very convenient to define the three-body interactions [1-4]. Although the type of the problem varies depending on the interaction potential, it is possible to create a general formalism.

In this study, after giving hyperspherical harmonics method, some solutions are given for atomic three body problems.

**Keywords:** Hyperspherical harmonics, three-body interactions

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**NEUTRON DETECTION SYSTEMS AND THEIR APPLICATION**

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**Abstract:** In order to understand the nuclear reaction and the reaction mechanism, we need different types of detection system. In order to understand the structure of reaction products, especially exotic nuclei, we definitely need an advanced detector system to detect gamma-rays, charged particles, and neutrons. In this study, the recent developments on neutron detector systems, specifically the NEDA (NEutron Detector Array) detector system, will be explained. The use of both detector system and its electronic system, including their performance from recent experiments, will be presented.

We acknowledge TUBITAK (project number 114F473 and 117F114)

**Keywords:** Neutron detection, exotic nuclei

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**EVALUATION OF MEASUREMENT UNCERTAINTY COMPONENTS OF  
<sup>230</sup>Th ACTIVITY CONCENTRATION IN SOIL**

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**Abstract:** The routine measurement of activity concentration of radionuclides in the nuclear and non-nuclear industry in which employees are exposed to radioactive materials such as thorium and its daughters is essential for protection of worker's health and safety issues related with harmful radiation doses exposure to the employees. Thorium is a naturally occurring radionuclide that is ubiquitous in soil, rocks, water, plants, and animals. Th decays to a number of daughters by emitting  $\alpha$ ,  $\beta$  and  $\gamma$  radiation. This decay series causes a health hazard to workers [1]. So the accurate and precise measurement of the activity concentration of Th isotopes at trace and ultra-trace levels is of great interest. The purpose of this study is to evaluate the measurement uncertainty associated with the activity concentration of <sup>230</sup>Th in soil sample. All the steps in the analysis method that contribute substantially to the combined measurement uncertainty are also addressed. Main uncertainty sources are identified as uncertainties associated with the counting rates which are very difficult to reduce.

**Keywords:** Measurement uncertainty, thorium isotopes, radioactivity measurement, alpha spectrometry

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**THE ROLE OF POTASSIUM CHANNELS IN CANCER**

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**Abstract:** Cancer is one of the most common diseases worldwide. Its incidence and mortality have increased considerably in the 20<sup>th</sup> century. After the time of diagnosis, the disease spreads and exhibits a marked insensitivity to chemotherapeutic/radiation therapy. More than 85% of these patients die due to metastasis within the first 5 years, and this last mortality has not changed significantly over the last thirty years.

Ion channels are expressed in almost all living cells and form a pathway for charged ions formed from dissolved salts, including calcium ( $\text{Ca}^{2+}$ ), potassium ( $\text{K}^+$ ), sodium ( $\text{Na}^+$ ) and chloride ( $\text{Cl}^-$ ) ions to pass through the lipid membrane [1]. The non-functional behavior of ion channels in any of its roles, such as regulating the cell cycle of proliferating cells, interacting with membrane potential, preventing apoptosis, altering intracellular  $\text{Ca}^{2+}$  balance, and adjusting cell contraction is thought to cause cancer. In the light of this information, the crucial roles of ion channel involvement in cancer mechanism have been revealed in the last few years and central to cancer pathophysiology [2].

In this study, it is aimed to understand the role of inwardly rectifying potassium channels (Kir channels) carrying ions into the cell by working as a diode. For this purpose, firstly the difference between the expression of mRNA and the expression of Kir proteins will be determined between the cancer lines to be prepared [3]. After selecting the Kir channel with significant differences, the effect of channel inhibitors/activators on gene will be examined due to possible up/down regulation in the channels. By using molecular biology techniques, the mRNA fragment encoding this channel protein is silenced and its genotoxic and cytotoxic effects on cells will be examined.

It is expected that the project outputs to be achieved by achieving the objectives stated in the proposed project will contribute to the literature on pharmacology and cancer studies, especially biotechnology.

**Keywords:** potassium channels, cancer, ion, protein expression.

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## MICROALGAE AND WASTEWATER TREATMENT

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**Abstract:** Due to population growth and technological developments, diversity in consumer goods is increasing day by day, this leads to an increase in the amount and characteristics of wastewater generated. These wastewaters are now commonly treated with conventional biological nutrient removal systems, which cause serious problems directly or indirectly on human health but biological sludge is formed which it must be disposed. In order to minimize these sludge disposal costs, many studies are being done in scientific and technical terms but serious investments are required for now [1,2]. In recent years, however, systems have been investigated that minimize or not occur sludge cost. The most noteworthy of these studies is the treatment of microalgae. Using nutrients for growth and development thanks to the microalgae, both wastewater treatment is carried out and microalgae biomass with many useful uses is formed [3]. The use of this biomass in food industry with additives, raw food in feed industry, additional resources in chemical and enzyme systems and its use in pharmacy is scientifically researched and transition to commercial production begins. In addition, biofuels are obtained from this biomass, which is an alternative and almost endless source of energy to petroleum-derived fuels [4,5]. In this review article, literature information and commercial production companies in Turkey and the world were used [6,7]. So in this way, the basic parameters for the growth and development of microalgae, open and closed (photobioreactor) microalgae production systems, harvesting methods of the obtained biomass, the role of microalgae in wastewater treatment and the basic information about the useful uses of the obtained biomass were compiled [8-11].

**Keywords:** Wastewater treatment, microalgae production, microalgae biomass, microalgae harvest, nutrient removal.

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## QUANTUM INFORMATION THEORY AND QUANTUM COMPUTERS

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**Abstract:** Advances in mathematics, materials science and computer science over 50 years have transformed quantum computing from theory to reality. Nowadays, real quantum computers can be accessed through the cloud, and thousands are using them to learn, research and deal with new challenges. A quantum computer is any computing device that enables the direct use of different quantum mechanical phenomena, such as superposition and entanglement, to process data. In a classical (or conventional) computer, information is stored as bits while in a quantum computer, it is stored as qubits (quantum bits). These computers are the new computational tools that the world expects with great interest in order to comprehend the universe, for the computational power required exactly to know the functioning and relations of the forces of nature, and the communication speeds required by the developing technological civilization. Their computing power and speed are theoretically tens of times higher than that of ordinary computers. The developments announced in recent years show that theoretical studies are rapidly approaching the results. In fact, in the field of quantum cryptography, the practice (experiment) goes even further than theory. Quantum computers, in the future, can revolutionize many disciplines, including the discovery of materials and drugs, optimization of complex systems, and artificial intelligence. In this presentation, some applications such as quantum cryptology and quantum teleportation will be explained by giving information about quantum computers.

**Keywords:** quantum computers, quantum information

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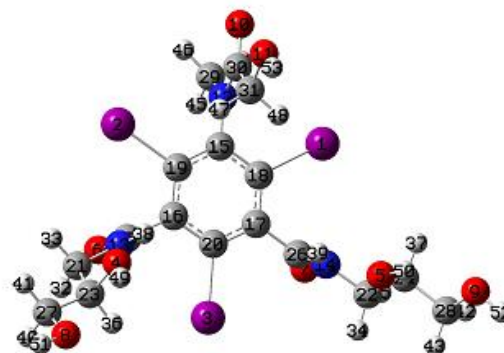
**STABILIZATION ENERGY STUDY OF THE CONTRAST AGENT  
IOMEPROL**

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**Abstract:** In general, the iodinated contrast agent classified into two different types, namely ionic and nonionic contrast agent plays an important role in digital subtraction angiography (DSA) and computed tomography angiography (CTA) examinations. Among these, the nonionic monomer, iomeprol, has been commercially marketed for a long time and their safety has been clinically verified [1]. The presence of a range of iodine concentrations in the iomeprol has been reported to show diagnostic activity equivalent to other nonionic contrast agents and a similar adverse event profile. It has also been found that iomeprol allows its use in a variety of diagnostic procedures and is suitable to use in diagnostic imaging, as well as in its class. In this study, the stabilization energy of iomeprol, one of the iodinated contrast agents, in gas phase was investigated using B3LYP/lanl2dz. The Natural Bonding Orbitals (NBOs) energetic importance estimation was done by second-order perturbation theory that for each acceptor NBO (j) and donor NBO (i), the stabilization energy related to electron delocalization between donor and acceptor was considered. In molecule iomeprol  $\sigma(I_1-C_{19}) \rightarrow \sigma^*(C_{17}-C_{22})$ , and  $\sigma(I_1-C_{19}) \rightarrow \sigma^*(C_{18}-C_{21})$  interactions have 7.06 and 7.07 kcal mol<sup>-1</sup> stabilization energy.



**Keywords:** Contrast agent, NBO, hyperconjugation

**Reference:**

[1] M. Dooley and B. Jarvis, Iomeprol A Review of its Use as a Contrast Medium, *Drugs* 59 (2000) 1169-1186

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**INVESTIGATION OF STRUCTURAL PROPERTIES OF RAPIDLY  
SOLIDIFIED Al-10La ALLOY**

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**Abstract:** Rapid solidification process for the manufacture of metallic alloys mechanical properties markedly the same composition is better than conventionally solidified alloy. Increased solid solubility limit, and better distribution of secondary phases in alloys due to rapid solidification improve mechanical properties. Moreover, it is possible to fabricate metastable samples such as, amorphous, nano-crystals and quasi-crystals alloys by cooling metallic melts at cooling rates over the  $10^6 \text{ Ks}^{-1}$ . Recently, many researchers have studied the effect of rare earth addition on aluminum alloys. Results indicated that the appropriate addition of La had an advantage in refining grain size, removing harmful impurity, improving tensile strength and elongation rate of aluminum alloys [1-3]. In this study, we examined the effect of rapid solidification production method on the morphological and microhardness of Al-10La alloys. The Al-10La alloy samples were produced by the conventionally casting (ingot) and melt spinning process at 10, 20 and 30 m/s. The phases existing in the Al-10La ingot alloy were precise to be  $\text{Al}_{11}\text{La}_3$  and  $\alpha\text{-Al}$  and while only  $\alpha\text{-Al}$  phases were identified in the melt-spinning alloy at 30 m/s. The average diameter sizes of the dendrite arm spacing are about 250-400 nm. The mechanical properties of the ingot and melt-spun alloy was measured by Vickers micro-hardness test method. The microhardness values of the rapidly solidified sample were found about two times higher than those of ingot counterpart sample.

**Keywords:** Al-La, Melt-spun, Vickers micro-hardness test

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**GROSS ALPHA AND GROSS BETA ACTIVITY LEVELS OF HOLOCENE  
SEDIMENTS BETWEEN ŞARKÖY AND MÜREFTE (TEKİRDAĞ)**

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**Abstract:** Background and human-made ionizing radiations are main sources of environmental radioactivity exposing humankind. Background radiation occurs as a result of cosmogenic and terrestrial radiation, while other is arisen from human-made activities [1,2]. In this context, gross alpha and beta activity of sea sediment samples collected at 7 different stations in the research region were analyzed using the low-background counter (Berthold, LB 770 10- channel  $\alpha$ - $\beta$  low-level counter). As a result, the average gross alpha and beta activity was determined as  $218.18 \pm 14.9$  Bq  $\text{kg}^{-1}$  and  $579.00 \pm 23.9$  Bq  $\text{kg}^{-1}$ , respectively. Maximum gross alpha value in investigation area  $301 \pm 15.9$  Bq  $\text{kg}^{-1}$  (Şarköy Port), and maximum gross beta value is  $989 \pm 16.5$  Bq  $\text{kg}^{-1}$  (Şarköy Port). When these values were compared with Bosna River results, both total alpha and total beta values were found to be high [3,4]. The main reason why total alpha and beta concentrations are generally high is that the fertilizers used in agriculture contain uranium, thorium and their degradation products and natural potassium-40.

**Keywords:** Gross alpha, Gross beta, Marmara Sea, Sediment, Radioactivity

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**STUDY OF THE EFFECTS OF ONE OF THE DERIVATIVES OF PYRIDINE  
ON THE BEHAVIOR OF MILD STEEL CORROSION IN HYDROCHLORIC  
ACID SOLUTION (1M)**

Khaled Saad Miled FERIGITA<sup>1,\*</sup>, Mothana Ghazi Kadhim ALFALAH<sup>1</sup>, Murat SARACOĞLU<sup>2</sup>,  
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**Abstract:** In this study, the effect of 1-amino-5-(4-methylbenzoyl)-4-(4-methylphenyl) pyrimidin-2(1H)-one [1] as corrosion inhibitor for mild steel in 1 M hydrochloric acid solution has been investigated. Corrosion inhibitor efficiency was performed by using potentiostat type (IVIUM). It was found that the 1-amino-5-(4-methylbenzoyl)-4-(4-methylphenyl)pyrimidin-2(1H)-one acts as a good corrosion inhibitor for mild steel in 1M HCl solution. The corrosion inhibition efficiency was found to be 90% at  $5 \times 10^{-4}$  M concentration. Both cathodic and anodic curves are significantly changed with more effect in anodic curve lead to reduce the current density and the corrosion rate for mild steel as well.

The increase in inhibition efficiency with increasing concentrations of inhibitor indicates that the inhibition effects are due to the adsorption on the steel surface. According to the experimental data, it is concluded that 1-amino-5-(4-methylbenzoyl)-4-(4-methylphenyl) pyrimidin-2(1H)-one can be used in the control of the corrosion of steel.

**Keywords:** Corrosion, Mild Steel, Pyrimidine, Acidic medium

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**References:**

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**ELECTROCHEMICAL INVESTIGATION OF NORBORNYL  
THIOSEMICARBAZIDE (NTSC) AS CORROSION INHIBITOR FOR  
COPPER IN 3.5% NaCl SOLUTION**

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**Abstract:** The fifth most famous metal in the world is copper that is valuable in pure or compound with other metal to create a new alloy. Copper is very important in our life as it has good mechanical and electrical properties and can be used in the construction of wire, plate and pipelines in the electronics industries, heat exchangers and cooling towers. Unfortunately, when Cu is exposed to an aggressive environment, it decomposes and degrades. Various types of organic compounds are widely used as corrosion inhibitors to protect metals from quality deterioration in such environments due to corrosion [1]. In this work, Norbornyl thiosemicarbazide (NTSC) as corrosion inhibitor for Cu in solution containing 3.5 % NaCl were studied. Impedance spectroscopy, linear polarization resistance, potential dynamic polarization were used to determine corrosion inhibitor efficiency. These electrochemical measurements were performed using an IVIUM type potentiostat. The results show that with increasing inhibitor concentration, corrosion inhibition increases. It has been predicted that a thin layer formed on the copper surface due to the adsorption of inhibitor molecules on the surface protects the Cu from aggressive chloride ions. Anodic plot has changed significantly, leading to a decrease in the current density. The highest efficiency was found to be about 95% at 0.01M inhibitor concentration. Adsorption on the surface obeyed Langmuir adsorption isotherm.

**Keywords:** Norbornyl thiosemicarbazide, Copper, LPR, EIS

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**References:**

[1] A. Khiati, *et. al.*, *Corros. Sci.* 53 (2011) 3092–3099.

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**EFFECT OF THE MACROCYCLE RING SIZE AND R-GROUP CHAIN LENGTH ON THE OPTICAL PROPERTIES OF THE CuPc THIN FILMS**

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**Abstract:** Spin-coated thin film characterization and optical properties of copper phthalocyanine (CuPc) are reported in this study. UV-visible spectroscopy and surface plasmon resonance (SPR) technique systems are used to investigate optical properties of CuPc thin films in the spectral range of 200-800 nm. Values of absorption A, reflectance R, refractive index n, extinction coefficient k, optical conductivity  $\sigma_{opt}$ , and optical band gap  $E_g$  are evaluated at different substrate rotational speed. Three versions of CuPc structures coded as CuPc I, II and III were investigated in which chemical structures differ from each other in terms of their macrocycle ring groups and peripheral groups attached to the same free base porphyrin skeleton. Optical properties of the three versions of CuPc structures were found to vary drastically based on the number of macrocycle ring groups and peripheral groups. Values of the direct optical band gaps of the three versions of CuPc structures were measured and found to be in the range of 1.5-3.7 eV.

**Keywords:** CuPc thin film, optical properties, R-group chain

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**THE COMPOSITION AND CHEMICAL ORDERING EFFECT ON THE  
MELTING TEMPERATURE OF 55 ATOM Au-Ag-Pt NANOALLOYS**

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**Abstract:** The classical molecular dynamics (MD) simulations [1-2] were carried out in canonical ensemble conditions (NVT) for investigation of the dynamical properties of trimetallic  $\text{Au}_n\text{Ag}_{(42-n)}\text{Pt}_{13}$  nanoalloy clusters with the interatomic interactions modeled by Gupta many-body potential [3]. The initial configurations for MD simulations were obtained by optimizing the chemical ordering using the basin hopping algorithm in a fixed icosahedral geometry. The composition dependence of melting temperatures of  $\text{Au}_n\text{Ag}_{(42-n)}\text{Pt}_{13}$  clusters have been investigated via traditional indicators like caloric curve and Lindemann index. The estimated melting temperatures for all compositions fluctuate around 700 K except  $\text{Au}_6\text{Ag}_{36}\text{Pt}_{13}$  with a pretty lower value. The performed Density Functional Theory (DFT) relaxations [4] introduced some new energetically favorable clusters with different chemical orderings. The melting temperatures have been investigated for all these new chemical orderings.

**Keywords:** Optimization, Melting, Gold, Silver, Platinum.

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**STRUCTURAL AND ENERGETIC STABILITY OF SILVER CLUSTERS: A  
MOLECULAR DYNAMIC STUDY**

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**Abstract:** The possibly lowest-energy structures of silver clusters,  $Ag_n$  ( $n = 2-50$ ), are predicted by using molecular-dynamics simulations via following rearrangement collision procedure given in references [1,2]. Atomic geometry, growing pattern, structural stability, energetics, and magic sizes have been investigated. Starting from the dimer configuration, following rearrangement collision of the system during a fusion process, and absorbing its energy step by step up to the value closer to 0 K, possible optimal stable structures of the clusters are identified via an empirical model potential energy function [3]. This approach serves an efficient alternative to the growing path determination and the optimization techniques. The determined configurations are displayed. It has been found that silver clusters prefer to form three-dimensional compact structures and five-fold symmetry appears on the spherical medium sizes which are in similar morphologies as reported in the literature [4].

**Keywords:** Silver clusters; empirical potentials; molecular dynamics

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**CRITICAL BEHAVIORS OF THE MIXED SPIN-1/2 AND SPIN-2 BLUME-  
CAPEL MODEL IN A RANDOM CRYSYAL FIELD**

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**Abstract:** The randomness effects on the thermal behaviors of the order-parameters for the mixed spin-1/2 and spin-2 Blume-Capel Ising ferrimagnetic system on the Bethe lattice are studied by using the exact recursion equations taking the coordination number  $q=4$ . All the functions of interest, the sublattice magnetizations and quadrupolar-order parameter are obtained in terms of these recursion relations. The second- and first-order phase transition lines, therefore the existence of the tricritical points are investigated in detail by studying the thermal variations of the sublattice magnetizations. Also, the compensation temperatures in the model are investigated in detail. It is found that the random crystal field considerably affects the thermal variations of net and sublattice magnetizations [1-4].

**Keywords:** Bethe-lattice, Random crystal field, Mixed spin compensation temperature

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**INVESTIGATION OF STRUCTURAL BEHAVIOR OF SOME  
ODD-EVEN SAMARIUM ISOTOPES**

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**Abstract:** In this study, some nuclear structural properties of Samarium nuclei were investigated, and it was tried to understand how they behave at A~150 region. This region is called as transitional region where the nuclei present different behaviors. The main purpose of this study is to investigate the nuclear structural properties of odd-A nuclei formed by single fermion coupled to even-even nuclei. Many experimental studies [1] were performed on odd-A nuclei having more complex structure than even-even nuclei. Parallel to the experimental studies, various theoretical models are also presented. In this study, we used the interacting boson fermion model (IBFM) [2] related to the interacting boson model (IBM) [3] based on Lie algebra. Firstly, even-even Samarium isotopes were investigated within the IBM-1 model. This model is still useful to explain the medium and heavy mass even-even nuclei especially in deformed regions. Then, the single fermion is coupled to bosonic core to form to odd-even Samarium isotopes and their structure nuclei were investigated within the IBFM-1 model. For this investigation, the energy levels and B(E2) values of these isotopes have been calculated in the scope of these algebraic models.

**Keywords:** nuclear structure, energy level, B(E2) value, interacting boson model

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**ELECTROCHEMICAL ACTIVITY OF V<sub>2</sub>O<sub>5</sub> FILMS OF DIFFERENT  
CURRENT DENSITIES BY ELECTRODEPOSITION METHOD**

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**Abstract:** Although vanadium pentoxide is an electrochromic material, it has a wide range of applications including electrochromic and thermochromic devices, solar cells, lithium batteries as electrodes, electronic and optical switching devices [1,2]. Therefore, vanadium pentoxide and dopants continue to be popular in research. Vanadium pentoxide (V<sub>2</sub>O<sub>5</sub>) films can be prepared by various methods. Chemical and physical vapor deposition techniques, pulsed laser deposition, RF magnetron sputtering, sol-gel, spray pyrolysis, thermal evaporation and DC ion beam sputtering are generally preferred [3]. In this work, ITO glasses were coated with vanadium pentoxide with different current densities by electrodeposition method. For each current density case, electrochemical activities were measured using a scan rate of 10 mV s<sup>-1</sup> through the voltage range of -0.5 V to 0.25 V. According to the results obtained, charge-carrying capacity of the coated films with different current densities were compared. Improvements were observed in the results obtained.

**Keywords:** Vanadium pentoxide, electrodeposition, electrochemical activity

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