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Seventh Bozok Science Workshop: Boron and Boron Containing Nanomaterials with Applications

Bozok Science Workshop 2018, Yozgat, August 8-10, 2018.

Preface to the Special Issue BSW2018

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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, BSW2018 (Seventh Bozok Science Workshop: Boron and Boron Containing Nanomaterials with Applications) held during April 08-10, 2018 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 and sixth 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 and “Studies from Nuclei to Nanomaterials with Applications” for BSW2017, respectively. "Boron and Boron Containing Nanomaterials with Applications" was considered as special topic for BSW2018. The studies on boron, computational chemical physics, atomic/molecular and cluster systems were stil welcome again to BSW2018.

As for the workshop planned to be held as BSW2018; the abstracts are prepared as a special issue of e-LSE. All referees (consisting 51 experts and 9 of them from out of Turkey) have been selected from the Scientific Committee (consisting 63 experts and 11 of them from out of Turkey) of

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BSW2018 to review the abstracts before the workshop. 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 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. Announcement on the special issue is on the workshop circulars right from the start, at web page and in the shared emails. In total, 42 selected abstracts from the reviewed and presented abstracts are published in this issue. 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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ULTRASONIC IRRADIATION ASSISTED SURFACE MODIFIED BARIUM BORATE SYNTHESIS

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Abstract: Barium borates ($BaB_2O_4 \cdot xH_2O$) are extensively used as a functional additives besides use of its beta form (β-BaB_2O_4 or BBO) in photonic industries. In general, reducing the particle sizes of chemical additives is essential in terms of increasing the effective surface area. Surface modified barium borate nanoparticles were synthesized in this regard via wet method in the presence of ultrasonic irradiation. H_3BO_3 and $BaCl_2 \cdot 2H_2O$ were used as starting materials. For the size limiting surface modifications, organic and inorganic additives were used to control the particle sizes and other properties. The ultrasonic irradiation of 20 kHz was provided by UIP2000 hdT generator. The effects of ultrasonic irradiation time and amplitude (in relation with power consumption), with and without the additives, on the particle size was investigated. X-ray diffraction (XRD), particle size distribution analysis, zeta potential measurements, and TG-DTA were used to characterize the microstructure, chemical composition, suspension stability, and the particle sizes. We report that organic modification of the particles with the ultrasonic aid reduced the particle sizes from approximately 12 μm to 100 nm within 2 h of reaction time. Zeta potential of the nanoparticles was found to be around 30 mV in methanol. With respect to surface modifications of similar barium borate synthesis, ultrasonic irradiation aid was found to be useful in terms of kinetics of size reduction and relatively large-scale synthesis.

Keywords: Barium Borate, β-BaB_2O_4, BBO, Surface Modifications, Nanoparticles, Ultrasonic Irradiation, Particle Size Distribution, Zeta Potential

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UTILIZATION OF BORON AS AN ENERGY MATERIAL

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Abstract: Turkey has 73% of the world's boron reserves, however, approximately 93.5% of boron treated in Turkey is known to be shipped [1]. In developed countries, boron materials produced from boron mine are the common value added materials used in many technologies from aircraft fuels to space technologies. Studies and ongoing research on boron will enable the exploration of new uses of boron compounds and boron-based materials in advanced products, and as the critical areas of use of boron mine increase, they will become a mine to overcome the international struggle over the next years as it is in oil. In recent years, the increase in the number of R & D studies and patents on the use of boron materials in power generation and energy storage systems is striking. Boron materials have been found to provide electrochemical performance, charge-discharge cycle life and thermal stability when used in lithium ion battery components as electrolyte salt, electrolyte additive and cathode active material. Lithium-ion batteries are the most efficient power sources for a variety of applications such as portable electronics, electric vehicles and large-capacity energy storage systems. The intense price competition in lithium-ion battery technology drives manufacturers to improve new chemistry technologies and improve processes to reduce production costs. In this study, the results of the use of boron compounds and materials in lithium ion battery technology in the world and in our country are given. Another use of boron products in energy technologies is to use them as fuel in fuel cells. In this context, sodium borohydride can be used directly as fuel in sodium borohydride fuel cells or as a hydrogen source in PEM fuel cells. Particularly sodium borohydride stands out as a good alternative because of its high volumetric and weighted hydrogen storage capacity. Sodium borohydride network can store 20% hydrogen, not flammable / explosive, the reaction can be easily controlled, half of the hydrogen comes from the water, the other half comes from water, the catalyst and sodium metaborate can be reused. The theoretical energy density and the theoretical specific capacity are 9.3 Wh/g [2] and 5.67 Ah/g [3], respectively. Especially in range-boosting vehicles, the

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transport of flammable / explosive fuels in pressurized tanks will provide the user with confidence and facilitate the spread of technology. Sodium borohydride is converted into hydrogen and metaborate by the hydrolysis reaction. In this study, products developed domestically are explained for both area of usage.

Keywords: Sodium Borohydride, Boron Usage, Energy Storing Materials, PEM Fuel Cell

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TRACE ELEMENT ENRICHMENT AND OCCURRENCE OF WESTERN ANATOLIAN BORATE DEPOSITS

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Abstract: Borate occurrences of western Anatolia were deposited in the intra-continental playa lake sediments during Miocene when the volcanic activity occurred from Paleogene to Quaternary. All mineralizations were associated with volcanic activity. Borate levels situated in the sequence that are intercalated with claystone, siltstone, tuff, marl and limestone. Western Anatolia borate deposits were formed in two types such as continuous and discontinuous. Emet, Bigadiç and Kestelek deposits have discontinuous while Kırka has continuous deposition in the region. Geological, petrological and mineralogical properties of these deposits have been studied by many authors[1-3]. However, geochemistry of these deposits have not been studied yet. The trace elements of Bigadiç borate deposits including Se, Sr, As, Sb, Mo, Li; Kestelek borate deposits containing Se, Sr, As, Sb, Cs, Li, Mo; Kırka borate deposits comprising Se, Cs, Sr, Li, As and Emet borate deposits involving As, Se, Cs, Li, Sr, Sb, Pb enrichments were determined with the averages of earth crust and andesite[4-8]. It can be concluded that based on the concentration of Se and Li elements can be gained into economical as by product, besides B.

Keywords: Western Anatolian, borate, geochemistry, trace element.

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ENHANCEMENT OF THE CRITICAL CURRENT AND TRAPPED MAGNETIC FIELD PROPERTIES OF THE PARTIAL DOPED AND SINTERED $MgTi_{0.06}B_2$ BULK SUPERCONDUCTOR USING NUMERICAL AND EXPERIMENTAL METHODS

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Abstract: Between the intermetallic superconductors, MgB_2 superconductor has superior properties, as the high critical temperature (T_c), critical current density (J_c), stable levitation force. The magnetic field trapping property of this superconductor makes these materials very promising candidates for technological applications, such as the next generation of medical MRI devices and super-magnets for Maglev systems. The trapped magnetic field B_{trap} on the sample axis of a MgB_2 superconductor, due to an induced persistent supercurrent, depends on the critical current density J_c, the sample diameter R and geometrical constant (or Levitation force F_L depends the shielding current density J_c, the critical current loop radius r, the sample geometry, sample volume and external magnetic field gradient) [1,2]. The studies, on the increasing of the trapped field value in literature, reported that the critical current density value decreases while going to the outer sample region [3] and the trapped magnetic field increases initially with increasing sample diameter but it gets saturation for the larger diameters [1]. In our previous study, on electromagnetic modelling of regional critical current and bulk trapped field, we determined that the tendency to saturation in the peak trapped field pointed out

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that the increasing of the bulk diameter alone does not have a significant effect on the value of the trapped magnetic field, unless the bulk superconducting current density was improved uniformly throughout the whole MgB_2 bulk [4]. Addition to the trapped magnetic modelling and the nanoparticle Ag doping (using the regional doping method) [2], in this study, we performed the Infrared (IR) line laser process on sample surface acted as a second sintering to further enhance the supercurrent density distribution uniformly of the bulk $MgTi_{0.06}B_2$ superconductor and so to increase the maximum trapped magnetic field value. After the laser treatment at 28 K it is seen that, the J_c improved both inner and outer sections for undoped Ag0 and doped Ag3 sample. Also the maximum J_c value increasing approximately two times for the inner region Ag3 (1) specimen and 1.2 times for the outer region Ag3 (2) specimen explains that the fast laser sintering process is much more effective at the non Ag added surface regions.

Keywords: Superconductor, MgB_2, Critical current, Levitation force

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EFFECT OF CeO_2 SUPPORTED La-Ni-Mo-B ON POTASSIUM BOROHYDRIDE HYDROLYSIS

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Abstract: One of the fundamental needs of the age we are in is energy. It has accelerated the shift to clean energy sources with the depletion of fossil fuels. One of the chemical compounds with high energy density, which removes the problem of the storage of hydrogen from the clean energy sources, is potassium borohydride [1-4]. The basic parameter that determines the hydrolysis of potassium borohydride, hydrogen production efficiency and reaction course is the catalyst. In this context, CeO_2 supported La-Ni-Mo-B catalyst was synthesized in this study. Then, the optimal metal ratio, the amount of catalyst, the concentration of different potassium borohydride, and the catalytic activity at different temperatures were examined for potassium borohydride hydrolysis. From here, kinetic first order and activation energy of the reaction were also 63,26 kj/mol calculated.

Keywords: KBH_4, La-Ni-Mo-B, Hydrogen, Catalyst, CeO_2

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BORON-ADDED PUMICE BRICK PRODUCTION: DETERMINATION OF PHYSICOMECHANICAL AND CHEMICAL PROPERTIES

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Abstract: In Turkey, colemanite and borax minerals are produced in boron processing plants located respectively in Emet and Kırka. In addition, there are lots of pumice deposits in various regions of the country. Within the scope of this work, it is aimed to produce bricks which are fireproof, light, with high strength, and earthquake resistant for building and construction sector by employing strategically important boron minerals as well as their wastes. Boron minerals were used within the pumice aggregate as much as 6-12% by taking advantage of its binding properties. Experimental studies were carried out in laboratories located at Mineral Research and Exploration General Directory. Appropriate sizes of pumice (0-8 mm) and other boron minerals were mixed in the presence of clay and carboxymethylcellulose, CMC, to prepare dry mixture. Sufficient amount water forming a semi-dry mixture was then added. The semi-dry mixture was then compressed into molds with 10-20 bar pressure. The green-bodies were subsequently left natural drying. The dried samples were fired at 700-850 ^{o}C for 2 h. The final composition containing pumice, tincal, colemanite, boron waste, clay, and CMC was determined at the end of the laboratory work. Specifically, CMC in the composition kept between 0.5-1.5%. Mechanical, physical, and chemical experiments were carried out on baked products according to Turkish Standards Institution and international standards. On the best sample, thermal conductivity (0.1939 W/mK) and compressive strength (3.63 MPa) were measured. The bulk density (0.62 g/cm^3), water absorption (32%) and apparent porosity (37.1%) by Archimedes method were determined. The results were also compared with similar bricks. It was determined that the bricks can be produced in industrial size (5x10x20 cm^3).

Keywords: Pumice brick, Boron, Boron minerals, Boron waste, Lightweight brick.

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INVESTIGATION OF THE USE OF BORON NANO MATERIALS IN TEXTILE BASED BALISTING PRODUCTS

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Abstract: In recent years, nanomaterials and nanotechnology have become very effective in obtaining highly functional products. Boron works show that boron gives superior properties to materials and products. Boron is used to improve material performance such as thermal insulation, electrical conductivity, strength enhancement, processability improvement. It is evident that boron is a very important material, and its importance and nano-size boron particles are characteristic. Boron is used from automotive to machine, textile to health. The use of boron as boron carbide, boron nitride, aluminum borate and borohydride is found in various investigations. Boron carbide stands out with its high hardness value and lightness.

Boroncarbide is used in the defense industry for the production of plates used as lightweight protective protective ballistic armor or vests. Boronnitride is hexagonal and cubic in structure, also known as white graphite because of its graphite resemblance. Boronnitride is the least dense material among ceramic materials (2.27 g / cm3) [1]. Boronnitrile nanofibers (BNNF) find applications in increasing the performance of high temperature ceramics. Aluminumborate (9Al2O3.2B2O3) is a material with high melting temperatures, low density, low thermal expansion coefficient and low friction resistance. Because of these properties, they are used as automotive, composite materials and electronic ceramic materials as oxygen resistant reinforcements [2]. Boronhydrides are the most stable and commercially available [3]. This material is used for bleaching paper clay, recovering precious metals such as gold, silver, etc. from the solutions; removal of heavy metals such as cadmium and mercury in waste water; are used in the production of chemicals. Boron is used as fiberglass in the textile sector due to its flame retardant property. In addition to this, it can be used in fabric dyeing and fabric finishing processes.

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Boron is used as matrix reinforcing reinforcements in the construction of composite materials with nano size shape and also as reinforcing element in the form of boron doped fibers. Use of boron materials in defense industry; protective textile products, protective vests and helmets [4,5,6,7]. In this study, it was aimed to strengthen the boron carbide nanoparticles to the aramid fabrics and to produce composite textile material to be used for vests, which can provide protection level III in the defense industry and to evaluate the ballistic performance of this composite textile product. Taking into consideration the lightness, price and performance indicators, it is aimed to reveal the optimum number of fabric coats and nano boron carbide ratio. In the study, a 200 g / m2 aramid fabric was selected and an experimental plan was developed in which the proportions of boroncarbide nanoparticles to be added to the composite resin were changed. The fabrics will be brought together on different floors to form a structure for protective vests. This composite textile structure will be subjected to ballistic tests with protection level III, and the performance of the product will be examined. The study will be carried out by applying optimization techniques from scientific research techniques.

Keywords: Boron, nanoparticle, aramid fabric, ballistic, composite

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Effect of Boriding and Plasma Nitriding Process on Gamma Attenuation Parameters of Hardox 400 Alloy

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Abstract: In this study, the effect of boriding (BRD) and plasma nitriding (PN) processes on the radiation shielding properties of Hardox 400 was investigated. Gamma attenuation measurements were made in a good transmission geometry using a HPGe detector. A 133Ba radioactive source which emits photons 81 keV, 276 keV, 302 keV, 356 keV and 383 keV was used to irradiate the samples. Linear attenuation coefficients (LACs) of alloys were measured. The obtained LACs were then used to calculate the tenth value layers (TVLs), half value layers (HVLs) and mean free paths (MFPs) for the alloys. The results were compared with as received form of Hardox 400. It was concluded that single BRD processing decreases the LACs in all measured energies. In contrast to single processing, the dublex processing (BRD and PN) tends to increase the LACs of the materials. These changes are due to changes in electron density and effective atomic number of the Hardox 400 with BRD and PN processing. In order to fully understand the effects of the BRD and PN on LACs, the measurements should be taken at a wider energy range depending on the different functions of the BRD and PN processes.

Keywords: Gamma attenuation, Hardox 400, Plasma Nitriding, Boriding

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CHARACTERIZATION OF A NOVEL NEUTRON SHIELDING MATERIAL CONSISTS OF POLYESTER AND BORON CARBIDE

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Abstract: Ionizing radiation has great benefits to humankind in a wide range of areas such as industry, medical applications, education and R&D fields etc. Beyond these benefits, exposure to excessive radiation doses uncontrollably could cause fatal harms to human body and environment. Radiation types can be named alpha, beta, gamma, neutron radiation and X-rays and all have different characteristics [1]. Among of these, only the neutrons can interact with the nucleus of atoms and change the structure of the nucleus, means a serious danger for living tissues. To ensure safe working conditions, along with distance and time limitations, shielding of the sources is one of the three important parts of As Low as Reasonably Achievable (ALARA) principles. Hence, the shielding material developed and characterized against neutron radiation and analyzed with both experiments and simulations. The basic principle for shielding design against neutron is well known; thermalizing the energetic particles with a good moderator, then absorb them with the second part of the shielding material, which has a high thermal neutron cross section. Polyester is a good moderator due to its high hydrogen content. In addition, it is easy to handle and cost effective matrix material [2]. Therewithal, boron carbide (B_4C) has high thermal neutron absorption cross section of 767 barn naturally because of ^{10}B isotope and well known for its hardness and mechanical strength, which makes it a precious material for neutron shielding applications [3]. 10 to 50 wt. % B_4C reinforcement 20, 40 and 60 mm-thick specimens were prepared and neutron shielding capabilities of B_4C reinforced polyester matrix materials were investigated because of the excellent properties, like nonradioactive capturing of boron carbide against neutron radiation and their characterization were studied with various characterization methods. After metallographic determination of microstructure, impurity analysis and neutron absorption characterizations, it was observed that, shielding capability of the composite material increased with increasing its thickness furthermore when the amount of B_4C reinforcement was increased, the shielding rate also increased, but when it was increased up to 40 and 50 %, a slight decrease was observed in the shielding ratio.

The simulation of the study, Fluka Monte Carlo (MCNP-5) was made, and experimental data were compared with those obtained by the simulation. The result we find out from this table is; we reached large absorption ratios with our specimens, which contains enriched ^{10}B, "Polyester-B_4C" shielding material.

Keywords: Nuclear reactors, neutron radiation, shielding, composite material

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SYNTHESIS OF SOME RARE EARTH BORIDES

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Abstract: There are many ways of synthesis of rare earth borides. In this work, we synthesized lanthanide (La, Gd, Eu, Sm, Nd and Tb) borides via magnesiothermic reduction in open air. Stoichiometric amounts of M_2O_3, B_2O_3 and Mg were mixed, where M is a lanthanide metal. Mixture was heated to 700 °C, 800 °C and 900 °C by Mg metal to form the metal borides.. Reaction temperature and reaction time were regulated to obtain nano and micro crystals with monodispersed and irregular particle morphology. Optimal conditions for the formation of metal borides were detected. It was found that optimum reaction temperature and reaction time of NdB_6 is 700 °C and 3 hour, for SmB_6 700 °C and 1 hour, for GdB_6 900 °C and 4 hour and for TbB_4 900 °C and 2 hour, 700°C and 4 hours for EuB_6 [1]. Produced structures were leached with concentrated HCl to get rid of impurities which may cause different chemical and physical features. . Crystal structure of metal borides were investigated by X-Ray Diffraction (XRD) spectroscopy in addition to Energy Dispersive x-ray spectroscopy (EDS). Scanning Electron Microscopy (SEM) was used to analyze the geometrical varions. It was detected that pure metal borides can be synthesized with irregular morphology in nano and micro sizes [2].

Keywords: Boride, Rare Earth, Boron

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FACILE SYNTHESIS and CHARACTERIZATION of 5-[(N-METHYL-N-(2-HYDROXYETHYL) -4-AMINO) -BENZYLIDENAMINO]-2-MERCAPTOBENZIMIDAZOLE. COMPOUND and ITS ELECTROCHEMICAL SENSOR APPLICATION

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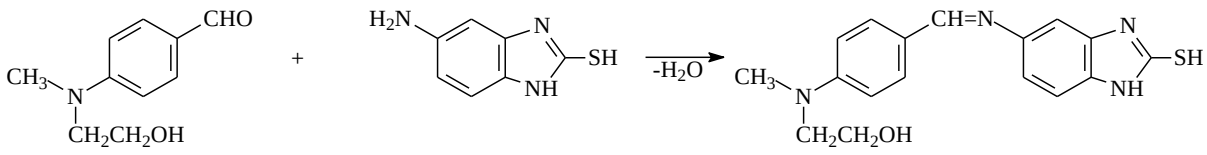
Abstract: Schiff bases are formed from a reaction of primary amines with aldehydes and ketones. Schiff bases have a wide range of usage, including medicine, industry, technology and many areas of chemistry. Therefore, in this study it was aimed to synthesize a novel mercaptobenzimidazole derivative Schiff base. 5-[(N-Methyl-N-(2-hydroxyethyl)-4-amino)-benzylidenamino]-2-mercaptobenzimidazole **(3)** was obtained from reaction of N-methyl-N-(2-hydroxyethyl)-4-aminobenzaldehyde **(1)** and 5-Amino-2-mercaptobenzimidazole **(2)**. The newly synthesized Schiff base compound was characterized by IR, 1H-NMR, 13C-NMR, UV-Visible and Elemental analyses techniques. Experimental measurements indicated that the synthesized compound exhibited a good activity for copper binding [2]. The synthesized compound was used as ionophore in the structure of potentiometric ion selective sensors. The prepared potentiometric ion selective sensors based on 5-[(N-Methyl-N-(2-hydroxyethyl)-4-amino)-benzylidenamino]-2-mercaptobenzimidazole **(3)** showed a selective potentiometric response for copper(II) ions. Additionally, the potentiometric performance characteristics such as linear working range, slope, detection limit, repeatability and pH range of the prepared sensors were investigated [3-5].



1 **2** **3**

Scheme 1. Synthesis stages of compound.

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Keywords: Schiff Base, Azomethine Group, Potentiometric Ion Selective Sensor, Copper(II) Determination.

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RADIOLOGICAL ASSESSMENT OF PHOSPHATE ROCKS IN SOME COUNTRIES

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Abstract: The phosphate rocks is used to manufacture phosphate fertilizers [1]. Radiological characterization of phosphate rocks in Turkey, Tunisia, Egypt, Morocco, Algeria and Syria were investigated using gamma ray spectrometry. The radioactivity concentration levels for ^{226}Ra, ^{232}Th and ^{40}K in all phosphate rock samples ranged from 250 to 1029 Bq/kg with a mean of 535 Bq/kg, from 5 to 50 Bq/kg with a mean of 20 Bq/kg and from 117 to 186 Bq/kg with a mean of 148 Bq/kg, respectively. The radium equivalent activity (Ra_{eq}), the total air-absorbed dose rate (D) and the annual effective dose (H_e) rate were also calculated using for ^{226}Ra, ^{232}Th and ^{40}K activity values. The calculated mean values of the Ra_{eq}, D and H_e for the phosphate samples were 575 Bq/kg, 266 nGy/h and 0.33 mSv, respectively. All the Ra_{eq} values of the samples except for Tunisia are higher than the recommended reference value 370 Bq/kg recommended by the Organization for Economic Co-operation and Development (OECD) [2]. Also, the computed values of H_e are lower than the recommended limit by the International Commission on Radiological Protection (ICRP) [3].

Keywords: Phosphate Rocks, Radioactivity, Radium Equivalent Activity, Annual Effective Dose

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INVESTIGATION OF OPTICAL PROPERTIES OF PETROLEUM PRODUCTS BY LIGHT SCATTERING

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Abstract: Computational modeling of light scattering and propagation through petroleum products, which take into account the shaped slab geometry, was studied. Light propagation through a slab has been represented via transmitted and reflected electromagnetic fields by using a finite thin petroleum cell model. Numerical aspects of the light scattering process, which are based on numerically solving Maxwell's equations, have been calculated for petroleum products. It has been described the computation details for the slab model for computing light scattering using specific petroleum products such as diesel, gasoline, oil, paraffin etc. to investigate the optical properties of these materials. The results of benchmark computations have been presented for the considered as shaped slab geometry. By the light scattering, we were able to set a standard for the quality of petroleum products, which matches our previous work on different geometries [1-4].

Keywords: Light Scattering; Slab; Computer Modelling; Petroleum Products

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ALKALI-Mg METAL INCORPORATED 211-MAX COMPOUNDS: Hf_2MgY (Y=B, C, N)

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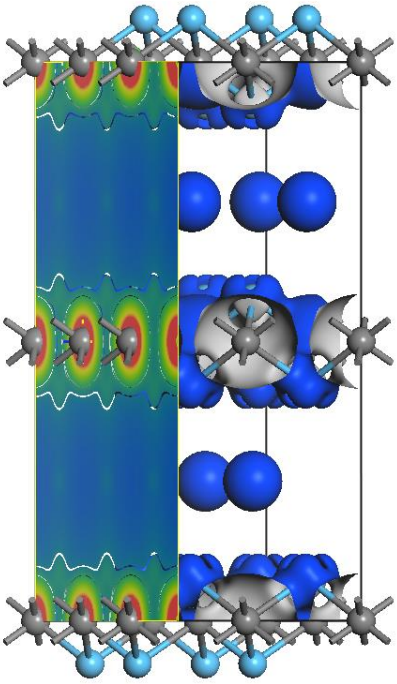
Abstract: 211-MAX phases are an important material family which is widely considered, because they form a bridge between physical properties of metals and ceramics [1]. They have wide range of physical properties such as most readily machinable, high efficiency engines, damage tolerant thermal systems, wear and corrosion protection, good electric and thermal conductivity [2, 3].



In this study, to reveal the effects of the alkali and light elements especially boron on the actual properties of 211-MAX phases, the structural, electronic, mechanical and dynamic properties of alkali metal (Mg)-incorporated Hf_2MgY, Y= B, C, and N compounds with nanolaminated Cr_2AlC-type structure (see Fig.) have been investigated by CASTEP based on first-principles density functional plane-wave pseudopotential calculations within generalized gradient approximation. From calculated formation enthalpies, all compounds are thermodynamically stable, and they have metallic behavior. From calculated elastic constants and phonon dispersion curves, it is shown that all compounds are mechanically stable, and Y=C, and N-incorporated compounds are dynamically stable. Boron-incorporated one is dynamically unstable due to the negative frequency around the Γ. At the same time, related mechanical properties such as bulk and shear moduli are calculated, and anisotropic properties are investigated. It is shown that Hf_2MgN has higher mechanical properties and lower anisotropic character. For further mechanical characterization, hardnesses of the compounds are determined theoretically.

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Keywords: DFT, MAX-borides, stability, mechanical properties.

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EXPERIMENTAL AND THEORETICAL INVESTIGATION OF AMINOPYRIMIDINE-CARBOXYL(ATE) INTERACTIONS IN TRIMETHOPRIM 1,2-CYCLOHEXANEDICARBOXYLATE

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Abstract: Trimethoprim [2,4-diamino-5-(3,4,5-trimethoxybenzyl)pyrimidine], TMP, containing pyrimidine ring play a significant role in many biological systems [1]. The pyrimidine ring system, present in nucleic acids, several vitamins, coenzymes etc., provides potential binding sites for metal ions. Trimethoprim is a well-known biological agent, also employed as a metabolic inhibitor of the dihydrofolic acid reductase enzyme [2].

TMP also showed complexing ability with various carboxylic acids [3]. In the complexes N-H…O hydrogen bonds were established between the pyrimidinic group of trimethoprim and the carboxylate group of some carboxylic acids. Hydrogen bonding is the most important noncovalent interactions. It plays a vital role in biological structure and functions, molecular design [4]. Hydrogen bonded motifs can self-organize in various ways, leading to a variety of supramolecular architectures [5].

In this study, a new trimethoprim-1,2-cyclohexanedicarboxylate salt was synthesized and characterized by analytic and spectroscopic methods. Then, a complete description of the structural properties of the compound through its consistency with the spectroscopic data has been presented by theoretical studies. Structural and energetic properties of the compound have been investigated by Density Functional Theory (B3LYP) with 6-311G(d,p) basis sets [6]. Bond lengths for $TMPH^+$ and $TMPH^+C_8H_9O_4^-$ have been given in (Fig 1)

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Atoms	$TMPH^+$(Å)	$TMPH^+C_8H_9O_4^-$(Å)	
N5-C18	1.366	1.353	
C18-N7	1.341	1.347	
C18-N4	1.318	1.343	
N4-C16	1.343	1.332	
C16-C1O	1.450	1.425	
C10-C17	1.355	1.378	
C17-N5	1.376	1.342	
C16-N6	1.330	1.364	$TMPH^+$
C10-C8	1.512	1.509	
N5-H40	1.624	1.624	
	$C_8H_9O_4^-$		
O41-H40		1.030	
C42-O41	1.247	1.317	
C42-O43	1.257	1.222	
C42-C44	1.581	1.531	
O43-H40		2.391	$TMPH^+C_8H_9O_4^-$

Figure 1. The optimized form and Bond lengths for $TMPH^+$ and $TMPH^+C_8H_9O_4^-$

Also theoretical calculation provides another method to investigate the important characters of materials. Calculation is an alternative option since it is difficult to directly measure hyperpolarization. The first order-hyperpolarizability and related properties of $TMPH^+$, $C_8H_9O_4^-$and $TMPH^+C_8H_9O_4$- were calculated using B3LYP/6-311G(d,p) basis set, based on the finite field approach. The mean first-order hyperpolarizability can be calculated using the following equations.

$$\beta_{total} = \sqrt{\beta_x^2 + \beta_y^2 + \beta_z^2}$$

$$\beta_x = \beta_{xxx} + \beta_{xyy} + \beta_{xzz}$$

$$\beta_y = \beta_{yyy} + \beta_{yzz} + \beta_{yxx}$$

$$\beta_z = \beta_{zzz} + \beta_{zxx} + \beta_{zyy}$$

Mean first order hyperpolarizability of $TMPH^+$, $C_8H_9O_4^-$and $TMPH^+C_8H_9O_4$- were calculated to be 3.68×10^{-30} esu 8.64×10^{-30} esu, 5.55×10^{-30} esu, respectively.

Molecules	Hyperpolarisibility
$TMPH^+C_8H_9O_4^-$	3.68
$TMPH^+$	8.64
$C_8H_9O_4^-$	5.55

Keywords: Trimethoprim, Hydrogen Bonding, HF, DFT.

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CLEAN LIGHT TECHNOLOGY

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Abstract: With Clean Light technology developed within the scope of an R & D project has been aimed both to save the energy and to remove the negative affects of the harmful micro-organisms on human health. It is also aimed to be able to maintain the flow and efficiency of daily life in a healthier environment. The photometric and the medium electromagnetic radiation measurements of the developed "Innovative Clean Light LED Technology" have stated the conformance to lighting standards and stated that the equivalent fluorescent luminaires are lower than the affects of the electromagnetic radiation [1]. In addition, the light intensity distribution of Clean Light LED luminaires is approximately 10.3% more symmetrical and brighter than the equivalent fluorescent luminaires. For antimicrobial efficacy tests, the resistance of three different pathogenic bacterial on the different surfaces was examined in a controlled manner. Tests on harmful microorganism agents in community habitats have shown that such microorganisms reduce their reproduction and spreading [2,3]. Clean light technology is prospective for contributing to all living creatures' living areas to be clean and healthy as well, and it has high economical value.

Keywords: Clean Light, LED, Lighting, Biotechnology

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STUDY OF INTERACTION BETWEEN TIGECYCLINE AND SULBACTAM

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Abstract: Drug interactions can have desired, reduced or unwanted effects. The probability of interactions increases with the number of drugs taken. Side effects or therapeutic drug interactions can increase or decrease the effects of one or two drugs. “Failure may result from clinically meaningful interactions.” Clinicians rarely use foreseeable drug-drug interactions to produce the desired therapeutic effect. For example, when we consider two drugs each causing, peripheral neuropathy increases the likelihood of neuropathy occurrence. The selection of alternative treatment options with antibiotic combinations may be used to successfully manage ultidrug-resistant Acinetobacter baumannii. Liu et al.,[1] studied combined therapy of tigecycline with cefoperazone–sulbactam and reported that it was seemingly superior treatment option compared with monotherapy or the combination of tigecycline with sulbactam alone. In this study geometry optimizations of tigecycline and sulbactam drugs and combination of them have been carried out with the evaluation of B3LYP/6-311G (d,p), B3LYP/6-311++G (2d,2p) levels, and the reaction mechanism at semi empirical PM6, which was parameterized for biochemical systems and B3LYP/6-311G (d,p) levels. The main objective of the present study is to understand the interaction of sulbactam with tigecycline, to describe energetic condition of bond formation and electronic structure (orders of the broken and formed bonds). The reaction mechanisms of sulbactam with tigecycline have been studied as stepwise and concerted mechanisms using semi-empircal PM6 and B3LYP/6-311G (d,p) levels and the energy of the reactants, intermediate, transition states and products are given in Figure 1.

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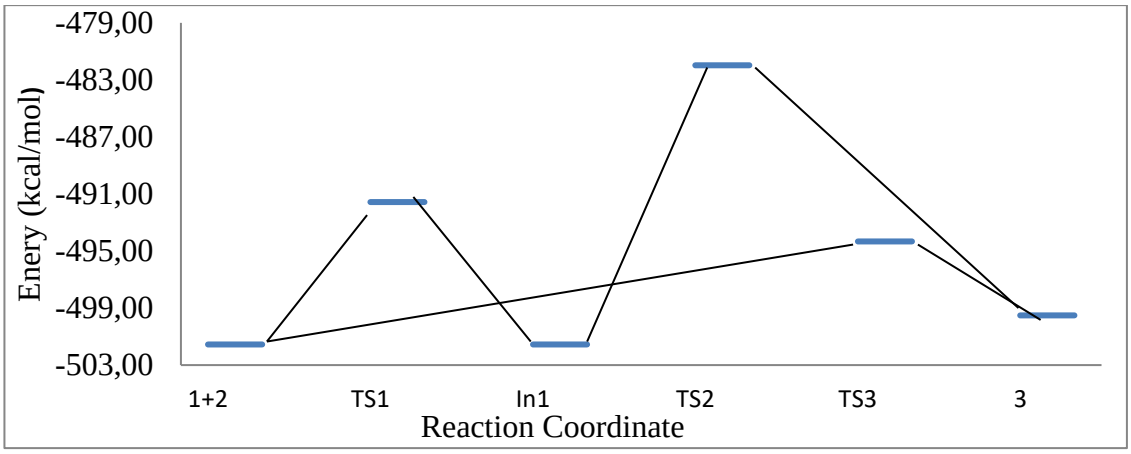

Figure 1 Energy Characteristics of the Systems Participating in the Reaction (Calculated by PM6)

Keywords: tigecycline, sulbactam, reaction mechanism

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MOLECULAR STRUCTURE AND ELECTRONIC PROPERTIES OF DIATRIZOATE, IOXAGLATE CONTRAST COMPOUNDS BY QUANTUM CHEMICAL CALCULATIONS

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Abstract: Iodinated radiographic contrast media for intravascular use are tri-iodinated derivatives of benzoic acid and they all have biological properties that may affect a variety of physiological processes [1]. The optimization of 1,3,5 tri-iodinated benzene, diatrizoate, ioxaglate contrast agent was done in order to calculate the energetic behavior and dipole moment of the title compound in gas phase and water. To support that we will comparing these results with UV-visible and IR excremental data. The total energy for different orbital transitions, energy gap between HOMO and LUMO, electro-negativity, chemical hardness, softness, electrophilicity index and dipole moment have been calculated with cep-4g, cep-31g, cep-121g and B3lyp/lanl2dz levels. The four important molecular orbitals (MO) for the title molecule: the second highest and highest occupied MOs and the lowest and the second lowest unoccupied MOs which were denoted as HOMO-1, HOMO, LUMO and LUMO+1, respectively are the critical parameter in determining molecular electrical transport properties because it is a measure of electron transition. The surfaces of HOMO-1, HOMO, LUMO and LUMO+1 for diatrizoate are given in Figure. 1 to understand the bonding scheme of present compound.

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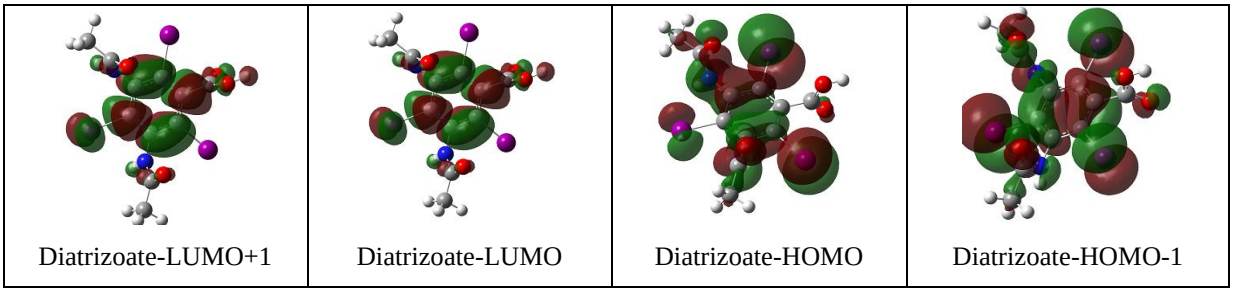

Figure 1. HOMO-1, HOMO, LUMO and LUMO+1 for diatrizoate

Keywords: Diatrizoate, Ioxaglate, CEP

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THYROZINASE, ANTIOXIDANT, TOXICITY EVALUATION OF THE NOVEL BORON COMPOUND OBTAINED FROM 3-METHOXY CATECHOL AND 4-METHOXYPHENYLBORONIC ACID

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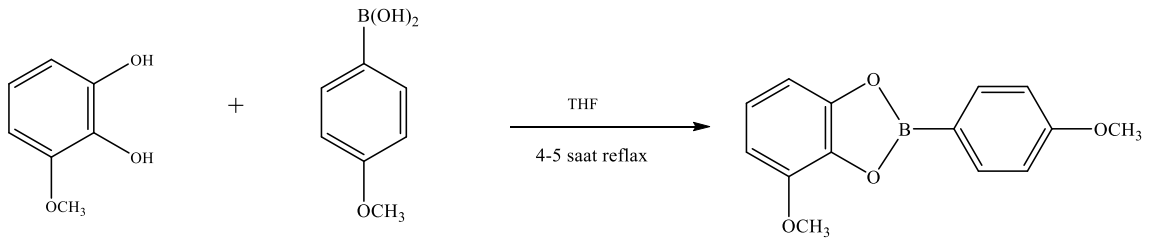
Abstract: Boron is an extremely valuable mineral and it is used in many products from cookware and medicine to nuclear waste storage and space exploration. Boron compounds are mainly used in borosilicate glass products, but are also used in agriculture, in fire retardants, and in soaps and detergents [1, 2]. In this study, new boron-derived compound synthesized by reacting 3-methoxy catechol compound with 4-methoxyphenylboronic acid and obtained compounds characterized by ^{1}H, ^{13}C NMR, UV-Vis., FTIR etc. Synthesis of ligand: 2 mmol (0.280 g) of 3-methoxy catechol was dissolved in 25 mL of THF. 1 mmol (0.152 g) of 4-methoxyphenylboronic acid was then dissolved in 10 mL of THF and added to the reflux flask. The reaction was maintained at 120 ° C for 4-5 hours. After heating, the solid substance in the solution was crystallized and washed in THF and dried. The cytotoxic activities of this new compound was evaluated by MTT method against 3 cell lines, antioxidant activities by ABTS cation radical decolorization method, cupric reducing antioxidant capacity assay and DPPH free radical scavenging activity methods. In addition, tyrosinase activities of this component was determined. As a result, the obtained new compound showed good degree activity in the three antioxidant activities. This compound is found to be more active than BHT and α-tocopherol in DPPH, ABTS and CUPRAC methods. The DPPH and ABTS methods of this compound was found to have IC50<1. In general, when looking at the cytotoxic and thyrozinase activities of this compound was found very low, despite this their antioxidant activities were found at high levels.



Scheme 1. Synthesis stages of compound.

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Keywords: Thyozinase, antioxidant, toxicity, 4-methoxyphenylboronic acid.

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DUMP OF THE BEAM AT LINEAR ACCELERATORS

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Abstract: Linear or circular accelerator systems are used to have very high energetic beams at the order of GeV or TeV. With the electromagnetic field applied to the Superconducting or normal conducting accelerating cavities allow the electron beam to gain energy, while the electron beam also loses some of its energies throughout the accelerating system. To trap the electron beam that lost its energy and to measure the beam current an instrument that is called Faraday Cup is placed under the ground in the accelerator system hall. In this study, electron beam parameters that are optimized by utilizing Astra Code are used to determine Faraday Cup's sizes and material properties [1]. Astra Code is used to track particles along the beamline and also transverse directions for all phase space. For whole accelerator system, Faraday Cup design is simulated and desired simulation measurement studies are configured in four location along the beamline. These four locations are at the exit of the photocathode gun, right after the buncher, entrance of the undulator, and after the undulator. At these locations, energy distribution of the beam versus beamline, radiation dose of the beam, and beam currents through the beam directions are studied and simulated in more detailed way by using FLUKA code [2]. Depending on the beam energy, Faraday Cup's sizes are changing to able to trap particles.

Keywords: Faraday Cup, Radiation Dose, Photocathode Gun, Linear Accelerator

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[2] https://www.fluka.org

* *Corresponding author; Tel.: 05359440088 E-mail:* hdyildiz@ankara.edu.tr

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INVESTIGATION OF NATURAL GAMMA DOSE RATES FOR EDİRNE, TURKEY

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[2] *Namık Kemal University, Environmental Engineering Department, 59860, Corlu, Tekirdağ, Turkey*
[3] *Yıldız Technical University, Faculty of Arts and Sciences, Physics Department, Davutpaşa Campus, 34220 Esenler, Istanbul, TURKEY*

Abstract: Edirne is a city in the eastern Thrace region of Turkey [1]. In this study, a total of 14 stations were selected from the central district of Edirne and measurements were taken with a scintillation detector SP6 (via using portable counter ESP2, Eberline). The measurements were performed to determine the natural background radiation level of the central district of Edirne. The average gamma dose rates obtained from 14 stations were calculated as 38,5 nGy/h. Also, the average annual effective dose equivalent to the public was calculated to be about 47,3 μSv/y. The results checked against the world average determined by UNSCEAR. In conclusion, results were evaluated to determine whether the region carries risk or not in terms of live health [2, 3].

Keywords: Scintillation detector, Gamma dose rate, Edirne, Turkey

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IBM-1 AND SM CALCULATIONS ON THE EVEN-EVEN Fe ISOTOPES

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[2] *Department of Physics, Sivas Cumhuriyet University, Sivas, Turkey*

Abstract: In this work, interacting boson model (IBM) [1] and shell model (SM) [2] calculations have been performed to investigate some nuclear properties of the even-even $^{50-52}$Fe and $^{56-70}$Fe nuclei along to Z=26 isotopic chain. For this investigation, the energy levels and B(E2) values of these isotopes have been calculated in the scope of interacting boson model-1 and the nuclear shell model. The multipole Hamiltonian form was selected for the IBM-1 calculations. For the shell model calculations, 20Ca nucleus was considered as inert core and pfg single particle orbitals on this core were used as the model space. Different nucleon-nucleon interactions were used for two-body effective interactions. KShell, NuShell and Bigstick softwares were used for the SM calculations. The obtained results have been compared with each other and the experimental data [3,4]. A good agreement was observed between them.

Keywords: Nuclear Structure, Energy Level, B(E2) value, Interacting Boson Model, Shell Model.

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MONOVACANCY IN PHOSPHORENE RIBBONS

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Gebze Technical University Physics Department 41400 Gebze KOCAELİ

Abstract: We have investigated the reconstruction, energetic and electronic structure of monovacancy in phosphorene [1] ribbons as the monovacancy moves from the ribbon center to the edge. We considered three type of ribbons with symmetric(armchair), asymmetric(zigzag) and cliff geometries, which are depicted in Figure 1. In this work all calculations were performed in Spanish Initiative for Electronic Simulations with Thousands of Atoms (SIESTA). The generalized gradient approximation (GGA) in the form of the Perdew Burke-Ernzerhof (PBE) functional was used. We used 120,110 and 100 atoms for asymmetric, symmetric and cliff geometries. All calculations which we performed in SIESTA are non-spin polarized. We find that monovacancy reconstructs and shows four-coordinated P atoms. The total energy exhibits an alternating behavior when the defect is shifted to next atomic site, revealing that the reconstruction strength depends on the defect orientation with respect to ribbon axis. Approaching the edge, total energy is reduced by ~1.5 eV in symmetric and asymmetric ribbons while energy gain by moving to edge for cliff ribbons is negligible. This is partly because of the structural instability of the cliff shaped ribbons. In symmetric and asymmetric ribbons, the reconstruction is seamless, and the defect state forms a delocalized state with a free electron-like dispersion near the Fermi level. Thus, the ribbon shows a metallic character although pristine ribbon is semiconductor. In cliff shaped ribbons, shown in Figure 1(c), the defect state is a localized state at the Fermi level with little or no dispersion, which depends on defect distance to the edge. Note that pristine cliff geometry is energetically less stable, reflecting the strain in this configuration. Such flat bands near the Fermi level indicate electronic instability that may lead to either spin polarization or symmetry lowering structural transitions. The profile of the ribbon determines if the defect heals seamlessly. The electronic structure is significantly modified by monovacancy.

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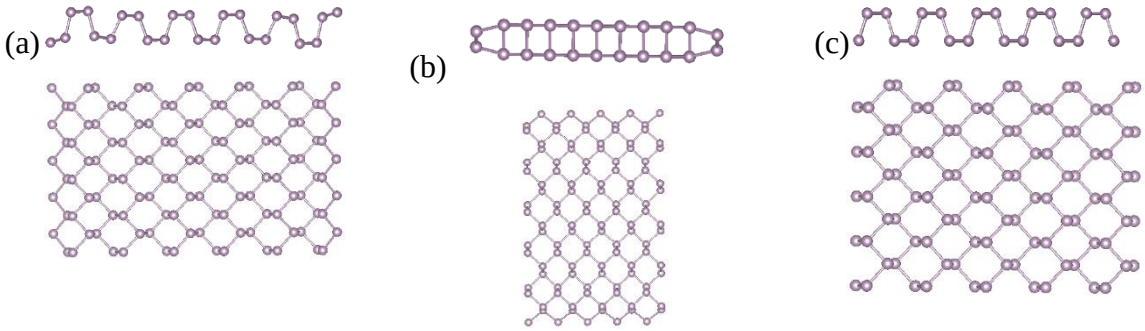

Figure 1. Atomic structures of (a) asymmetric, (b) symmetric and (c) cliff phosphorene ribbons are depicted as ball-and-stick models from top and side view.

Keywords: Phosphorene , Armchair , Zigzag, Cliff , SIESTA, GGA, PBE, Monovacany, Semi,Conductor, Metallic

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ANALYZING THE RELATIONSHIP BETWEEN SUNSPOT NUMBERS AND THUNDERSTORMS OVER TURKEY CASE STUDY; ANKARA REGIONAL STATION AND ANKARA ESENBOĞA AIRPORT STATION

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[2] *Turkish State Meteorological Service Research Department Hydrometeorology Division*

Abstract: This study aimed to understand the relationship between sunspot numbers and thunderstorms that are under both Space Weather and Atmospheric Electricity for Turkey. For this purpose, weather stations of Turkish State Meteorological Service at Ankara Regional Directorate and Ankara Esenboğa Airport were chosen. Counts of thunderbolt/lightning between 1960 and 2017 were prepared as annual and monthly time series and Pearson Correlation is calculated for relationship and Mann Kendall method is used for the trend. It has been observed and determined that there is positive and weak correlation between sunspot numbers and thunderstorms in 57 years. However, when the sunspot cycles between two maxima or two minima have been evaluated, the relationship can be both negative and positive. When results of this study are merged with the results of other countries in literature, it will contribute the global understanding of the behavior of thunderstorms with observing sun and forecasts of sunspot numbers. Additionally, the relationship between thunderstorms and climate causing extreme rain events can be determined and used as initial conditions for forecasting thunderstorms to mitigate loss of lives and properties.

Keywords: Thunderstorms, Sunspot Numbers, Mann Kendall, Pearson Correlation, Atmospheric Electricity

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CUBIC BORON NITRIDE (c-BN) HOLLOW NANOPARTICLES IN WATER: A MOLECULAR DYNAMICS STUDY

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Abstract: Cubic Boron Nitride (c-BN) is the second highest hardness material which ranks next to diamond. However, size of c-BN material reduced below the 10nm scale, is rather challenging, its interesting properties can be explored [1].

Herein, a computational model is first presented to investigate the stability and structural properties of the spherical hollow c-BN nanoparticles in water by classical molecular dynamics (MD) simulations. The SPC water model is used for the model interactions in water. The two hollow c-BN NPs, sub<5nm constructed with different shell thicknesses were simulated under continuous heating. The pair radial distribution functions (RDF) and self-diffusion coefficients of the free-standing hollow c-BN NPs have computed at 300K and compared with those obtained in water. We have observed the comparatively strong interactions between B and N atoms in the c-BN hollow NPs with diameters sub<2nm. The small phase separated boron clusters have formed at around the hollow interior of the nanoparticles in water. The coordination of B-N atoms for the hollow BN-NPs –water system has rather changed in comparison without water. The results show that the hollow c-BN NPs with diameters of sub<2nm can be an easily solved in water. However, there have no reported studies so far on the transport and structural properties of spherical hollow c-BN NPs in water for comparison.

Keywords: Cubic Boron-Nitride, Hollow Nanoparticles, c-BN-water, MD simulations

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INVESTIGATION OF THE STRUCTURAL PROPERTIES OF $(Au\text{-}Co\text{-}Pd)_N$ TERNARY NANOALLOYS

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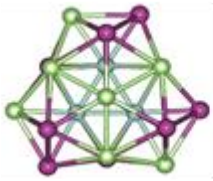
Abstract: Alloys and nanoalloys receive much attention because of their numerous potential applications in various fields like metallurgy, catalysis, magnetism, optics and health [1]. One of the main scientific challenge is to model their structure and properties as accurately as possible for experimentalists to the design of new materials with targeted properties. This study focuses on the structural properties of (Au-Co-Pd)N (N=19,23,26,34,38,55) ternary nanoalloys. To determine the most stable structures, the optimizations were performed by the Basin-hopping algorithm [2][3]. The Gupta many-body potential [4] was used to model interatomic interactions. To investigate the effects of composition on structural properties, the number of cobalt atoms was fixed, and the number of palladium and gold atoms was varied for all other compositions. It was predicted that the Pd and Au atoms mainly occupy the surface sites and Co atoms tend to be in the core of the ternary nanoalloys due to the lower surface and cohesive energy in comparison with palladium and gold. As a result of the performed geometry optimization, we obtained polyicosahedral structures for N=19, 23, 26 and 55 atoms. Relative stability investigation were performed using excess energy calculations. Common neighbor analysis (CNA)[5] signatures have been used for structural classifications. As a results of excess energy analyses, we obtained the most stable compositions for fixed number of Co atoms.

$Au_{10}Co_2Pd_7$



$Au_{10}Co_3Pd_{10}$

$Au_{10}Co_4Pd_{12}$

$Au_{19}Co_{13}Pd_{23}$

Keywords: Ternary Nanoalloys, Optimization

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AB INITIO INVESTIGATION into STRUCTURAL, MECHANICAL and ELECTRONIC PROPERTIES of W_5GE_3

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Abstract: Germanides formed by transition metals commonly exhibit outstanding thermal stability, oxidation resistance, high stress and compressive strength, which is quite suitable for the applications at elevated temperatures [1]. W5Ge3 have been synthesized [2-4] at high pressure (0.75-7.7 GPa) and at high temperature (600-2500 C) long time ago. In this study we report a compherensive theoretical study on the mechanical and electronic properties of W_5Ge_3 within the framework of density functional theory, as implemented in the VASP package [5]. Generalized gradient approximation has been used for modelling exchange-correlation effects. The Elastic constants, Bulk modulus, Shear modulus, Young's modulus, Poisson's ratio, Debye temperature, Shear anisotropic factors and the Elastic anisotropy are obtained and analyzed for the first time. Furthermore, electronic band structure calculations have been done and also discussed.

Keywords: First-principles, W_5Ge_3

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THERMAL STABILITY of ICOSAHEDRAL SHAPED $Pd_mPt_{(13-m)}Ag_{42}$ TERNARY NANOALLOYS: A MOLECULAR DYNAMICS STUDY

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Abstract: In this study, the structural and dynamical properties of 55 atom $Pd_mPt_{(13-m)}Ag_{42}$ ternary nanoalloys were investigated theoretically. In atomistic simulations, the Gupta many-body potential has been employed to describe the interatomic interactions [1][2]. The global minimum optimizations were performed by using the Basin-hopping algorithm [3]. It was resulted that all compositions of $Pd_mPt_{(13-m)}Ag_{42}$ ternary nanoalloys were obtained as icosahedral. Silver atoms predominantly segregate to the surface due to the lower surface and cohesive energy in comparison with palladium and platinum. We used classical Molecular Dynamics (MD) simulations in canonical ensemble conditions (NVT) to investigate the melting temperatures of ternary $Pd_mPt_{(13-m)}Ag_{42}$ nanoalloys. MD simulations were performed by DL_POLY_4 software [4]. The optimized icosahedral structures were taken as the initial configurations for MD simulations. The heating was started from Global Minimum structure to 1300 K with the increments of 1 K for avoiding the large temperature fluctuations. The traditional indicators of melting, Lindemann criterion and caloric curves were used to determine the melting temperatures. No simple correlation has been determined between alloy composition and melting temperatures. The highest melting temperature is about 734 K for $Pd_9Pt_4Ag_{42}$ composition. $Pd_8Pt_5Ag_{42}$ is the most stable composition according to the relative stability investigation. The simulation results showed that the melting takes place as a whole without any surface premelting.

Keywords: Optimization, Melting, Palladium, Platinum, Silver.

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ADVANCED TECHNIQUES IN MOLECULAR DYNAMICS, APPLICATION TO A SOLID MATTER

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Abstract: It is important to make a simulation prior to an experiment to test experiment conditions, and to reduce expenditures, and also for the cases where an experiment implanting is impossible. There exist many simulation techniques which achieve satisfactorily good results with that of experiments. However, physics behind the methodology of simulations contains some artefacts. Aim of this review is to clarify those effects, and to explain so far known solutions particularly for Molecular Dynamics (MD). The artefacts have two main sources: Firstly, from the nature of simulation, where the number of particles in the sample is much fewer than the real experiments [1,2]. To solve that problem some models are being used, however they bring some artefacts together. In this work, simple solutions to avoid these will be shown [3]. Second source is due to inherent properties of MD simulations, one of which is the lack of ergodicity [1,2]. An ergodicity model solution to implant in an MD code was introduced by Hundur [3], the results were in good agreement with the available experiments [4,5].

Keywords: Simulation artefact, molecular dynamics, ergodicity model

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QUANTUM CHEMICAL STUDY ON RELATIONSHIP BETWEEN STRUCTURE OF SOME THISEMICARBAZIDE AND TETRAZOLE DERIVATIVES AND THEIR INHIBITION PERFORMANCE

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Abstract: Semicarbazide, known as carbohydrazide, is the chemical compound with the formula $OC(NH_2)(N_2H_3)$. It is a water-soluble white solid. It is a derivative of urea prepared by treating urea with hydrazine. A thiosemicarbazide is the analog with sulfur atom in place of oxygen atom. Semicarbazones are derived by the condensation reaction between a ketone (or aldehyde) and a semicarbazide. Thiosemicarbazide derivatives were tested as corrosion inhibitors for steel in HCl, HNO3 environments, however, very little work was published on copper in chloride environments.

In the present work, relationships between corrosion inhibition efficiency of two thiosemicarbazide and based compounds namely; 4-phenyl thiosemicarbazide (PTSC), Salicylaldehyde thiosemicarbazone (STSC) and one tetrazole derivative; 5-phenyl-1-H-tetrazole (PTAH), and their molecular electronic properties have been theoretically studied at the level of DFT/B3LYP with 6-31+G (2d, 2p) base sets. These compounds are also tested as corrosion inhibitors for copper in sea water using polarization techmiques. The structural parameters, such as energy, highest occupied molecular orbital (HOMO) energy and lowest unoccupied molecular orbital (LUMO) energy, the charge distribution of the studied inhibitors, the absolute electronegativity (χ) values were calculated and discussed using linear regression analysis to determine the most effective parameters to establish inhibition efficiency.

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The calculated and experimentally measured inhibition efficiencies (Table 1) show that PTAH posses the highest inhibition efficiency (93%), followed by TSCS (81%), while PTSC gives very low inhibition efficiency (16%). The table shows an agreement between the theoretical and experimentally measured inhibition efficiencies.

Table (1): Calculated and measured inhibition efficiencies

rb3lyp/6-311++g(2d,2p)	**β-Total**	**Calculated IE%**	**Measured IE%**
PTAH	0.624317772	93	91
STSC	71.46529503	81	81
PTSC	8.329364392	16	0.0

Keywords: Quantum chemical calculations, inhibition efficiency, corrosion inhibitors, copper.

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Ge QUANTUM DOTS (QDs) ENCAPSULATED IN FULLERENE C_{720}

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Abstract: A size dependent stability of quasi-spherical Germanium Nanoparticles Ge-NPs with a diameter of sub<5nm, which is different from the cubic diamond structure of bulk crystalline Ge [1,2] have investigated by molecular dynamics simulations under continuous heating. In order to understand the quantum size effect on the thermal stability and atomic structure of nano size Ge, carbon based nanostructures such as a carbon nanocage is used. The monocrystalline Ge quantum dots (QDs) were carried out with a high fullerene C_{720} in MD simulations. The stability of Ge QDs @C_{720} core-shell structures with diameters of between 2-2.4nm are first reported. Results are compared with those obtained for free standing Ge QDs.

The stability of free standing and fullerene encapsulated Ge QDs was observed to be dependent on the nanoparticle size with smaller nanoparticles exhibiting less stability. The hollow carbon C720 cage affects more amorphous phase transformation for the Ge QDs while comparing the atomic structure and cohesive energy of free and encapsulated QDs each other.

Keywords: Ge quantum dots, Ge nanoparticles, Fullerene C_{720}

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ICOSAHEDRAL BORON CARBIDE NANOCRYSTALS GROWN INSIDE DLC TEXTURE BY HFCVD

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Abstract: In this research, carbon nanostructures doped by boron atoms to synthesize Boron doped diamond like carbon (BDDLC), through DLC texture grown icosahedral boron carbide nanostructure to achievement used hot filament chemical vapor deposition (HFCVD) regime. Raman spectroscopy of BDDLC revealed two broad peaks centered on 1334 cm^{-1} and 1573 cm^{-1}, the origin of which is sp^3 hybrid of disorder (D-band) and sp^2 hybrid of graphite (G-band), respectively (Fig. 1). These peaks stem from aromatic compounds with sp^2 hybrid, demonstrating a local collection of amorphous B_4C on the substrate surface. Furthermore, D and G peaks are illustrative of more damage inside the structure. X-ray diffraction (XRD) characterization indicated significant peaks assigned to icosahedral ($B_{13}C_2$) structures in planes (012), (021), and (024). Particles size calculated by Debye-scherrer formula is between 0.8-7 nm. Additionally, Tuinstra – Koenig formula at a 42-73 nm interval, evaluated the graphite grain size. The decrease observed in the intensity of G and D peaks may stem from disrupting the vibrational behavior of the film and diminution of polarizability in the molecules of the lattice. One of the factors inducing the decrease of polarizability may be the promotion of a great fraction of δ bonds between B-C atoms. Through cauliflowers morphology observed in field emission Scanning electron microscopy (FE-SEM) images (Fig. 2), it could be apparently seen that the increase of boron concentration leads to the augmentation of chain crack on the surface and raising the amount of doped boron gives rise to a smoother and more uniform surface. It was observed that the cracks on the surface increase by increasing boron doped in the grown film, as seen in Fig. 2 (a)-(d).

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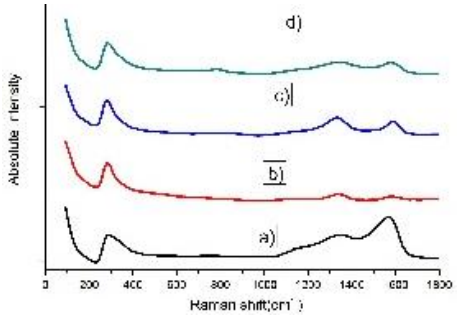

Figure 1. Raman spectra with 532 nm wavelength from samples shows evolutions in positions, boron doped in DLC films.

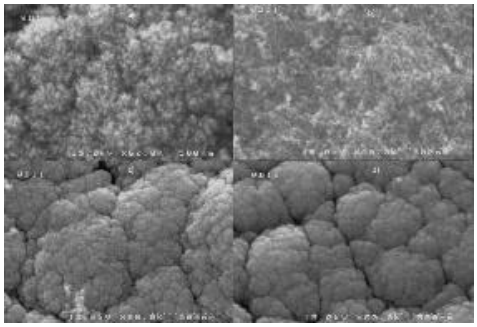

Figure 2. FE-SEM images show boron doped DLC films in different contents a) 0.00625, b) 0.0125, c) 0.025 and d) 0.05 molar.

Keywords: Diamond like carbon (DLC), Icosahedral, Cauliflowers

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THEORETICAL AND EXPERIMENTAL STUDIES FOR THE CORROSION INHIBITION POTENTIALS OF (4-(2-METHOXYPHENYL)-3-THIOSEMICARBAZIDE) FOR MILD STEEL IN 1.0 M HCL

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Abstract: The adsorption behavior and inhibition mechanism of (4-(2-Methoxyphenyl)-3-thiosemicarbazide) (2Metho-TSC) on corrosion of mild steel in HCl were studied by potentiodynamic polarization AC resistance and current voltages in 1.0 M HCl at 293 K. While Ecorr value was -0.518 mV in uninhibited solution, it shifted slightly in the positive direction in inhibited solutions with the increase of inhibitor concentration. The currents density of anodic and cathodic regions has lower compared to that of 1.0 M HCl solution. icorr value was 158.78 $\mu A \cdot cm^{-2}$ in uninhibited solution and 15.64 $\mu A.cm^{-2}$ at the 1×10^{-2} M concentration of 2Metho-TSC. When the inhibitor concentration increases, the corrosion current density value decreases, and the suppression efficiency value increases. The percentage inhibition efficiency values ranged of 2Metho-TSC from 68 to 90 %. The values of R_{pblank} and R_{pinh} are 110 and 1019 $\Omega.cm^{-2}$, CPE_{blank} and CPE_{inh} are 348 and 15 $\mu F.cm^{-2}$ respectively. As the Rp value increases, the CPE value decrease as the inhibitor concentration increases, most likely due to decreased local dielectric constant and/or increased thickness of the metal/solution interface. The adsorption of corrosion inhibitor on the surface of mild steel conforms to the Langmuir model [1]. Adsorption equilibrium constant and adsorption free energy were determined. The value of $\Delta G°_{ads}$ is -37.8 $kJ.mol^{-1}$ of 2Metho-TSC, it is suggested that the adsorption of these inhibitors involve two types of interactions chemisorption and physisorption.

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The density functional theory (DFT) at the B3LYP functionals with the 6-311G (d,p) basis set were performed for 2Metho-TSC.

Table 1. The calculated parameters by B3LYP/6-311G (d, p) of molecules.

6-311g(d,p)	HOMO (eV)	LUMO (eV)	Energy gap (eV)	Hardness(eV)	Softness(eV)
2-Meth	-5.606	-0.684	4.922	2.461	0.203
2-Meth-wat	-5.965	-0.995	4.970	2.485	0.201
2-Meth-p	-9.307	-5.245	4.062	2.031	0.246
2-Meth-wat-p	-6.379	-1.815	4.564	2.282	0.219

Keywords: Corrosion, Inhibition, Mild steel, Thiosemicarbazide, Quantum chemical studies.

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OPTIMIZATION and MELTING DYNAMICS of PtAlCu TERNARY NANOALLOY

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Abstract: Ternary nanoalloys are mainly formed by the combination of three different metals and they have attract great interests due to their potential applications in optical, electronic, magnetic, and catalytic fields [1,2]. Important effects in catalytic activities on metal surfaces are the alloying effect, size and composition [3,4]. Especially, the Pt-alloy catalysts have drawn most of attention. Since the surface structures of Pt-alloys strongly affect the catalytic performance, a thorough study of their surface structures is important for the syntheses and applications of Pt-alloy catalysts [5].

In this study, a theoretical investigation of PtAlCu ternary nanoalloys, consisting of N = 38 and N = 55 atoms, was carried out by modeling interatomic interactions with the Gupta many-body potential energy function [6,7]. The lowest energy structures for all compositions of $Pt_6Al_nCu_{32-n}$ (n=0-32) and $Pt_{13}Al_nCu_{42-n}$ (n=0-42) ternary nanoalloys were obtained using the Basin Hopping algorithm [8,9]. $Pt_6Al_{17}Cu_{15}$ was determined the most stable structure for $Pt_6Al_nCu_{32-n}$ and $Pt_{13}Al_{25}Cu_{17}$ was determined to be the most stable structure for $Pt1_3Al_nCu_{42-n}$. The melting behavior of the most stable $Pt_6Al_{17}Cu_15$ and $Pt_{13}Al_{25}Cu_{17}$ ternary nanoalloys, found by optimization, were investigated using the Canonical Molecular Dynamics Simulation method [10]. We obtained the melting temperatures of the $Pt_6Al_{17}Cu_{15}$, $Pt_{13}Al_{25}Cu_{17}$ to be 610 K and 620 K, respectively.

The simulation results show that the melting temperatures of PtAlCu nanoalloys vary depending on the composition. Molecular dynamics simulations allow ones to synthesize and develop a new functional nanostructured material by controlling atom types in nanoalloys and by increasing the size of nanoalloys to guide the experimentalists.

Keywords: Ternary nanoalloy, Molecular dynamics simulation, Gupta potantial, Global optimization

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LATEST RESULTS ON ASSOCIATED PRODUCTION OF A VECTOR BOSON JETS FOR STANDARD MODEL PHYSICS

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Abstract: The production of vector bosons (V = W, Z or γ) associated with jets (V+Jets) is very important for both the Standard Model(SM) and the Beyond the Standard Model(BSM) searches. V+ Jets searches provide precision tests for Monte Carlo based event generators and perturbative Quantum ChoromoDynamics (pQCD) calculations [1, 2]. It is also important for most of the SM and BSM analysis because it is very common background source for many analysis decay channels like Higgs Searches, Supersymmetry(SUSY) searches etc. The production cross section of highly boosted vector bosons recoiling against jets is studied, differentially as function of the transverse momentum and angular correlations of the final state particles [1]. The measurements are confronted with different state-of-the-art theory predictions that include next-to-leading order calculations and matrix-element plus parton shower event simulations.

Keywords: Standard Model, Perturbative QCD, Vector Boson plus Jets,

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INVESTIGATION OF OPTICAL PROPERTIES OF LIQUID CRYSTALS IN HEXAGONAL STRUCTURE BY LIGHT SCATTERING

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Abstract: The computer modeling of light scattering and its propagation through columnar disc liquid crystal, shaped hexagonal is presented. Light propagation through a columnar disc 2,3,6,7,10,11-hexaheptyloxytriphenylene format in H7T is represented by using a cylindrical model by using the transverse magnetic (TM) and the transverse electric (TE) conditions. Numerical aspects of the light scattering process, which are based on numerically solved Maxwell's equations, are calculated for a hexagonal liquid crystal. We described in detail how we computed the circular cylindrical model of light scattering from a columnar hexagonal liquid crystal and presented results of benchmark computations for our model. These results are associated with our previous studies on liquid crystals [1-3].

Keywords: Light Scattering; Liquid Crystal; Columnar Disc; Computer Modelling

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DIELECTRIC PROPERTIES OF MOS DEVICE BASED ON TiO_2/SiO_2 OXIDE LAYER

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Abstract: The metal-oxide-semiconductor (MOS) structure consists of a metal contact separated from the semiconductor by a dielectric material. In this study, the MOS device with double oxide layer was fabricated. The dielectric properties of the MOS device based on TiO_2 (100 nm)/SiO_2 (10 nm) oxide layer have been investigated by using the frequency dependent admittance (Y=G+iωC) measurements. For electrical measurements, the both ohmic back and rectifier front contacts were formed by thermal evaporation system using high purity Au (99.999%) metal with thickness of 150 nm. The admittance measurements were carried out in the frequency range of 1 kHz – 5 MHz and at room temperature. The values of dielectric parameters such as dielectric constant (ε'), loss (ε''), loss tangent ($tan\ \delta$), ac conductivity (σ_{ac}) and complex modulus (M^*) of the MOS device were calculated using the capacitance and conductance data [1-3]. The experimental results show that the ε' and ε'' values decrease with increasing frequency. Moreover, the σ_{ac} value increases with increasing frequency.

Keywords: MOS structure, admittance measurements, dielectric constant and loss, ac conductivity, modulus.

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DETERMINATION of OUTDOOR GAMMA DOSE RATES in YALOVA, TURKEY

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Abstract: Today, environmental radiation measurements are made in order to investigate the radioactivity levels of a region. By measuring natural background radiation, it is possible to show how much radiation people are exposed to [1, 2].

Yalova is a city located at the entrance of the Izmit bay and coastline to the Marmara Sea [3]. The main purpose of this study is to determine the natural background radiation level of Yalova. For this aim, 36 different stations were determined from the districts of Yalova and measurements were taken with a portable scintillation detector SP6 (via using portable counter ESP2, Eberline). When the measurements are analyzed, outdoor gamma dose rates in air were found ranging from 27.7 nGy/h to 64 nGy/h. And, the average gamma dose value of the study area was calculated as 48.1 nGy/h. Also, the mean equivalent dose rate expected to be taken annually by a person was calculated as 60.65 μSv/y. In conclusion, this study was compared with different studies and UNSCEAR report.

Keywords: Gamma dose rates, Scintillation detector, Yalova, Turkey

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HF and DFT STUDIES of DISODYUM OKTABORAT TETRAHIDRAT

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Abstract: Inorder to obtain abundant and high quality products, Nitrogen, Phosporus and Potassium based fertilizers are not enough to provide balanced nutrition in plants [1]. In modern agricultural industry, there are some elements, which should not be inevitable for feeding of the plants. On the top of these elements, bor directly affect the quality of products, but the amount of it should be determined carefully. Its possible side effects can be reduced by decreasing or increasing the amount of the H_2O molecule [2]. As a preliminary work, in this study, Disodyum Oktaborat Tetrahidrat (Figure 1) used as boron fertilizer are optimized via performing Hartree–Fock (HF) and DFT (B3LYP) methods with STO-3G and 6-311++G(d,p) basis set [3]. The energetic and structural quantities such as, HOMO-LUMO energies, zero point energies, vibrational frequencies, bond lengths and bond angels fort he obtimized compounds were examined and it was investigated the changes in the values of the considered parameters with respect to the different amount of H_2O molecules. It is observed that the considered molecular systems can be studied with the selected methodolgy.

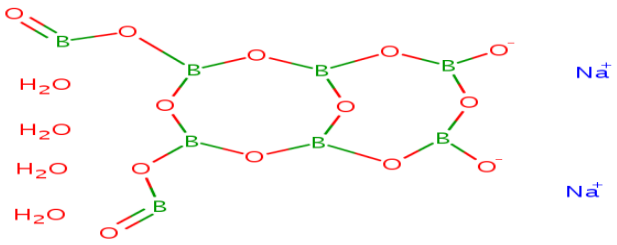

Figure 1 Disodyum Oktaborat Tetrahidrat

Keywords: Disodyum Oktaborat Tetrahidrat, HF, DFT.

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EFFECT OF SYNTHESIS TEMPERATURE ON THE PARTICLE SIZE AND OPTICAL ENERGY BAND GAP OF Ni DOPED CdS NANOPARTICLES

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Abstract: In the present study, Ni-doped CdS nanoparticles (NPs) were synthesized at 55 ^{0}C and 100 ^{0}C via wet chemical precipitation method [1, 2]. The particle size of Ni-doped CdS NPs prepared at 55 ^{0}C and 100 ^{0}C was calculated as 1.9 and 2.2 nm, respectively using the Scherrer's equation. This result indicates that the XRD patterns of Ni-doped CdS NPs get broader upon decreasing the synhtesis temperature. In other words, it can be said that the size of NPs decreases as the synthesis of temperature decreases. The energy band gap of NPs was determined from the UV-Vis spectroscopy. It was observed that the energy band gap of Ni-doped CdS prepared at different temperatures increase with the decrease in the particle size owing to quantum confinement effect. Our results suggest that the synthesis temperature can be an alternative method to alter particle size and energy band gap of NPs [3,4].

Keywords: Band gap, characterization, nanoparticles, particle size, synthesis

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RF FIELDS AND ACCELERATING PARTICLES

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Abstract: We study simulation of the effect on the RF field to accelerate the particles. RF field is applied to the accelerator cavities in order to obtain uniform electromagnetic field distribution inside the cavity. Nowadays, particle beams can be accelerated up to 20 GeV in the Linac Coherent Light Source at SLAC and Eurofel Facilities by using superconducting Tesla type cavity technologies [1,2]. In our studies, we obtained in our simulation studies approximately 4 GeV electron beam energy by using superconducting Tesla type accelerator cavities. In this study, in addition to acceleration of electron beam dynamics by utilizing RF, we also present field problems and mechanical problems that effect beam acceleration of the system. One can be placed many accelerator cavities with beam diyagnostics system, cooling system, and other accelerator components on a beamline by using Superfish/Poisson and Computer Simulation Technology Codes. When the particles from photocathode gun passes through to the accelerator cavities, many beam, accelerator, and field parameters are studied in more detail, optimized and will be presented.

Keywords: RF Fields, Superconducting Accelerator Cavities, Photocathode Gun, Beam Dynamic

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THE OPTICAL AND STRUCTURAL PROPERTIES OF ZnO NANORODS

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Abstract: In photovoltaic (PV) devices, a transparent conducting oxide (TCO) film is used as a transparent electrode which permits sun rays to reach to the photoactive semiconducting layers and also to collect the photogenerated electrons. Also, transparent conductive oxides (TCOs) are a very important part of solar cells substructure [1]. Among the conductive oxides, ZnO is a remarkable preferred transparent conductive oxide because of its beneficial electrical and optical features [2,3]. For their optoelectronic features nanostructures zinc oxide (ZnO) materials are used as a plentiful and economic option for TCOs.

In this work, ZnO thin films were produced in nanorod form on lamellar glass by using hydrothermal and spin coating techniques. The ZnO thin films were defined using UV-Vis spectra, field emission electron microscopy (FE-SEM) and X-ray diffractometer (XRD). The XRD peaks were determined as a hexagonal wurtzite cell structure. The FE-SEM photograph illustrated that the structure of samples has nanorod shape particles. The average size of the nanorod diameter is between 50 and 100 nm. Also, the ZnO samples are highly transparent and the optical transmittance values is over 85%.

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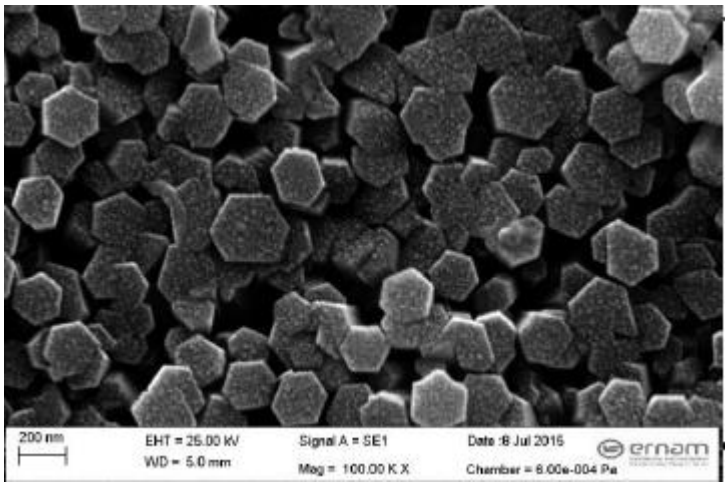

Scheme 1. FE-SEM image of ZnO nanorod.

Keywords: ZnO, TCOs, Hydrothermal Method, Spin Coating Method.

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