

5th



30 October – 01 November, 2020

**Istanbul Ayvansaray
University
Istanbul, Turkey**



ABSTRACTS BOOK

 / taegcenter

 / taeg_center

 / taegcenter

GC-MAS 2019 Participants Flags



GC-MAS 2020

GC-MAS 2020

www.gc-mas.org





**5th Global Conference on Materials Sciences
(GC-MAS 2020)**

30 October – 01 November, 2020

Istanbul Ayyansaray University
Istanbul, Turkey

ABSTRACTS BOOK

Organized by

Istanbul Ayvansaray University

Association for Human, Science, Natura, Education and Technology

Chair

Dogan Ibrahim, Near East University, Cyprus

International Program Committee

Adem Karahoca, Bahcesehir University, Turkey

Adisa Dabardini, Albanian University, Albania

Ahmed Mancy Mosa, Al Mansour University College

Aslıhan Tüfekçi, Gazi University, Turkey

Blerta Prevalla, AAB College, Republic of Kosovo

Ergun Gide, CQUniversity Sydney, Australia

Lejla Abazi, South East European University, Republic of Macedonia

Mehmet Karamanoglu, Middlesex University, UK

Mentor Hamiti, South East European University, Macedonia

Nihat Ekizoğlu, Ataturk Teacher Training Academy

Tahir Tavukcu, Cyprus Social Sciences University, Cyprus

Organizing Committee

Dr. Blerta Prevalla Etemi, AAB University

PhD Candidate. Beria Gökaydın, Near East University, Cyprus

PhD Candidate Semih Çalışkan, Istanbul Aydın University

PhD Candidate Zeynep Genç, Istanbul Aydın University

PhD. Daniel Sekyere-Asiedu, Near East University, Cyprus

Florijeta Hulaj, AAB College

Lilia Trushko, Girne American University

Metin Berk Odabası, Warwick University, UK

Secretariat

Pembe Mehmet, Cyprus International University, Cyprus

gcmass.info@gmail.com

International advisory board

Prof. Dr. Adam Lee, Cardiff University, UK

Prof. Dr. Anthony Cheetham, University of Cambridge, UK

Prof. Dr. Börje Sellergren, Technische Universität Dortmund, Germany

Prof. Dr. Cetin Bolcal, Istanbul Kültür University, Turkey

Prof. Dr. Chang-jun Liu FRSC, Tianjin University, China

Prof. Dr. Dietmar Hutmacher, Queensland University of Technology, Australia

Prof. Dr. Ehud Gazit, Tel Aviv University, Israel

Prof. Dr. Fahrettin Yakuphanoglu, Firat University, Turkey

Prof. Dr. Gianluca Ciardelli, Politecnico di Torino, Italy

Prof. Dr. Greta R. Patzke, University of Zurich, Switzerland

Prof. Dr. Hasan Mandal, Sabancı University, Turkey

Prof. Dr. James Durrant, Imperial College London, UK

Prof. Dr. Jin Young Kim, University of Toronto, Canada

Prof. Dr. Jöns Hilborn, Uppsala University, Sweden

Prof. Dr. Kunio Awaga, Nagoya University, Japan

Prof. Dr. Lapo Bogani, University of Stuttgart, Germany

Prof. Dr. Markus Antonietti, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Prof. Dr. Mehmet Ozer, Istanbul Kültür University, Turkey

Prof. Dr. Michael Guiver, National Research Council of Canada, Canada

Prof. Dr. Neil Hyatt, The University of Sheffield, UK

Prof. Dr. Patrick Grant, University of Oxford, UK

Prof. Dr. Peter Skabara, University of Strathclyde, UK

Prof. Dr. Rasit Turan, Middle East Technical University, Turkey

Prof. Dr. Richard Gross, NYU Poly, USA

Prof. Dr. Stephen Mann FRS, University of Bristol, UK

Prof. Dr. Steven McIntosh, Lehigh University, USA

Prof. Dr. Thomas Albrecht-Schmitt, University of Notre-Dame, USA

Prof. Dr. Timothy Swager, Massachusetts Institute of Technology, USA

KEYNOTES



Prof. Dr. Osman Adigüzel

Department of Physics, Firat University
23169 Elazig, Turkey

Keynote Title: “Lattice Reactions and Interactions Governing Phase Transformations in Shape Memory Alloys”

Bio: Dr. Osman Adiguzel was born in 1952, Nigde, Turkey. He graduated from Department of Physics, Ankara University, Turkey in 1974 and received PhD- degree from Dicle University, Diyarbakir-Turkey in Solid State Physics with experimental studies on diffusionless phase transformations in Ti-Ta alloys in 1980. He studied at Surrey University, Guildford, UK, as a post-doctoral research scientist in 1986-1987, and his studies focused on shape memory alloys. He worked as research assistant, 1975-80, at Dicle University, Diyarbakir, Turkey. He shifted to Firat University in 1980, and became professor in 1996, and He has already been working as professor. He published over 45 papers in international and national journals, He joined over 60 conferences and symposia in international and national level with contributions of oral or poster, and He supervised 5 PhD- theses and 3 M.Sc theses.

Dr. Adiguzel served his directorate of Graduate School of Natural and Applied Sciences, Firat University in 1999-2004. He received a certificate which is being awarded to him and his experimental group in recognition of significant contribution of 2 patterns to the Powder Diffraction File – Release 2000. The ICDD (International Centre for Diffraction Data) also appreciates cooperation of his group and interest in Powder Diffraction File.

Scientific fields of Dr. Adiguzel are as follow: Martensitic phase transformations and applications to copper-based shape memory alloys, molecular dynamics simulations, alloy modeling, x-ray diffraction, and electron microscopy.



Prof. Dr. Adem KARAHOCA

Istanbul Nişantaşı University
Istanbul, Turkey

Keynote Title: “Smart Technologies and Big Data”

Abstract: Smart cities are enabler of the smart technologies to improve outcomes across every aspect of city operation to give feasible service to residents. Making cities smart can be enabled by using full potential of technology and innovation ecosystems in cities. Implementation of IoT (internet of things) devices, sensors and other methods and approaches to get data from the city operations trigger operational data size and increases the big data. To give real time decisions for the city operations, smart applications and data enabled capabilities must be supported

with big data sets. In this study, smart technologies and big data interaction was analyzed to improve city operations for providing more benefits and opportunities for city residents.

Bio: Adem Karahoca is currently a full-time professor in the Department of Computer Eng. And dean of Engineering and Architecture Faculty, Nisantasi University, Istanbul, Turkey. He received his B.Sc. degree in Mathematical Engineering from Istanbul Technical University, M.Sc. and Ph.D. degrees in Software Engineering from Istanbul University. He has published 20 IT related books in Turkish and edited 4 IT related books in English. His research interests are data mining, fuzzy systems, information systems, business intelligence, computers in education, human computer interaction and big data. His research papers have published in Expert Systems with Applications, Applied Soft Computing, Soft Computing, Neural Computing and Applications, Journal of Biomedical Informatics etc.



Assoc. Prof. Dr. Murat TEZER

Near East University
North Cyprus

Keynote Title: “Teachers’ Opinions on WEB 2.0 Tools And Use In Mathematics Teaching During The Pandemic Period”

Abstract: An important feature of successful math teachers is that they can provide a variety of activities that support students’ learning and assessment. Web 2.0 applications are known to provide a variety of tools to help produce creative activities. A Web 2.0 tool enables the student to enter data and create multimedia products using text, graphics, sound, and video. The possibilities for creativity and variety are unlimited. As a standard, students are expected to demonstrate reasoning and intuition and understanding when solving math exercises. The aim of this study is to examine teachers’ opinions about WEB 2.0 tools and use in mathematics teaching in distance education during the pandemic period. As a research method, interview technique, one of the qualitative research methods, was used in this research. The working group of the research consists of 12 classroom teachers working in primary schools. Suggestions were given as a result of the findings of the research in which the semi-structured interview form was used to collect the data.

Bio: He was born in Nicosia in 1972. After completing his primary education, he completed his high school at Nicosia Turkish Lycee in the year of 1990. In the same year, he started to Hacettepe University at Ankara for BA and graduated in 1994. He completed his MA (1996) and Ph.D. (2003) at the Faculty of Arts and Sciences, Applied Mathematics and Computer Sciences Department of Eastern Mediterranean University. He gave his Ph.D. Thesis about “Cycle Decompositions and Labeling of Graphs” in 2003. Between the years 1994 and 2003, he worked as full-time instructor in the same university. Between the years in 2010-2014 he worked as a project advisor and project assistant at Yenyüzyıl Kindergarten, Karaođlanođlu Primary School, Gönyeli Primary School, amlıbel Primary School, Őehit Hüseyin Ruso Secondary School, Yeşilyurt Primary School in Northern Cyprus and Kurtuluş Lycee and under

the grant program supported by the European Union and also gave these school teachers Smart Board lessons. He gives in-service training courses (statistical software SPSS, further evaluation and assessment, and office programs) to the teachers these working in schools affiliated to the Ministry of Education.



Assoc. Prof. Dr. Nazım Kaşot

Keynote Title: “Teaching Environmental Education Through Technology”

Abstracts: It is very important to share information about the environment, to create awareness and to ensure its sustainability, to connect with and touch people. People need to know that the environment must be protected in order to survive. Addressing environmental problems and eliminating these problems can only be possible if people have environmental awareness. Various media tools and technologies can be used to spread environmental

awareness among people. Everybody knows that social media raise awareness of the public by examining environmental problems. For this reason, it can be said that the easiest way to share information about the environment is social media. Increasing environmental knowledge and awareness with technologies that can be used alongside the media has become one of the important issues of today’s world. Despite different opinions, the Covid-19 pandemic has shown that digital learning has become a part of our lives and will be used more often in the future. In this presentation, methods that will facilitate the learning of environmental issues with the help of technology will be mentioned and examples will be given.

Bio: Nazım Kaşot studied biology at the Ege University between the years 2003 and 2007. His graduation project was about the biology of stripe necked terrapin (*Mauremys rivulata*). He was ranked third in the class and the fourth of section Nazım Kaşot, Kıbrıs Adası’nda Dağılım Gösteren Çizgili Kaplumbağa’nın (*Mauremys rivulata*) Ekolojisi ve Biyolojisi Hakkında Bir Ön Çalışma with 85/100 points. He has the master degree on Secondary Education Field Teaching at Atatürk Teacher Training Academy between the years 2010 and 2011 and then worked as a biology and science teacher at the Bekirpaşa High School, Mehmetçik Secondary School, Mağusa Vocational High School, Haspolat Vocational High School and Gazi Mağusa Türk Maarif College. He had many experiences in the field of secondary education and combined his experiences to improve the environmental education in secondary schools. He was graduated from the master program on environmental education at the Near East University in 2012. He was also graduated from his PhD program on the same area in 2016 at the same university. He is now working for University of the Mediterranean Karpasia as an associate professor. He is conducting researches especially on environmental education and biodiversity issues. He has lots of academic papers and books in the field of environmental education and biodiversity.

ABSTRACTS

INHIBITIVE EFFECT OF AN ORGANIC COMPOUND ON THE CORROSION OF CARBON STEEL IN DEMINERALIZED WATER

Nadia HAMMOUDA, 20 Août 1955 University

Abstract

The study of corrosion inhibition of C-1026 carbon steel in demineralized water by morpholine was carried out using different techniques: stationary electrochemical methods (free potential: E-t, polarization curves: E-i, the Tafel rights and the Rp) and non-stationary electrochemical methods (EIS). The results obtained show that the addition of morpholine as an organic inhibitor to our medium, considerably slows down the corrosion process, this has been confirmed by the noble values of the corrosion potential (E_{corr}) and the low values of the corrosion current (i_{corr}). The immersion time only decreases the inhibitory efficiency. The inhibitory action of our organic compound is related to the formation (by adsorption) of a more or less continuous barrier, but of finite thickness, which prevents access of the solution to the metal. The characterization of the surface was carried out using an optical microscope.

ADDRESS FOR CORRESPONDENCE: Nadia HAMMOUDA, 20 Août 1955 University

E-Mail Address: hammoudanad@yahoo.fr

Development of Modified Zeolite Based Adsorbents for High-Performance Desulfurization

Betül Bulut, Istanbul Technical University

Abstract

Due to the combustion of sulfur-rich compounds, SO_x has become one of the most serious problems in the world as it causes significant pollution in the atmosphere, global warming and acid rain. Therefore, reducing sulfur levels in fuels and using low sulfur fuels are on the agenda to improve the air quality and carbon footprint. Sulfur removal by adsorption is considered as an effective and reliable method for removal sulfur compounds that are difficult to remove conventional methods due to their properties such as low energy consumption, operation at relatively low temperature and pressure and regeneration. Among the various porous materials, zeolites are promising for adsorption of sulfur compounds due to their high ion exchange, size-selective adsorption capacities, thermal and mechanical stability. Also, the addition of various metals to the structure of zeolites by surface modification process increases the pore volume and the number of active sites for adsorption, thereby improving the capacity of these adsorbents. In this study, adsorptive removal of two sulfur compounds which can be found in fuels and are difficult to remove by traditional methods, namely dimethyl disulfide (DMDS) and thiophene (TP), is studied. NaX type zeolite has been used and new adsorbents have been developed by loading the zeolite with Cu, Zn and Cu-Zn metal ions through liquid phase ion exchange (LPIE) method. Crystal structure, ion exchange rate and adsorption mechanism of materials were determined by XRD, ICP and FT-IR analysis of modified adsorbents, respectively. In addition, DMDS and TP dosed fuel samples containing 350 ppm sulfur were prepared and desulfurization experiments of zeolites were carried out by static method. The sulfur removal performance of the adsorbents was determined by measuring the amount of sulfur in fuel with Gas Chromatography (GC) and adsorption performances of commercial and modified zeolites were compared.

ADDRESS FOR CORRESPONDENCE: Betül Bulut, Istanbul Technical University

E-Mail Address: btl.bulut@gmail.com

Structural and Magnetic Properties of NdFe_{10.5-x}Al_{1.5}B_x (x = 0, 1, 2, 3) Alloys

Gülten Sadullahođlu, Zonguldak Bülent Ecevit University

Abstract

The aim of this study is to investigate the effect of boron addition on structural and magnetic properties of Nd(Fe,Al)₁₂ alloy. The ingots with nominal compositions of NdFe_{10.5-x}Al_{1.5}B_x (x = 0, 1, 2, 3) were prepared by arc melting method under Ar atmosphere followed by heat treatment at 700 °C for 2 h under vacuum. The changes in the structures of the samples were measured by X-ray diffraction at room temperature. The microstructures of the materials were characterized by Scanning Electron Microscope (SEM). Curie temperatures of the samples were determined by AC magnetic susceptibility measurements by heating the samples up to 350 °C under Argon atmosphere. Magnetic properties were measured by using Vibrating Sample Magnetometer (VSM) with a maximum magnetizing field of 10 kOe at room temperature. For all the samples, soft magnetic α -Fe was detected as a major phase in XRD analysis. According to the magnetization measurements, for the undoped sample, the shape of hysteresis curve shows that magnetization was not saturated under the externally applied magnetic field of 10 kOe. With boron addition Ms value increased from 104 emu/g to 130 emu/g at x = 1, with the further increase in boron addition, the highest saturation magnetization (Ms) of 142 emu/g was obtained at x = 3. Hc values are low due to the existence of soft magnetic phase in the microstructures detected by X-ray diffraction in all the samples. The micro images of the samples examined by using Scanning Electron Microscope (SEM) showed that an eutectic like lamellar structure was formed in the microstructure by adding boron to the alloy and it expanded to larger regions with the further amount of boron in the alloy. In this study, boron substitution was resulted in an evolution of the phase formation and morphological changes in the microstructures that caused variations in the magnetic properties of the NdFe_{10.5-x}Al_{1.5}B_x (x = 0, 1, 2, 3) alloys. The further investigations about this study including heat treatments at different temperatures above 700 °C and for longer periods can provide more detailed and systematic knowledge to obtain optimum magnetic properties.

ADDRESS FOR CORRESPONDENCE: Gülten Sadullahođlu, Zonguldak Bülent Ecevit University

E-Mail Address: gultensadullah@gmail.com

Growth of single crystal Ga₂O₃ by customized low pressure chemical deposition

Fatih Akyol, Yıldız Technical University

Abstract

Besides excellent chemical and thermal stability up to 1400 °C, monoclinic Gallium Oxide (β -Ga₂O₃) has been shown to be grown from melt which gives it the privilege to be the only cost-effective ultra-high bandgap (~4.8 eV) material. Growth of β -Ga₂O₃ using thin film growth techniques is also a point of interest as customized epitaxial designs are required for device applications. Although homo-epitaxial Ga₂O₃ is commercially available the price is still much higher than conventional low cost substrates such as sapphire. Also, thin film heteroepitaxial growths on large diameter substrates is a point of interest. In this work, overview of heteroepitaxial Ga₂O₃ thin film growths are discussed and compared with β -Ga₂O₃ single crystal layers grown on c-plane sapphire with our customized low pressure chemical vapor deposition (LPCVD) system. Unlike conventional solid source LPCVD growth, our customized system delivers oxygen gas via dedicated line to the substrate surface which enables effective control of oxygen concentration on the growth surface and minimize unwanted gas phase reactions between reactants before reaching the substrate, thus ensures highly efficient reactant transfer. The grown β -Ga₂O₃ thin films were found to be single crystal and (-201) oriented. We can precisely adjust growth rate between 0-4 micron/hr by changing the growth temperature, O₂ flow rate and Ga crucible temperature. Growth surface under optimized conditions shows atomically flat terraces. Absorption spectra reveals the bandgap of the films around 4.7-4.8 eV as expected.

ADDRESS FOR CORRESPONDENCE: **Fatih Akyol**, Yıldız Technical University

E-Mail Address: akyolf@yildiz.edu.tr

Investigation of Microstructure and Mechanical Performances of Nozzles Produced from DIN 1.3343 Steel with Heat Treatment and Coated with TiN

Muhammet Ahmet SÖYLER, Turkey

Abstract

It is very important in terms of cost, time, and quality in the related sectors to prevent high import costs of atomization nozzles, which are widely used in different fields of the industry and inevitably needed in the glazing processes of production of tableware porcelain products, increasing their working performance and extending their life. Instead of importing wolfram carbide (WC) glaze throwing nozzles made of powder metallurgy, its mechanical properties are improved by coating the nozzle produced from heat treated high speed steel with known coating methods. The type of coating material and the coating efficiency are important factors for coating performance. The wear resistance of substrate has the same wear resistance with the coating material if it is made of the same material. Coating process needs less material than producing the tool from the same material. Therefore, coating process has lower cost. In this study, the most preferred coating material TiN is investigated in terms of microstructure and mechanical performances. TiN coated and uncoated heat treated high speed steel glaze shot nozzles are experimentally compared with each other.

Keywords: Stainless steel, TiN, surface coating, glaze shot nozzle, PVD

ADDRESS FOR CORRESPONDENCE: Muhammet Ahmet SÖYLER, Turkey

E-Mail Address: ahmetsoyler@ngkutahya.com

Diffusion properties of barium disilicate glass-ceramics for dental applications

BURCU ERTUĞ, Nişantaşı University

Abstract

The aim of the present study is to produce and characterize the stoichiometric barium disilicate glasses of the BaO-SiO₂ binary system. The optimum controlled crystallization parameters were defined according to a number of Differential Thermal Analysis (DTA) studies. A double-step thermal treatment was applied to all glass samples. Density and the crystallization results indicated a densification throughout the glass-ceramic. Scanning Electron Microscope (SEM) images showed that the nuclei transformed into well-grown barium disilicate crystals. SiO₂76-dimmer units were determined to be the predominant species by Fourier Transform Infrared (FTIR) Spectroscopy analysis. Barium disilicate samples showed a similar crystalline structure by X-ray diffraction (XRD) and the composition to the previous dental materials. The diffusivity (D) increased exponentially with the nucleation temperature. The thickness also increased with the temperature due to the thermal diffusion of Ba cations into the quartz crystal. It can be concluded that the present barium disilicate glass-ceramic can be considered as a potential dental implant material for further investigations.

ADDRESS FOR CORRESPONDENCE: BURCU ERTUĞ, Nişantaşı University

E-Mail Address: burcu.ertug@nisantasi.edu.tr

TEMPORARY SPATIAL SOLUTIONS and The New Approaches to Design | How social innovation and collaborative services can reshape Balat, Istanbul for children's everyday sense of well-being?

Yasemin Albayrak Kutlay, Izmir University of Economics

Abstract

Nowadays, triggering temporary and pop-up initiatives through community's engagement is recognized as an effective way to design the surrounding environment in urban areas. Re-conceptualizing the neighbourhoods according to the efforts of creative and productive individuals who have limited resources, is important to create livable cities and encourage the citizens about decision making processes to take back control of the public realm. Moreover, this culture of inspiring bottom-up initiatives and pop-up projects affects the way urbanites use and make the cities by showing innovation and passion of individuals. This thesis discusses how living spaces are becoming more and more temporary, adaptable and fluid to create an encouraging ground for innovative and inspirational community activities to foster spontaneous human actions in hybrid spaces by linking multiple functions and services. Recognizing the connection and relationship between people and their spatial setting plays a significant role in creating a sense of place for promoting individual's and communities' wellbeing. The importance of the physical and social environment around urbanites is non-negligible for the future of communities living in cities. In order to encounter in this elaborate context, collaborative design activities and participatory design research methods are considered the most suitable methodology for conducting spatial and ethnographic research. Within the framework of these criteria, the thesis focuses on the Balat-Fener District in Istanbul and aims to increase the quality level of social interactions for the Minik Kalpler organization by promoting social capital and better civic behaviour with an adaptive approach. The approach uses a place-based dimension that has been called a "sense or spirit of the place", emphasizing how social urban spaces mean for people who create their individual and collective identities and how the local communities can help in overcoming challenges for underprivileged children in Balat. This study sheds new light on increasing the everyday sense of wellbeing of the mini-community in Balat with the help of social innovation and driving positive change with small temporary spatial footprints.

ADDRESS FOR CORRESPONDENCE: Yasemin Albayrak Kutlay, Izmir University of Economics

E-Mail Address: yaseminn.albayrak@gmail.com

A Detailed Study of Hydrogen Treatment of Iron Catalyst for Carbon Nanotube Synthesis

Osman Tolga Gul, Ankara Haci Bayram Veli University

Abstract

Vertical Carbon nanotube (VCNT) synthesis is a multistep process that consists of several chemical steps. Catalyst treatment and formation are the first steps after catalyst layer deposition. H₂ treatment of catalysts provides formation of small catalyst islands which initiate and maintain VCNT synthesis. Moreover, H₂ treatment removes oxide layers on catalysts that forms immediately when they exposed to air and ensures oxygen free Fe catalysts. However, H₂ treatment parameters need optimizations in order to form homogeneous and active catalyst particles prior to VCNTs synthesis. We have studied the effect of some H₂ treatment parameters on VACNT synthesis such as H₂ treatment temperature and H₂ treatment duration. We have found that H₂ treatment temperature has a great impact on shaping catalyst particles. Low treatment temperatures induced smaller and homogeneous catalyst islands while larger catalyst islands formation was observed at higher treatment temperatures. At VACNT growth side, small catalyst particles mediate growth of longer VACNT forests. On the other hand, we have observed that H₂ treatment duration is another important factor on catalyst particles formation. Longer H₂ treatment causes aggregation of catalyst particles and formation of very large catalyst islands. These large islands are not favourable for VACNTs formation and resulted with short VACNT forests.

ADDRESS FOR CORRESPONDENCE: Osman Tolga Gul, Ankara Haci Bayram Veli University

E-Mail Address: tolga.gul@hbv.edu.tr

Improved thermo-hydraulic performance of an Aluminum hemispherical pin fins heat sink

BELLAHCENE LAHCENE, Laboratoire de mécanique, Université Amar Telidji-Laghouat, Algeria

Abstract

The main objective of this work is to numerically study the thermal and hydraulic performances of aluminum hemispherical pin fins heat sink. The geometry design of the heat sink is made to reduce the volume of cooling air. The k- ϵ two-equation numerical turbulence model was used to describe the phenomenon of flow. The effect of the thickness of the trench on the thermal and hydraulic fields of the flow was studied to avoid areas of stagnation of the flow. The results obtained show that the use of aluminum hemispherical pin fins heat sinks optimized by a trench in the middle considerably increases the heat transfer zones between the cooling air and the Aluminum heat sink. The results indicate that for a half-sphere heat sink of $e = 1\text{mm}$, the Nusselt number increases by 45% and the thermal resistance decreases by 42% with a pressure of 50%.

ADDRESS FOR CORRESPONDENCE: **BELLAHCENE LAHCENE**, Laboratoire de mécanique, Université Amar Telidji-Laghouat, Algeria

E-Mail Address: i.bellahcene@lagh-univ.dz

Basic Properties of double Perovskites (La_{0.25}Bi_{0.75})₂FeCrO₆ by the FPLMTO-(GGA+U) Method

Melouka Bellil, Mustapha Stambouli University of Mascara

Abstract

This work presents a study of the generalized gradient approximation (GGA), plus a Hubbard correlation ($U = 4.1$ eV), of the alloy (La_{0.25}Bi_{0.75})₂FeCrO₆, in the pnma / order ferrimagnetic structure of the rare earth d-La electrons of transition. This study shows an optimal optical absorption of about 10^3 cm⁻¹ near an ideal band gap around 1.52 eV, with local magnetic moments of (Cr³⁺, Fe³⁺) proven (- 2.56, 4.14) μ_B , which makes it a promising candidate for photovoltaics and photoferroics. Tun-gap La-Bi₂FeCrO₆ active layer which is expected to possess better light absorption and greater carriers mobility, could be a suitable light absorber and should be an effective alternative to many absorbers such as the broadband chalcopyrite prohibited for solar cells, without achieving the highest efficiency or even with their counterparts perovskite metal – organic halide .

ADDRESS FOR CORRESPONDENCE: Melouka Bellil, Mustapha Stambouli University of Mascara

E-Mail Address: meloukabellil@yahoo.fr