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Web of Science
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**Record 1 of 50****Title:** Gamma glycine crystal for efficient second harmonic generation of 1064 nm Nd:YAG laser light**Author(s):** Anis, M (Anis, Mohd); Baig, MI (Baig, M. I.); Muley, GG (Muley, G. G.); Rabbani, G (Rabbani, G.); Shirsat, MD (Shirsat, M. D.); Shkir, M (Shkir, Mohd.); Ghramh, HA (Ghramh, H. A.)**Source:** MATERIALS LETTERS **Volume:** 233 **Pages:** 238-241 **DOI:** 10.1016/j.matlet.2018.09.013 **Published:** DEC 15 2018**Abstract:** The organic crystals with abundance of donor-acceptor moieties readily facilitate the mechanism of charge transfer which aids for grooming the nonlinear optical (NLO) effects and hence core investigation on glycine crystal is deliberately needed for visualizing its compatibility for frequency conversion device applications. In this communication the gamma glycine (GG) crystal has been firstly grown in presence of salicylic acid and priority is given to explore its optical properties. The structural parameters and space group of GG crystal has been confirmed by single crystal X-ray diffraction analysis. The qualitative analysis of GG crystal has been performed by means of fourier transform infrared spectroscopy. The color centered luminescence emission profile of GG crystal has been assessed by means of photoluminescence study. The UV-visible spectral analysis has been employed within 200-1100 nm to examine the optical transparency of GG crystal. The linear optical parameters of GG crystal has been evaluated using the transmittance data. The large enhancement in second harmonic generation (SHG) efficiency of GG crystal with reference to KDP and ADP crystal has been confirmed by Kurtz-Perry test. The competency of GG crystal for NLO device application has been proposed in vision of obtained results. (C) 2018 Elsevier B.V. All rights reserved.**Accession Number:** WOS:000446244700061**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Ghramh, Hamed	L-4152-2019	
Shirsat, Mahendra	AAC-5814-2021	0000-0002-4216-2919
Anis, Mohd	I-9741-2019	
Muley, Gajanan G	K-4699-2017	0000-0001-5977-6987
, Mirza Irshad Baig Mirza Sadik Baig		0000-0002-2704-253X
Anis, Mohd		0000-0003-2106-9093

ISSN: 0167-577X**eISSN:** 1873-4979**Record 2 of 50****Title:** Effect of calcination and carbon incorporation on NiO nanowires for photodiode performance**Author(s):** Soylu, M (Soylu, M.); Dere, A (Dere, A.); Al-Sehemi, AG (Al-Sehemi, Abdullah G.); Al-Ghamdi, AA (Al-Ghamdi, Ahmed A.); Yakuphanoglu, F (Yakuphanoglu, F.)**Source:** MICROELECTRONIC ENGINEERING **Volume:** 202 **Pages:** 51-59 **DOI:** 10.1016/j.mee.2018.10.007 **Published:** DEC 15 2018**Abstract:** We report the effect of calcination and carbon (C) incorporation on the characteristic properties of nickel oxide (NiO) consisting of nanowires. The identification of NiO is carried out at room temperature using X-ray diffraction (XRD) and Raman spectroscopy. The images of NiO nanowires are investigated by scanning electron microscope (SEM). It has been observed that the morphology is affected by calcination and carbon incorporation. The optical band gaps vary in the range of 3.22 to 3.42 eV. NiO-based heterojunction is obtained by inserting nanowire structured NiO layer between Al electrode and Si. NiO/p-Si heterojunction shows rectifying behavior in the dark and exhibits prominent photovoltaic response under light. The photovoltaic performance of the NiO/p-Si isotype heterojunction diode is significantly changed with calcination and carbon (C) incorporation of NiO. Results imply that the characteristic properties of NiO as transparent electrode can be improved by doping and calcination for efficient optoelectronic applications.**Accession Number:** WOS:000452572700008**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Al-Sehemi, Abdullah	AAK-5902-2020	
Al-Sehemi, Abdullah	J-9967-2012	
al-sehemi, Abdullah	AAM-4039-2020	
Al-Sehemi, Abdullah		0000-0002-6793-3038

ISSN: 0167-9317**eISSN:** 1873-5568**Record 3 of 50****Title:** Quantum chemical investigation on molecular structure, vibrational, photophysical and nonlinear optical properties of L-threoninium picrate: an admirable contender for nonlinear applications**Author(s):** AlFaify, S (AlFaify, S.); Shkir, M (Shkir, Mohd.); Arora, M (Arora, M.); Irfan, A (Irfan, Ahmad); Algarni, H (Algarni, H.); Abbas, H (Abbas, Haider); Al-Sehemi, AG (Al-Sehemi, Abdullah G.)**Source:** JOURNAL OF COMPUTATIONAL ELECTRONICS **Volume:** 17 **Issue:** 4 **Pages:** 1421-1433 **DOI:** 10.1007/s10825-018-1230-9 **Published:** DEC 2018**Abstract:** In this work, very first attempt has been made to investigate the electronic, spectroscopic and nonlinear optical properties of L-threoninium picrate (LTHP) molecule by exploiting vital computational methods such as HF, B3LYP and range-separated functionals (CAM-B3LYP and LC-BLYP) with 6-31G* basis set. The calculated values of IR and Raman vibrational frequencies were found to be in a good agreement with experimental results. Time-dependent density functional theory has been applied to calculate the electronic and photophysical properties such as excitation energy, dipole moment and frontier molecular orbital (FMO) energies of LTHP. The excitation energy value calculated by CAM-B3LYP is at similar to 351 nm that in close harmony with experimental value (i.e., 356 nm). Total/partial DOS was determined using GGA/BLYP. The values of $\mu(\text{tot})$, $\alpha(\text{tot})$, $\Delta\alpha$, $\beta(0)$ and $\beta(\text{tot})$ were estimated and discussed. The $\mu(\text{tot})$ and $\beta(\text{tot})$ are found to be 3 and 51 times higher than urea molecule, respectively. The FMOs, molecular electrostatic potential and

global reactivity descriptors were also calculated and discussed. All these results suggest that the LTHP would be a good candidate for optoelectronic applications.

Accession Number: WOS:000456674800003

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Al-Sehemi, Abdullah	J-9967-2012	
al-sehemi, Abdullah	AAM-4039-2020	
Irfan, Ahmad	R-7642-2019	0000-0001-6941-6934
Al-Sehemi, Abdullah		0000-0002-6793-3038

ISSN: 1569-8025

eISSN: 1572-8137

Record 4 of 50

Title: Magnetic Field Effect on the Double Diffusive Natural Convection in Three-Dimensional Cavity Filled with Micropolar Nanofluid

Author(s): Abidi, A (Abidi, Awatef); Raizah, Z (Raizah, Zehba); Madiouli, J (Madiouli, Jamel)

Source: APPLIED SCIENCES-BASEL **Volume:** 8 **Issue:** 12 **Article Number:** 2342 **DOI:** 10.3390/app8122342 **Published:** DEC 2018

Abstract: This article presents a three-dimensional numerical investigation of heat and mass transfers and fluid flow in a cavity filled with an Al₂O₃/water micropolar fluid under uniform magnetic field. To solve the governing non-dimensional equations, Finite Volume Method (FVM) based on 3-D vorticity-vector potential formulation has been employed. The effects of various parameters such as buoyancy ratio ($-2 \leq N \leq 0$), Rayleigh number ($10(3) \leq Ra \leq 10(5)$), Hartmann number ($0 \leq Ha \leq 60$), nanoparticles volume fraction ($0 \leq \phi \leq 0.06$) and micropolar material parameter ($0 \leq K \leq 5$) on flow structure and on heat and mass transfers are presented. The results illustrate that for the micropolar nanofluid model, both heat and mass transfer rates and three-dimensional character of the flow are smaller when compared with the pure nanofluid model. It is also observed that increase and decrease in heat and mass transfer rates is experienced due to increase in Rayleigh number and Hartmann number, respectively. It is also noted that increase in vortex viscosity parameter reduces the average heat and mass transfer rates and is more evident when the magnetic field is imposed. Combined effects of magnetic field and nanoparticles volume fraction on heat and mass transfers are also explored.

Accession Number: WOS:000455145000010

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Madiouli, Jamel	AAS-9088-2020	
Raizah, Zehba A	V-7556-2018	0000-0002-6529-8050
Madiouli, Jamel		0000-0003-1426-961X

ISSN: 2076-3417

Record 5 of 50

Title: Assessment of natural radioactivity levels and radiation hazard indices for soil samples from Abha, Saudi Arabia

Author(s): Ibraheem, AA (Ibraheem, Awad A.); El-Taher, A (El-Taher, Atef); Alruwaili, MHM (Alruwaili, May H. M.)

Source: RESULTS IN PHYSICS **Volume:** 11 **Pages:** 325-330 **DOI:** 10.1016/j.rinp.2018.09.013 **Published:** DEC 2018

Abstract: The natural level of radioactivity in the soil is one of the main causes of external gamma exposure. It was considered necessary to measure concentrations of gamma ray activity due to naturally occurring, potentially hazardous radionuclides from, Ra-226, Th-232 and K-40 for soil samples collected from different locations (Abha, Khamis Mushait and Muhail Asir) in Asir region. The samples were analyzed for its naturally occurring radionuclides by gamma-ray spectrometry using NaI (TI). The results show that the average values of activity for Ra-226, Th-232 and K-40 in range of 38.2 ± 0.1 - 44.1 ± 0.1 , 23.49 ± 0.20 - 41.9 ± 0.2 and from 182.5 ± 1.0 to 251.5 ± 1.3 Bq Kg⁻¹ respectively. Also the frequency distribution for all radioactive variables in soil was analyzed. Additionally evaluations have been made of the radiological hazards and it's diagramed by Surfer program in maps. These data will serve as the baseline level of radionuclides that occur naturally in the study area and will be useful for tracking and assessing any pollution inventory in the environment of this region.

Accession Number: WOS:000454026000048

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ISSN: 2211-3797

Record 6 of 50

Title: Tuning the optoelectronic and charge transport properties of 2,5-di(pyrimidin-5-yl)thieno[3,2-b]thiophene by oligocene end cores substitution

Author(s): Irfan, A (Irfan, Ahmad); Chaudhary, AR (Chaudhary, Aijaz Rasool); Muhammad, S (Muhammad, Shabbir); Al-Sehemi, AG (Al-Sehemi, Abdullah G.); Bo, H (Bo, Hu); Mumtaz, MW (Mumtaz, Muhammad Waseem); Qayyum, MA (Qayyum, Muhammad Abdul)

Source: RESULTS IN PHYSICS **Volume:** 11 **Pages:** 599-604 **DOI:** 10.1016/j.rinp.2018.09.052 **Published:** DEC 2018

Abstract: With the focus on tuning the charge transport and optoelectronic properties, various new derivatives were designed by substituting the oligocene moieties at end cores of 2,5-di(pyrimidin-5-yl)thieno[3,2-b]thiophene (Comp. 1). The end core substitution effect of benzene, naphthalene, anthracene, tetracene, pentacene and hexacene on Comp. 1 was comprehensively studied on the structure-property relationship, electro-optical properties, ionization potential (IP), electron affinity (EA) and hole/electron reorganization energies ($\lambda_{h(e)}$). The injection barrier was reduced by introducing the

oligocene units at end cores. The substitution of anthracene, tetracene, pentacene and hexacene at end cores of Comp. 1 significantly minimized the polarization resulting smaller $\lambda(h)$ (Comp.1c - Comp.1f) than the referenced compound, i.e., pentacene. The smaller $\lambda(h)$ values are illuminating that newly designed derivatives might be superior/analogous to pentacene, i.e., frequently used hole transport material. The fluorescence spectra, dipole moment, IP, EA and $\lambda(h)$ values showed that targeted molecules would be not only good for organic light emitters but also efficient for organic semiconductors and photovoltaic devices.

Accession Number: WOS:000454026000090

Author Identifiers:

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Al-Sehemi, Abdullah	J-9967-2012	
Al-Sehemi, Abdullah		0000-0002-6793-3038

ISSN: 2211-3797

Record 7 of 50

Title: Assessment of health risk due to the exposure of heavy metals in soil around mega coal-fired cement factory in Nigeria

Author(s): Kolo, MT (Kolo, Matthew Tikpangi); Khandaker, MU (Khandaker, Mayeen Uddin); Amin, YM (Amin, Yusoff Mohd); Abdullah, WHB (Abdullah, Wan Hasiah Binti); Bradley, DA (Bradley, David A.); Alzimami, KS (Alzimami, Khalid S.)

Source: RESULTS IN PHYSICS **Volume:** 11 **Pages:** 755-762 **DOI:** 10.1016/j.rinp.2018.10.003 **Published:** DEC 2018

Abstract: Mobilization and dispersion of potentially toxic elements into the atmosphere and human environment due to industrial and anthropogenic activities have been associated with significant human health challenges. In this investigation, 20 surface soil samples collected around a coal-fired cement factory in northeast Nigeria were analysed for their heavy metal (Cr, Pb, Ni, Cu, Zn and Mn) concentrations using inductively coupled plasma mass spectrometry. The results showed that mean concentrations of heavy metals, except for Cr were lower than their normal backgrounds (Cr= 76.44 > 64 mg kg⁻¹, Pb= 19.32 < 70 mg kg⁻¹, Ni= 29.09 < 50 mg kg⁻¹, Cu= 5.03 < 63 mg kg⁻¹, Zn= 10.15 < 200 mg kg⁻¹) provided in the Canadian soil quality guidelines. Potential health risk assessment for adults and children for lifetime exposure through ingestion, inhalation and dermal contact were estimated. Statistical analysis identified anthropogenic activities as the principal source of metal contamination in the studied soils. Risk assessments indicated that ingestion pathway is the primary exposure route for both adults and children. Children were found to be prone to higher health risk possibly due to their hand-to-mouth dietary habits. Carcinogenic and non-carcinogenic health risk values were within safety limits for all the metals, though Cr showed a high potential for occurrence of non-carcinogenic health effects in the subpopulations.

Accession Number: WOS:000454026000114

Author Identifiers:

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Khandaker, Mayeen Uddin	F-5376-2011	0000-0003-3772-294X

ISSN: 2211-3797

Record 8 of 50

Title: Studies on the photoelectric properties of crosslinked-poly(acrylamide co-acrylic acid) for photo detector applications

Author(s): Ashraf, IM (Ashraf, I. M.); El-Zahhar, AA (El-Zahhar, Adel A.)

Source: RESULTS IN PHYSICS **Volume:** 11 **Pages:** 842-846 **DOI:** 10.1016/j.rinp.2018.10.048 **Published:** DEC 2018

Abstract: The co-polymer, polyacrylamide co-acrylic acid-P(AM-AA) was prepared by chemical polymerization of acrylamide with acrylic acid in presence of methylene bisacrylamide as a crosslinker. The copolymer was analyzed using FTIR, XRD and DTA. The I-V characteristics of the copolymer were studied and proved that the recombination process is dependent on the presence of traps distributed in the energy gap. The results showed that the traps contribute significantly in the increased photosensitivity of the co-polymer. The behaviors of both dark and photoconductivity with temperature showed linear relations at different light intensities and proved an activated conduction with single activation energy. The activation energy (E-a) at different light intensity was found to follow Meyer Neldel rule (MN rule) and the intercept σ_0 (pre factor) as well. The characteristic energy of exponential traps was found to be within 0.0134-0.009 eV, at different light intensities. The transient photoconductivity studies on the co-polymer confirmed the presence of traps. Where, the high photosensitivity and the presence of traps may contribute to the development of the improved performance of photo detectors.

Accession Number: WOS:000454026000127

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
El-Zahhar, Adel	AAT-6245-2020	
Ebrahim, Ashraf Mahmoud	AAT-6263-2020	

ISSN: 2211-3797

Record 9 of 50

Title: Study of the optical properties of amorphous As-Se-S thin films

Author(s): Aly, KA (Aly, Kamal A.); Hegazy, HH (Hegazy, H. H.); Dahshan, A (Dahshan, A.); Shaaban, KS (Shaaban, Kh. S.); Saddeek, Y (Saddeek, Y.); Alharbi, SR (Alharbi, S. R.); Ali, AM (Ali, Atif Mossad); Amin, SA (Amin, S. A.)

Source: APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING **Volume:** 124 **Issue:** 12 **Article Number:** 868 **DOI:** 10.1007/s00339-018-2278-x **Published:** DEC 2018

Abstract: This study investigates the effects of substitution of selenium by sulfur on the optical constants of amorphous (a-)As₂₀Se_{80-x}S_x films (x=0, 4, 8, 12, 16, and 20at%), where the coordination number for both Se and S is the same. The absorption coefficient, α , and the index of refraction, n, were derived using

the transmission spectra in a wide range of wavelengths from 400 to 2500nm. This revealed that the index of refraction for the a-As₂₀Se_{80-x}S_x system decreases with increase in sulfur content throughout the range under study. The effective coordination number of As has been determined based on the refractive index dispersion analysis. A decreasing in N-c from 4.022 to 3.752 with increase content of sulfur from 0 to 20at% has been recorded. In addition, the optical bandgap, E-g, of the a-As₂₀Se_{80-x}S_x thin films increases with increase in S content which can be explicated in terms of the chemical bond approach.

Accession Number: WOS:000452109300005

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ISSN: 0947-8396

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Record 10 of 50

Title: A study on structural, spectral, and magnetic properties of Pr-Bi co-doped M-type barium-strontium hexaferrites via the solid-state reaction method

Author(s): Yang, YJ (Yang, Yujie); Shao, JX (Shao, Juxiang); Wang, FH (Wang, Fanhou); Batoo, KM (Batoo, Khalid Mujasam); Adil, SF (Adil, Syed Farooq); Bhat, BH (Bhat, Bilal Hamid); Want, BA (Want, Basharat Ahmad)

Source: APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING **Volume:** 124 **Issue:** 12 **Article Number:** 854 **DOI:** 10.1007/s00339-018-2271-4 **Published:** DEC 2018

Abstract: Pr-Bi co-doped M-type Ba-Sr hexaferrites with nominal compositions Ba_{0.35}Sr_{0.65-x}Pr_xFe_{12.0-x}Bi_xO₁₉ (0.00x0.40) were synthesized for the first time by the solid-state reaction method. These hexaferrites were characterized by X-ray diffractometer (XRD), Fourier transformer infrared (FT-IR) spectroscopy, field emission scanning electron microscopy (FE-SEM), vibrating sample magnetometer (VSM) and thermogravimetric analyzer (TGA). XRD patterns showed that the single M-type hexaferrite phase was obtained only if Pr-Bi content (x)0.24. FT-IR frequency bands in the range (608-610) cm⁻¹ and (445-447) cm⁻¹ correspond to the formation of tetrahedral and octahedral clusters of metal oxides in the hexaferrites, respectively. FE-SEM micrographs indicated that the grains were of platelet-like shapes. The saturation magnetization (M_s), remanent magnetization (M_r), magnetic anisotropy field (H_a), first anisotropy constant (K₁) and coercivity (H_c) first increased with Pr-Bi content (x) from 0.00 to 0.08, and then decreased when Pr-Bi content (x)0.08. The Curie temperature (T_c) decreased with increasing Pr-Bi content (x) from 0.00 to 0.40.

Accession Number: WOS:000451672700002

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Batoo, Khalid Mujasam	F-2086-2015	0000-0001-8264-8203

ISSN: 0947-8396

eISSN: 1432-0630

Record 11 of 50

Title: Effect of TiO₂ Nanoparticles Addition on the Thermal, Microstructural and Room-Temperature Creep Behavior of Sn-Zn Based Solder

Author(s): Yassin, AM (Yassin, A. M.); Zahran, HY (Zahran, H. Y.); Abd El-Rehim, AF (Abd El-Rehim, A. F.)

Source: JOURNAL OF ELECTRONIC MATERIALS **Volume:** 47 **Issue:** 12 **Pages:** 6984-6994 **DOI:** 10.1007/s11664-018-6624-8 **Published:** DEC 2018

Abstract: The effect of adding TiO₂ nanoparticles as well as aging time on the thermal, microstructural and creep properties of Sn-6.5Zn solder was studied. The Sn-6.5Zn composite solders were prepared by mechanically dispersing different weight percentages (0.0wt.%, 0.25wt.%, 0.50wt.%, 0.75wt.% and 1.0wt.%) of TiO₂ nanoparticles into Sn-6.5Zn solder. After being solution heat treated at 453 K for 4h, specimens were cooled by water quenching at 273 K. Specimens were artificially aged at 393 K for durations ranging from 15 to 120 min, followed by water quenching at 273 K to cease further aging. The thermal behavior of the composite solders was investigated using differential scanning calorimetry (DSC). X-ray diffraction (XRD) and scanning electron microscopy (SEM) were used to observe the microstructure of the solders. The mechanical properties were characterized using tensile creep tests and correlated with microstructural features. The investigation revealed that the minimum creep rate of solders decreased with the increase in the content of TiO₂, while it increased with increasing aging time. The data from microstructure-properties analysis showed that the nano-TiO₂ particles had significantly refined the microstructure and improved the creep resistance in comparison with the Sn-Zn solder. The calculated stress exponent values were close to 7.

Accession Number: WOS:000448979100005

Author Identifiers:

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Yahia, Ibrahim Sayed	G-4458-2011	
El-Rehim, A. Abd	M-4861-2019	

ISSN: 0361-5235

eISSN: 1543-186X

Record 12 of 50

Title: Cadmium Oxide: Titanium Dioxide Composite Based Photosensitive Diode

Author(s): Karabulut, A (Karabulut, Abdulkemir); Dere, A (Dere, A.); Al-Sehemi, AG (Al-Sehemi, Abdullah G.); Al-Ghamdi, AA (Al-Ghamdi, Ahmed A.); Yakuphanoglu, F (Yakuphanoglu, F.)

Source: JOURNAL OF ELECTRONIC MATERIALS **Volume:** 47 **Issue:** 12 **Pages:** 7159-7169 **DOI:** 10.1007/s11664-018-6647-1 **Published:** DEC 2018

Abstract: Cadmium oxide:titanium dioxide (CdO:TiO₂) composite thin films with various ratios of CdO contents were prepared on p-type silicon semiconductor substrates by the sol-gel spin coating method. Al/CdO:TiO₂/p-Si/Al heterojunction devices exhibited optoelectronic device behavior due to their photocurrent under solar light illuminations. The photoresponse behavior of the diodes is controlled by changing the molar ratio of CdO to TiO₂. The fabricated CdO:TiO₂ (2:1) based device exhibited the highest photoresponse of about 7.5×10^3 . The interface properties of the devices are changed with the molar ratio of CdO:TiO₂. The obtained results suggest that CdO:TiO₂ composite film/p-type Si structure can be used in optoelectronic applications.

Accession Number: WOS:000448979100024

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Al-Sehemi, Abdullah	J-9967-2012	
Al-Sehemi, Abdullah	AAK-5902-2020	
al-sehemi, Abdullah	AAM-4039-2020	
Yakuphanoglu, Fahrettin	C-8365-2012	
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ISSN: 0361-5235

eISSN: 1543-186X

Record 13 of 50

Title: Selective CUT-OFF laser filters using brilliant green-doped PMMA polymeric composite films: sensing approach

Author(s): Abutalib, MM (Abutalib, M. M.); Yahia, IS (Yahia, I. S.)

Source: JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 29 **Issue:** 23 **Pages:** 19798-19804 **DOI:** 10.1007/s10854-018-0106-x **Published:** DEC 2018

Abstract: Brilliant green doped poly(methyl methacrylate) (BG/PMMA) films were prepared by using a simple casting method. XRD patterns support the amorphous structure of both pure PMMA and its BG-doped PMMA polymeric composite films. The transmittance $T()$ and absorbance (abs) were directly measured and investigated. From the analysis of transmittance curves of BG/PMMA, we can notice that the addition of BG to the PMMA matrix creates multi-bands of the absorption measurements in the wavelength range 215-610nm. The absorption valley of BG/PMMA can be summarized as follows: 740-489nm, 489-362nm, and 362-261nm. The BG/PMMA have a CUT-OFF of transmittance in the wavelength region 585-645nm suitable for He-Ne laser of wavelength=632nm as an example. Optical parameters were calculated for the BG/PMMA polymeric composite films. AC electrical conductivity, dielectric constant, and dielectric loss were measured and analyzed according to the applied models in the field of polymeric materials. The studied samples are suitable to be applicable in selective laser CUT-OFF filters and solar cell applications as identified using optical limiting effect.

Accession Number: WOS:000448831000021

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Yahia, Ibrahim Sayed	G-4458-2011	

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eISSN: 1573-482X

Record 14 of 50

Title: The pressure-induced indirect to direct bandgap transition and thermoelectric response in SrTiO₃: An ab-initio study

Author(s): Batool, A (Batool, Abeeha); Faridi, MA (Faridi, M. A.); Mahmood, Q (Mahmood, Q.); Ul Haq, B (Ul Haq, Bakhtiar); Laref, A (Laref, A.); Awan, SE (Awan, Saeed Ehsan)

Source: JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS **Volume:** 123 **Pages:** 70-75 **DOI:** 10.1016/j.jpcs.2018.07.008 **Published:** DEC 2018

Abstract: In this paper, we investigate the electronic structure, optical and thermoelectric properties of the SrTiO₃ (STO) at a variant pressure from 0 to 120 GPa. The thermodynamic and structural stability has been confirmed by the enthalpy of formation and tolerance factor. The implementation of pressure has been found to shift the indirect bandgap to direct bandgap at 107 GPa to tune the optical and thermoelectric properties. The optical behavior of STO has been discussed by the dielectric constant and refraction of light in the visible and ultraviolet region. Furthermore, the thermoelectric behavior has been explored by investigating the electrical conductivity, thermal conductivity, Seebeck coefficient and power factor. The thermal efficiency has been elaborated from the figure of merit, which shows the studied materials are highly valuable for energy device applications.

Accession Number: WOS:000446145300011

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Author	Web of Science ResearcherID	ORCID Number
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Ul Haq, Bakhtiar		0000-0001-9058-2080

ISSN: 0022-3697

eISSN: 1879-2553

Record 15 of 50

Title: Linear and nonlinear optical properties of nano-spherical Perylenetetracarboxylic dianhydride/ITO as a new optical system

Author(s): Abuelwafa, AA (Abuelwafa, A. A.); Abd El-Sadek, MS (Abd El-Sadek, M. S.); Yahia, IS (Yahia, I. S.)

Source: OPTICS AND LASER TECHNOLOGY **Volume:** 108 **Pages:** 241-246 **DOI:** 10.1016/j.optlastec.2018.06.055 **Published:** DEC 2018

Abstract: In the current work, the thermal evaporation method was used to deposit the Perylenetetracarboxylic dianhydride (PTCDA) into conductive glass titled (ITO glass) as a new trend in the optical spectroscopy nowadays. X-Ray Diffraction (XRD) was evidenced that the PTCDA/ITO thin film has had a nanostructural characteristic, and the crystalline part of the film oriented with (1 0 2) plane. Atomic Force Microscopes (AFM) was definite that the

morphology containing nano-spherical particles. The absorption spectra were examined in the UV-Vis-NIR regions and determined the significant parameters such as molar extinction coefficient ϵ (molar), oscillator strength f , electric dipole strength $q(2)$ and optical energy gap. The linear optical constant; extinction coefficient, (k) , and refractive index (n) were measured using spectrophotometric measurements in the wavelength range 300-2500 nm. The real part and imaginary parts of the dielectric constant and optical conductivity were evaluated and discussed. The third order non-linear susceptibility, $\chi^{(3)}$ and nonlinear refractive $n^{(2)}$ were estimated based on generalized Miller's rule and linear refractive index at photon energy from 0.5 to 4 eV. All possible linear and nonlinear parameters are reported for using this material in OLED devices. PTCDA is a promising organic semiconductor for wide-scale application in organic devices and engineering. (C) 2018 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000443664100029

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ISSN: 0030-3992

eISSN: 1879-2545

Record 16 of 50

Title: Influence of Dy doping on key linear, nonlinear and optical limiting characteristics of SnO₂ films for optoelectronic and laser applications

Author(s): Shkir, M (Shkir, Mohd.); Khan, MT (Khan, Mohd Taukeer); Ganesh, V (Ganesh, V.); Yahia, IS (Yahia, I. S.); Ul Haq, B (Ul Haq, Bakhtiar); Almomhammedi, A (Almomhammedi, Abdullah); Patil, PS (Patil, Parutagouda Shankaragouda); Maidur, SR (Maidur, Shivaraj R.); AlFaify, S (AlFaify, S.)

Source: OPTICS AND LASER TECHNOLOGY **Volume:** 108 **Pages:** 609-618 **DOI:** 10.1016/j.optlastec.2018.07.039 **Published:** DEC 2018

Abstract: In the present work, pure and dysprosium (Dy) doped SnO₂ films have been fabricated through sol-gel spin coating technique. Strong influence of Dy doping is observed on structural, morphological, vibrational, linear and nonlinear optical properties of SnO₂ films. X-ray diffraction study revealed that deposited films exhibit tetragonal crystal structure with preferentially grown along (2 0 0) plane. With increase of doping concentration in SnO₂, the crystallite size decreases while dislocation density and lattice distortion ratio increases. The characteristics Raman peaks of doped SnO₂ thin films broaden, shifted and intensity decreases as compared to pure film which confirm the bonding between Dy and SnO₂. Optical study shows that the prepared thin films are highly transparent and absorption increases with doping concentrations owing to increase of defects states. It is also observed that the optical band gap first increases and then lessens with rise of Dy-doping concentration which attributed to the Burstein-Moss (BM) effect. Additionally, dielectric constant and refractive index first decreasing with small doping concentration (1-3%) due to increase of carrier concentration, and then increases for higher doping (5-7%) due to increase of defect in SnO₂ lattice. The values $\chi^{(3)}$ and β obtained by Z-scan measurement are observed in range of 0.31×10^{-7} to 1.28×10^{-7} and 1.27 to 5.32×10^{-4} CM W⁻¹, respectively. The limiting threshold of pure and Dy doped SnO₂ nanostructured films were calculated to be in the range of 5.37-11.18 kJ/cm². (C) 2018 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000443664100074

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ISSN: 0030-3992

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Record 17 of 50

Title: Characterization and radiation detection application of ZnS(Ag) nanoparticles

Author(s): Abdalla, AM (Abdalla, Ayman M.); Ali, AM (Ali, Atif M.); Al-Jarallah, M (Al-Jarallah, M.)

Source: PHYSICA B-CONDENSED MATTER **Volume:** 550 **Pages:** 235-243 **DOI:** 10.1016/j.physb.2018.09.024 **Published:** DEC 1 2018

Abstract: In this study, pure and transition-metal (silver (Ag)) activated zinc sulfide (ZnS) nanoparticles were prepared using a hydrothermal technique. The particles have spherical shape. The average crystallite size value of ZnS:Ag nanoparticles estimated from the XRD patterns is 4.2 nm. Our results also show that the prepared ZnS has a zinc blende structure. An absorption peak at 350 nm was observed from UV-Vis spectrum for 0.05 mol% Ag doped ZnS which is related to the cubic phase of bulk ZnS. A typical Raman peak of ZnS:Ag crystal at around 346 cm⁻¹ is detected. An optimum activating level of Ag for improved photoluminescence (PL) property is found by measuring the fluorescence of samples. The PL spectra of ZnS:Ag nanoparticles showed a new PL band at 473 nm. Results of ZnS:Ag nanoparticles preparation and optimization, along with structural and optical estimation are discussed and addressed thoroughly. A linear relationship between PMT counts and the flounces of alpha particles has been achieved. The detection efficiency of Lucas cell coated with the prepared samples has been determined.

Accession Number: WOS:000452280400031

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ISSN: 0921-4526

eISSN: 1873-2135

Record 18 of 50**Title:** Structural, morphological, optical and third order nonlinear optical response of spin-coated NiO thin films: An effect of N doping**Author(s):** Ganesh, V (Ganesh, V); Haritha, L (Haritha, L.); Anis, M (Anis, Mohd); Shkir, M (Shkir, Mohd); Yahia, IS (Yahia, I. S.); Singh, A (Singh, Arun); AlFaify, S (AlFaify, S.)**Source:** SOLID STATE SCIENCES **Volume:** 86 **Pages:** 98-106 **DOI:** 10.1016/j.solidstatesciences.2018.10.009 **Published:** DEC 2018**Abstract:** The present work deals with the deposition of NiO and Nitrogen (N)-doped NiO thin films by sol-gel spin coating technique. Structural, morphological, linear and non-linear optical characteristics of undoped and N-doped (1-15 wt%) NiO films were studied. From XRD measurements, it is evident that single phase nano crystalline NiO is formed for all doping concentrations. Surface morphology study shows that higher concentration of N doped NiO thin films were of high quality and EDX mapping confirmed the doping of Nitrogen in films. The Raman spectra of the studied films were analyzed over the range of 1400-200 cm⁻¹. The optical studies confirm that as doping increases, transparency of the film decreases (except at 10% N doping) and the band gap narrows. Nonlinear parameters such as refractive index and susceptibilities also depend on N dopant concentration. Z-scan studies viz., absorption index, nonlinear refractive index were carried out on undoped and N-doped NiO samples and the results were matched with theoretical calculated values.**Accession Number:** WOS:000451050400014**Author Identifiers:**

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ISSN: 1293-2558

eISSN: 1873-3085

Record 19 of 50**Title:** Optical spectroscopy and electrical analysis of La³⁺-doped PVA composite films for varistor and optoelectronic applications**Author(s):** Ali, HE (Ali, H. Elhosiny); Khairy, Y (Khairy, Yasmin); Algarni, H (Algarni, H.); Elsaedy, HI (Elsaedy, H. I.); Alshehri, AM (Alshehri, A. M.); Yahia, IS (Yahia, I. S.)**Source:** JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 29 **Issue:** 23 **Pages:** 20424-20432 **DOI:** 10.1007/s10854-018-0176-9 **Published:** DEC 2018**Abstract:** Poly(vinyl alcohol), PVA, a matrix with 0, 0.185, 0.37, 1.85, 3.7 and 18.5wt% of lanthanum (III) nitrate were synthesized by the traditional casting method. The order of the crystal structure and the interaction between the mixtures of the investigated materials were analyzed by X-ray and Fourier transform infrared (FT-IR) spectroscopies, while the Scanning Electron Microscopy (SEM), was used to study the surface images of them. Moreover, the optical filtering via UV/Vis/NIR spectroscopy, dielectric constant as well as the D.C. resistivity measurements that arose by the composite films with various wt% of La³⁺ ion were carried out. The structure study of these samples reveals that not only a cluster arises via La³⁺ ion on the SEM surface, but also, the semi-crystalline phases were confirmed by analyzing the pattern of the XRD and FT-IR. However, due to the complex formation of La³⁺ content in PVA matrix, there is an increment in the transitions strength, E-d, and the oscillator wavelength, (0) as well as the index of refractions, while the band gap and the average excitation energy, E-s, were decreased. Furthermore, there is a facility of moving charge carriers across the bands that contribute to the small energy gap via La³⁺-ion contents which clearly noticed in the dielectric and nonlinear I-V characteristics. The forward I-V measurement of the samples exhibited two distinct regions with different slopes, which is typical as nonlinear behavior for varistor with high applied voltage. Therefore, we can say that our samples have properties make them suitable to use in the applications of optoelectronic and varistor device.**Accession Number:** WOS:000448831000088**Author Identifiers:**

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ISSN: 0957-4522

eISSN: 1573-482X

Record 20 of 50**Title:** Effects of methyl violet dye on the growth and properties of zinc (tris) thiourea sulfate single crystals**Author(s):** Shkir, M (Shkir, Mohd); Ganesh, V (Ganesh, V.); Yahia, IS (Yahia, I. S.); Yahia, IS (Yahia, I. S.); Abd-Rabboh, HSM (Abd-Rabboh, Hisham S. M.); AlFaify, S (AlFaify, S.)**Source:** JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS **Volume:** 123 **Pages:** 336-343 **DOI:** 10.1016/j.jpccs.2018.08.021 **Published:** DEC 2018**Abstract:** In this study, we investigated the monocrystal growth and characteristics of pure and methyl violet (MV) dyed zinc(tris) thiourea sulfate (ZTS) large size single crystals. The morphology of ZTS was modified in the presence of MV dye. The crystals were crushed for a finite time to obtain powders for X-ray diffraction analysis and the lattice parameters were determined. The crystals were analyzed based on Fourier transform-Raman spectroscopy measurements and the vibrational modes were identified. Some extra vibrational modes were observed due to the presence of the MV dye. Ultraviolet visible near infrared optical absorbance measurements were recorded and the band gap was calculated. A large band gap similar to 4.31 eV was obtained for the ZTS crystals, which supports their possible application in electro-optic devices. Two absorption bands at around 584 nm (sharp) and 362 nm (broad) were also observed in the dyed crystals but not in the pure crystals, thereby indicating the interaction between the dye and ZTS. Photoluminescence (PL) emission studies were conducted at an excitation wavelength of 360 nm. PL emission peaks were observed at similar to 433 nm in the pure crystals, and at similar to 421 and 444 +/- 5 nm in the dyed crystals. Differential scanning calorimetry demonstrated the increased melting temperature of ZTS in the presence of the dye. The dielectric constant, ac electrical conductivity, and mechanical strength were higher for the dyed crystals. Our results suggest that the dyed crystals may be more suitable for applications in opto-electronic devices compared with the pure crystals.

Accession Number: WOS:000446145300043

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ISSN: 0022-3697

eISSN: 1879-2553

Record 21 of 50

Title: Influence of plasma functionalization treatment and gold nanoparticles on surface chemistry and wettability of reactive-sputtered TiO₂ thin films

Author(s): Achour, A (Achour, A.); Islam, M (Islam, M.); Solaymani, S (Solaymani, S.); Vizireanu, S (Vizireanu, S.); Saeed, K (Saeed, Khalid); Dinescu, G (Dinescu, G.)

Source: APPLIED SURFACE SCIENCE **Volume:** 458 **Pages:** 678-685 **DOI:** 10.1016/j.apsusc.2018.07.145 **Published:** NOV 15 2018

Abstract: Amorphous titanium oxide (TiO₂) thin films were deposited on silicon substrates by DC-magnetron sputtering at room temperature. The surface of thin films were treated in argon plasma admixed with ammonia or nitrogen or oxygen or hydrogen. It was found that plasma treatments did not influence micron and nanometer-scale surface morphology of the treated films, as examined by atomic force microscope. However, the X-Ray photoelectron spectroscopy (XPS) showed that oxygen groups have been incorporated in various amounts. In contrast with untreated TiO₂ which is hydrophobic, the plasma treatments improved the TiO₂ hydrophilicity persistently up to 77%. The wettability of the thin films, as determined from water contact angle measurements, is discussed with reference to changes in surface chemistry after plasma treatment. In addition, deposition of gold (Au) nanoparticles (NP) onto TiO₂ samples and their interaction with TiO₂ has been discussed through XPS results. It was demonstrated that in its reduced state, TiO₂ promotes electron donation to Au, whereas oxygen content does not seem to affect the interaction between Au NP and the TiO₂ support.

Accession Number: WOS:000441400000079

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ISSN: 0169-4332

eISSN: 1873-5584

Record 22 of 50

Title: An investigation on SnS layers for solar cells fabrication with CdS, SnS₂ and ZnO window layers prepared by nebulizer spray method

Author(s): Arulanantham, AMS (Arulanantham, A. M. S.); Valanarasu, S (Valanarasu, S.); Kathalingam, A (Kathalingam, A.); Shkir, M (Shkir, Mohd.); Kim, HS (Kim, Hyun-Seok)

Source: APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING **Volume:** 124 **Issue:** 11 **Article Number:** 776 **DOI:** 10.1007/s00339-018-2164-6 **Published:** NOV 2018

Abstract: The preparation of SnS, CdS, SnS₂ and ZnO thin films by nebulizer spray method, and their characterization is reported. The size of crystallites, dislocation density, texture coefficient and strain were estimated using XRD data. SEM study revealed good surface morphology of films. Optical properties of deposited SnS, CdS, SnS₂ and ZnO films were estimated using the optical absorption measurements. The calculated optical energy gaps of CdS, SnS₂, ZnO and SnS films were, respectively, found as 2.45, 2.41, 3.2 and 1.45eV. Hall effect measurements exhibited p-type conductivity for SnS and n-type conductivity for CdS, SnS₂, ZnO thin films. The grown SnS thin films showed resistivity and carrier concentration as 0.0689cm and 1.04x10¹⁹cm⁻³, respectively. Heterojunction solar cells of FTO/CdS/SnS, FTO/SnS₂/SnS, and FTO/ZnO/SnS were also fabricated and their properties studied. The fabricated FTO/ZnO/SnS heterojunction solar cell presented a superior performance with conversion efficiency (0.96%) greater than other structures.

Accession Number: WOS:000448470600001

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ISSN: 0947-8396

eISSN: 1432-0630

Record 23 of 50

Title: Designing Magnetic Layered Double Hydroxides and Two-Dimensional Magnetic Nano-Nets of Cobalt Ferrite through a Novel Approach

Author(s): Saber, O (Saber, Osama); Aljaafari, A (Aljaafari, Abdullah); Asiri, S (Asiri, Sarah); Batoo, KM (Batoo, Khalid M.)

Source: APPLIED SCIENCES-BASEL **Volume:** 8 **Issue:** 11 **Article Number:** 2099 **DOI:** 10.3390/app8112099 **Published:** NOV 2018

Abstract: The present study has a dual aim of supporting magnetic nanoparticles over the nanolayers of LDHs and designing two-dimensional magnetic nano-nets of cobalt ferrite. In this trend, nanoparticles of CoFe₂O₄ were prepared and supported by Co-Fe LDH through urea hydrolysis. The nanolayered structures of Co-Fe LDH were confirmed by X-ray diffraction, energy-dispersive X-ray spectrometry, FT-IR spectra, thermal analyses, and transmission electron microscopy. In addition, they indicated that 13.2% CoFe₂O₄ were supported over Co-Fe LDH. Transformation of the nanolayered structures of Co-Fe LDH to nano-nets was achieved by the catalytic effect of the supported CoFe₂O₄ nanoparticles through solvent thermal technique. X-ray diffraction patterns and transmission electron microscopy images confirmed the transformation of the supported Co-Fe LDH to nano-nets of cobalt ferrite. In order to indicate

the effect of the LDH for designing the nano-nets, nanoparticles of cobalt ferrite were prepared by the same technique without LDH. The magnetic behavior of the nano-nets and the supported Co-Fe LDH were measured and compared with the nanoparticles through vibrating sample magnetometer technique. The magnetic parameters indicated that the prepared nano-nets have ferromagnetic behavior and high coercivity. However, the prepared nanoparticles revealed a superparamagnetic state and low coercivity. The experimental results concluded that the incorporation of nanoparticles with nanowires into nano-net structures has been found to be an efficient way to improve their magnetic properties and prevent their agglomerations. Finally, layered double hydroxides are an important source for constructing magnetic nanolayered structures and nano-nets.

Accession Number: WOS:000451302800089

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eISSN: 2076-3417

Record 24 of 50

Title: EFFECT OF Sn ADDITION ON PHYSICAL AND OPTICAL PROPERTIES OF Ge-Se-Sb-Sn THIN FILMS

Author(s): Dahshan, A (Dahshan, A.); Hegazy, HH (Hegazy, H. H.); Aly, KA (Aly, K. A.)

Source: CHALCOGENIDE LETTERS **Volume:** 15 **Issue:** 11 **Pages:** 545-553 **Published:** NOV 2018

Abstract: The present work aims to study theoretically the effect of Sn content on many physical parameters, such as coordination number (CN), constraints number (CON), overall mean bond energy (<E>) and cohesive energy (CE) for Ge₂₅Se₆₅Sb₁₀-xSn_x (where 0 ≤ x ≤ 10 at. %) glasses. Likewise, optical constants of the thin films were evaluated via the use of the Swanepoel technique. It is found that, CN, CON, <E>, and CE increase by increasing the Sn content. This behavior is obvious evidence for increasing the rigidity of the Ge₂₅Se₆₅Sb₁₀-xSn_x glasses by increasing the Sn content. The chemical bonds occurred within the Ge₂₅Se₆₅Sb₁₀-xSn_x glasses have been estimated. It was found that, the heteropolar bonds occurred in the examined glasses are Sn-Se, Ge-Se and Sb-Se which have energies 58.818, 49.441 and 43.981 kcal/mol., respectively. The obtained values of the refractive index (n) of the films were fitted to the two-term Cauchy dispersion equation to get the single oscillator (E-o) and dispersion (E-d) energies. In addition, values of the absorption coefficient (alpha) are obtained using the conditions suggested by Connell and Lewis. An increase of the Sn content from 0 to 10 at. % prompts a decrease of the energy gap (E-g) from 1.79 to 1.40 eV.

Accession Number: WOS:000452411600003

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ISSN: 1584-8663

Record 25 of 50

Title: Convective Heat and Mass Transfer in Magneto Jeffrey Fluid Flow on a Rotating Cone with Heat Source and Chemical Reaction

Author(s): Saleem, S (Saleem, S.); Al-Qarni, MM (Al-Qarni, M. M.); Nadeem, S (Nadeem, S.); Sandeep, N (Sandeep, N.)

Source: COMMUNICATIONS IN THEORETICAL PHYSICS **Volume:** 70 **Issue:** 5 **Pages:** 534-540 **DOI:** 10.1088/0253-6102/70/5/534 **Published:** NOV 2018

Abstract: The present paper addresses the magneto-hydrodynamic Jeffrey fluid flow with heat and mass transfer on an infinitely rotating upright cone. Inquiry is carried out with heat source/sink and chemical reaction effects. Further, constant thermal and concentration flux situations are imposed. Optimal homotopy analysis method (OHAM) is employed to achieve series solutions of the concerned differential equations. Important results of the flow phenomena are explored and deliberated by means of graphs and numerical tables. It is perceived that thermal boundary layer thickness possess contrast variations for the heat source and heat sink, respectively. The chemical reaction enhances the heat transfer rate but decline the mass transfer rate. Moreover, the precision of the existing findings is verified by associating them with the previously available work.

Accession Number: WOS:000451760400005

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ISSN: 0253-6102

eISSN: 1572-9494

Record 26 of 50

Title: Low Cost Alcoholic Breath Sensor Based on SnO₂ Modified with CNTs and Graphene

Author(s): Morsy, M (Morsy, M.); Yahia, IS (Yahia, I. S.); Zahran, HY (Zahran, H. Y.); Ibrahim, M (Ibrahim, M.)

Source: JOURNAL OF THE KOREAN PHYSICAL SOCIETY **Volume:** 73 **Issue:** 10 **Pages:** 1437-1443 **DOI:** 10.3938/jkps.73.1437 **Published:** NOV 2018

Abstract: In this work, SnO₂ modified with reduced graphene oxide (rGO) and carbon nanotubes (CNTs) separately and combined sensitized by using the co-precipitation method and their sensing behavior toward ethanol vapor at room temperature were investigated. An interdigitated electrode (IDE) gold substrate is very expensive compared to a fluorine doped tin oxide (FTO) substrate; hence, we used the latter to reduce the fabrication cost. The structure and the morphology of the studied materials were characterized by using differential thermal analyses (DTA) and thermogravimetric analysis (TGA), transmission electron microscope (TEM), X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, Brunauer-Emmett-Teller surface area and Barrett-Joyner-Halenda (BJH) pore size measurements. The studied composites were subjected to ethanol in its gas phase at concentrations from 10 to 200

ppm. The present composites showed high-performance sensitivity for many reasons: the incorporation of SnO₂ and CNTs which prevents the agglomeration of rGO sheets, the formation of a 3D mesoporous structure and an increase in the surface area. The decoration with rGO and CNTs led to more active sites, such as vacancies, which increased the adsorption of ethanol gas. In addition, the mesopore structure and the nano size of the SnO₂ particles allowed an efficient diffusion of gases to the active sites. Based on these results, the present composites should be considered as efficient and low-cost sensors for alcohol.

Accession Number: WOS:000451051900005

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ISSN: 0374-4884

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Record 27 of 50

Title: Structural, Electronic and Nonlinear Optical Properties of Novel Derivatives of 9,12-Diiodo-1,2-dicarba-closo-dodecaborane: Density Functional Theory Approach

Author(s): Chaudhry, AR (Chaudhry, Aijaz Rasool); Muhammad, S (Muhammad, Shabbir); Irfan, A (Irfan, Ahmad); Al-Sehemi, AG (Al-Sehemi, Abdullah G.); Ul Haq, B (Ul Haq, Bakhtiar); Hussain, S (Hussain, Sajjad)

Source: ZEITSCHRIFT FUR NATURFORSCHUNG SECTION A-A JOURNAL OF PHYSICAL SCIENCES **Volume:** 73 **Issue:** 11 **Pages:** 1037-1045 **DOI:** 10.1515/zna-2018-0123 **Published:** NOV 2018

Abstract: Using density functional theory (DFT) methods, we shed light on the structural, optical, electronic, and nonlinear optical (NLO) properties of three derivatives of 9,12-diiodo-1,2-dicarba-closo-dodecaborane(12) (C₂H₁₀B₁₀I₂). The DFT and time-dependent DFT methods are considered very precise and practical to optimize the ground and excited state geometries, respectively. A vibrant intramolecular charge transfer from highest occupied molecular orbitals (HOMOs) to the lowest unoccupied molecular orbitals (LUMOs) was observed in all compounds. The geometrical parameters of the experimental crystal structure, i.e. bond lengths/angles, have been successfully reproduced. The HOMO and LUMO energies, as well as their energy gaps (E-g), were also calculated and compared with each other for all derivatives. The effect of attached groups on electronic, optical, and NLO properties along with detailed structure-property relationship was discussed. For NLO response, the CAM-B3LYP functional along with relatively larger basis set 631+G** (for hydrogen, carbon, boron, and oxygen atoms) and LANL2DZ (for iodine atoms) have been used to optimize the compounds at ground states. The calculation of second-order NLO polarizabilities (beta(tot)) shows that compounds 2 and 3 possess the beta(tot) amplitudes of 3029 and 4069 a.u., respectively, with CAM-B3LYP method that are reasonably larger than similar prototype molecules. Owing to their unique V-shapes, the nonlinear anisotropy values are found to be 0.63, 0.34, and 0.44 for compounds 1-3, respectively, which show the significant two-dimensional character of these compounds. Thus, the NLO amplitudes as well as the nonlinear anisotropies indicate that the above-entitled compounds are good contenders for optical and NLO applications.

Accession Number: WOS:000448415900006

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Al-Sehemi, Abdullah	J-9967-2012	
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ISSN: 0932-0784

eISSN: 1865-7109

Record 28 of 50

Title: Structural and magnetic study of Mn_{0.5}Zn_{0.5}Cu_xFe_{2-x}O₄ nanoferrites synthesized via solution combustion method

Author(s): Sharma, A (Sharma, Anjana); Batoo, KM (Batoo, Khalid Mujasam); Raslan, EH (Raslan, Emad H.); Adil, SF (Adil, Syed Farooq); Kumar, G (Kumar, Gagan)

Source: VACUUM **Volume:** 157 **Pages:** 422-427 **DOI:** 10.1016/j.vacuum.2018.09.015 **Published:** NOV 2018

Abstract: In the present work, Mn_{0.5}Zn_{0.5}Cu_xFe_{2-x}O₄ (x = 0.0, 0.1, 0.2 & 0.3) nanoferrites have been synthesized via solution combustion technique. X-ray diffraction (XRD), vibrating sample magnetometer (VSM) and Mossbauer spectroscopy techniques have been employed to explore the structural, cation distribution and magnetic behaviour of the synthesized nanoferrites. Rietveld refined XRD confirmed the cubic spinel phase of the nanoferrites with Fd3m space group. A reduction in particle size (51-40 nm) has been observed with the addition of copper ions. The Nelson Riley plots have been used to estimate the lattice parameter and the same has been observed to increase (8.40-8.46 angstrom) with the increasing substitution of copper content. The addition of copper ions has been observed to decrease the saturation magnetization (0.89-0.76 emu/g) and magnetic hyperfine field. Magnetization method has been used to predict the distribution of cations. The distribution of cations has been further utilized to investigate various structural parameters.

Accession Number: WOS:000449569600058

Conference Title: International Symposium on Functional Materials (ISFM) - Energy and Biomedical Applications

Conference Date: APR 13-15, 2018

Conference Location: Chandigarh, INDIA

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ISSN: 0042-207X

Record 29 of 50**Title:** Novel rare earth Gd and Al co-doped ZnO thin films prepared by nebulizer spray method for optoelectronic applications**Author(s):** Anand, V (Anand, V.); Sakthivelu, A (Sakthivelu, A.); Kumar, KDA (Kumar, K. Deva Arun); Valanarasu, S (Valanarasu, S.); Ganesh, V (Ganesh, V.); Shkir, M (Shkir, Mohd); Kathalingam, A (Kathalingam, A.); AlFaify, S (AlFaify, S.)**Source:** SUPERLATTICES AND MICROSTRUCTURES **Volume:** 123 **Pages:** 311-322 **DOI:** 10.1016/j.spmi.2018.09.014 **Published:** NOV 2018

Abstract: In this study, for the first time, rare earth element gadolinium and aluminum co-doped zinc oxide (Gd:AZO) films were prepared on insulating glass plates using cost-effective nebulizer spray method with various Gd co-doping levels (0, 0.5, 1 and 1.5 at.%). The deposited films were characterized using X-ray diffraction, FT-Raman, AFM, EDAX, UV-VIS spectroscopy, Photoluminescence (PL) spectrum and Hall Effect measurement at room temperature. From XRD study, it is confirmed that the Gd and Al ions are incorporated into ZnO lattice. Film crystallinity is slightly reduced due to Gd content by increasing lattice defects. Topology of AFM images displays a slight increase of Gd:AZO thin film roughness from 20 nm to 36 nm, with an increase of thickness from 232 to 324 nm respectively. Elemental mapping and EDAX studies confirmed the existence of Zn, O, Al and Gd elements in the prepared Gd:AZO thin films. Spray deposited pristine AZO films showed maximum optical transmittance similar to 91% in entire wavelength spectrum and energy gap value similar to 3.31eV. The observed PL spectra showed as a UV emission at 387 nm for deposited films. The obtained minimum resistivity and maximum figure of merit values are 3.42×10^{-4} Omega cm, and 18.68×10^{-3} (Omega/sq)⁻¹, respectively for 1.5 at.% Gd co-doped AZO thin film. Both values are decent enough for optoelectronic devices.

Accession Number: WOS:000448229500037**Author Identifiers:**

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AlFaify, S	ABF-3895-2020	0000-0002-8920-5891
Santiago, Valanarasu		0000-0001-7315-2126

ISSN: 0749-6036

Record 30 of 50**Title:** Optical and microelectronic analysis of rhodamine B-based organic Schottky diode: a new trend application**Author(s):** Salem, GF (Salem, G. F.); El-Shazly, EAA (El-Shazly, E. A. A.); Farag, AAM (Farag, A. A. M.); Yahia, IS (Yahia, I. S.)**Source:** APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING **Volume:** 124 **Issue:** 11 **Article Number:** 744 **DOI:** 10.1007/s00339-018-2151-y **Published:** NOV 2018

Abstract: The spin-coating technique was effectively used to prepare a good adherent and uniform thin films of rhodamine B (Rh.B). The investigation of the optical absorption revealed indirect energy gap of 2.1eV and Urbach energy of 29meV. The investigation of the electrical characteristics of the heterojunction-based Rh.B was achieved to extract the important parameters and identify the predominant conduction mechanism. Dark forward and reverse biasing current density-voltage characteristics showed notable rectification characteristics. The heterojunction conduction mechanism of Rh.B/p-Si confirms that observed mechanisms depend on the applied voltage range. The capacitance-voltage characteristics, measured at different signal frequencies, indicated the occurrence of an abrupt type of heterojunction. The frequency dependence of some heterojunction parameters like barrier height, maximum electric field, the width of the depletion region, and carrier concentration gives an indication for the type of interfacial layer of the heterojunction. A high dependence of the capacitance and conductance on both the biasing voltage and the applied frequency was observed. Moreover, the measured series resistance emphasizes the strong effect on the extracted parameters of the studied Schottky diode. Rh.B-based Schottky diode is a promising for multi-applications in an electronic device.

Accession Number: WOS:000446968100001**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Yahia, Ibrahim Sayed	G-4458-2011	

ISSN: 0947-8396

eISSN: 1432-0630

Record 31 of 50**Title:** Investigations of half-metallic ferromagnetism and thermoelectric properties of cubic XCrO₃ (X = Ca, Sr, Ba) compounds via first-principles approaches**Author(s):** Noor, NA (Noor, N. A.); Saddique, MB (Saddique, M. Bilal); Ul Haq, B (Ul Haq, Bakhtiar); Laref, A (Laref, A.); Rashid, M (Rashid, Muhammad)**Source:** PHYSICS LETTERS A **Volume:** 382 **Issue:** 42-43 **Pages:** 3095-3102 **DOI:** 10.1016/j.physleta.2018.07.045 **Published:** OCT 26 2018

Abstract: In this paper, the physical aspects of the cubic phase XCrO₃ (X = Ca, Sr, Ba) perovskites are studied by employing full-potential linearized augmented plane wave plus local orbital (FP-LAPW + lo) method. These compounds have been found stable in ferromagnetic (FM) phase since they possess lower energy in FM phase compared to non-FM phase and their stability is also confirmed by calculating the enthalpy of formation (Delta H). The electronic structures of these compounds are analyzed with Trans and Blaha modified Becke-Johnson potential (TB-mBJ) for both spin up and spin down channels, which indicate their half-metallic characters. Analysis of density of states (DOS) shows major contributions of O-2p states in the valence band and Cr 3d-state in conduction band. A comparative analysis of crystal field effect (Delta E-crystal) and the exchange energies (direct Delta(x)(d) and indirect Delta(x)(pd)) tells about the main part of electronic spin in ferromagnetic character. The calculated magnetic moments make these compounds favorable for spintronic applications. In the end, thermoelectric parameters are computed for 200 K-800 K temperature range to explore potential of these compounds for applications in renewable energy devices. (C) 2018 Elsevier B.V. All rights reserved.

Accession Number: WOS:000446145100009

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Ul Haq, Bakhtiar		0000-0001-9058-2080

ISSN: 0375-9601

eISSN: 1873-2429

Record 32 of 50

Title: Effect of size and location of solid on conjugate heat transfer in porous cavity**Author(s):** Azeem (Azeem); Badruddin, IA (Badruddin, Irfan Anjum); Nik-Ghazali, N (Nik-Ghazali, N.); Idris, MYI (Idris, Mohd Yamani Idna); Anqi, AE (Anqi, Ali E.); Ahmed, NJS (Ahmed, Salman N. J.); Kamangar, S (Kamangar, Sarfaraz); Al-Rashed, AAAA (Al-Rashed, Abdullah A. A. A.)**Source:** INDIAN JOURNAL OF PURE & APPLIED PHYSICS **Volume:** 56 **Issue:** 10 **Pages:** 792-801 **Published:** OCT 2018

Abstract: The highlight of this article is the influence of a solid over heat transfer characteristics in a square porous cavity. The solid placed inside the porous medium is fraction of the whole domain whose size is varied at 5 different locations of the cavity such as left ($\bar{x} = 0$), center ($\bar{x} = 0.5$), right ($\bar{x} = 1$), mid of left and center ($\bar{x} = 0.25$), mid of center and right ($\bar{x} = 0.75$) wall of cavity. The equations that govern the physical phenomenon have been simplified using popular numerical technique such as finite element method. These simultaneous equations are solved for the solution variables such as temperature and the stream function. The physical domain is divided into smaller segments with the help of triangular elements. The left and right vertical surfaces of cavity are maintained at hot and cold temperature T_h and T_c such that $T_h > T_c$.

Accession Number: WOS:000448627100007

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Ahmed, Salman	AAC-3716-2020	

ISSN: 0019-5596

eISSN: 0975-1041

Record 33 of 50

Title: Face-to-Face Collisions of Bright and Dark Ion Acoustic Solitons in Superthermal Electrons for Different Geometrical Configurations**Author(s):** El-Shamy, EF (El-Shamy, E. F.); El-Bedwehy, NA (El-Bedwehy, N. A.); Shokry, M (Shokry, M.); El-Labany, SK (El-Labany, S. K.)**Source:** ZEITSCHRIFT FUR NATURFORSCHUNG SECTION A-A JOURNAL OF PHYSICAL SCIENCES **Volume:** 73 **Issue:** 10 **Pages:** 893-904 **DOI:** 10.1515/zna-2018-0124 **Published:** OCT 2018

Abstract: The face-to-face collision of ion acoustic solitons (IASs) in superthermal plasmas composed of positive and negative ion fluids and superthermal electrons is investigated for different geometrical configurations. For the generic case, the extended Poincare-Lighthill-Kuo (EPLK) analysis is employed to obtain the extended Korteweg-de Vries (EKdV) equations and phase shift equations. The non-linear propagation and the face-to-face collision of bright and dark IASs are studied. In addition, when the concentration of ion reaches the critical value, the EPLK method is applied to obtain the modified Korteweg-de Vries (mKdV) equations and the phase shift relations, which govern the excitation and the face-to-face collision of bright and dark IASs. Appropriately, the effects of several parameters such as the electron concentration, the superthermality of electrons and the diversity in the system's geometry under consideration on the trajectories of IASs after the collision are discussed. Numerical calculations lead to some highlights on the properties of bright and dark IASs (e.g. in laboratory plasmas such as laser-matter/plasma interaction experiments and in astrophysical environments such as lower part of magnetosphere).

Accession Number: WOS:000445783400002

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ISSN: 0932-0784

eISSN: 1865-7109

Record 34 of 50

Title: A comprehensive investigation on core optoelectronic and laser properties of ZTS single crystals: an effect of Mg²⁺ doping**Author(s):** AlFaify, S (AlFaify, S.); Shkir, M (Shkir, Mohd.); Ganesh, V (Ganesh, V.); Anis, M (Anis, Mohd.); Yahia, IS (Yahia, I. S.)**Source:** APPLIED PHYSICS B-LASERS AND OPTICS **Volume:** 124 **Issue:** 10 **Article Number:** 196 **DOI:** 10.1007/s00340-018-7066-y **Published:** OCT 2018

Abstract: The synthesis and large-sized single crystals of pure and Mg²⁺-doped zinc (tris) thiourea sulfate has been developed using slow evaporation methods at 300 K. The size of the grown crystal for pure, 2% Mg and 5% Mg-doped ZTS is found to be similar to 15 mm x 17 mm, similar to 20 mm x 18 mm, and 22 mm x 10 mm, respectively. The crystal structural and vibrational modes are identified by powder X-ray diffraction, FT-IR and FT-Raman analyses. The grown crystal with 5% Mg doping possesses higher optical transparency (67%). Optical energy band gap is found similar to 4.36 eV for 2% Mg and similar to 4.41 eV for 5% Mg-doped crystals. Enhancement in PL intensity of UV band was observed due to doping. The third-order nonlinear susceptibility, $\chi^{(3)}$ is found to be enhanced due to doping which is in the order of 10^{-3} esu. DSC study confirms that the 5% MgZTS crystals possess higher thermal stability than

pure as well as 2% MgZTS. Furthermore, the dielectric study confirms that the grown crystals possess low defects. The microhardness is also found to be enhanced due to doping. All the properties of ZTS are found to be enhanced by Mg doping and make it more suitable for optoelectronic and nonlinear applications compared to pure.

Accession Number: WOS:000444803200001

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ISSN: 0946-2171

eISSN: 1432-0649

Record 35 of 50

Title: Effect of organic dyes on structural properties, linear optics and impedance spectroscopy of methyl orange (Cl acid orange 52) doped polyvinyl alcohol composite thin films

Author(s): Jilani, W (Jilani, W.); Bouzidi, A (Bouzidi, A.); Yahia, IS (Yahia, I. S.); Guermazi, H (Guermazi, H.); Zahran, HY (Zahran, H. Y.); Saker, G (Saker, G.)

Source: JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 29 **Issue:** 19 **Pages:** 16446-16453 **DOI:** 10.1007/s10854-018-9736-2 **Published:** OCT 2018

Abstract: The effect of methyl orange (MEO) dye on structural properties, linear optics and impedance spectroscopy of the polymer poly(vinyl alcohol) (PVA) is studied. MEO/PVA composite thin film was prepared via casting technique. The changes in the structures of the samples were characterized by XRD, which revealed that the internal strain improved the growth of the crystal imperfection and distortion with increasing MEO content in the composite samples. The UV-Vis-NIR spectroscopy was used to study the effect of MEO organic on the optical properties of composite thin films. The samples enhanced more potent light UV-Visible absorption and have very effective prohibition UV-light effect even with incorporating MEO content in the range between 190 and 535 nm. The gap energy leads to a decrease in the visible region which could be attributed to the decrease in crystallite sizes with increasing MEO content. Normalized power characteristics of the films at various MEO concentrations were studied. The normalized power is the very interesting behavior to correlate the optical UV-Vis transmittance and the optics limiting effect of the samples. The dependence of frequency on the conductivity has analyzed in phases of an empirical Jonscher's law. The impedance spectra were analyzed in terms of equivalent circuits involving resistors, capacitors and constant phase elements. Dielectric parameters infer that the incorporating MEO organic dye inside the PVA matrix may be affected by the faster charge transfer properties and behave like a non-ideal capacitor.

Accession Number: WOS:000444763400032

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ISSN: 0957-4522

eISSN: 1573-482X

Record 36 of 50

Title: Photodiode based on Pb_{0.9}Cd_{0.1}S ternary alloy semiconductor for solar tracking systems

Author(s): Wageh, S (Wageh, S.); Karabulut, A (Karabulut, Abdulkarim); Dere, A (Dere, A.); Al-Sehemi, AG (Al-Sehemi, Abdullah G.); Al-Ghamdi, AA (Al-Ghamdi, Ahmed A.); El-Tantawy, F (El-Tantawy, Farid); Yakuphanoglu, F (Yakuphanoglu, F.)

Source: JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 29 **Issue:** 19 **Pages:** 16880-16893 **DOI:** 10.1007/s10854-018-9783-8 **Published:** OCT 2018

Abstract: The fabrication and photoelectrical properties of the photodiodes based on the ternary alloy of semiconductor nanocrystallite Pb_{0.9}Cd_{0.1}S with coumarin dopant were investigated. The structure, stability, melting temperature and optical bandgap of the prepared nanostructure were characterized by X-ray diffraction, thermogravimetric analysis, Infrared, Raman spectroscopy and UV-VIS-NIR spectroscopies. The characterization of the ternary alloy indicates that the crystal structure of the ternary alloy is cubic with some distortion in (111) direction and has a nanosize of 9 nm. The photoelectrical characteristics of fabricated Si-based photodiodes with coumarin doped PbCdS interfacial layers were investigated by using current-voltage, transient photocurrent and capacitance/conductance-voltage measurements. Some electrical parameters and the effects of illumination on these parameters have been determined from these measurements. Consequently, results of experiments suggest that the ternary alloy Pb_{0.9}Cd_{0.1}S nanocrystallite based photodiode can be suitable for optoelectronic applications.

Accession Number: WOS:000444763400078

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Swelm, Wageh	I-8349-2012	
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ISSN: 0957-4522

eISSN: 1573-482X

Record 37 of 50**Title:** Magnetic Properties of Some Tellurite Glasses**Author(s):** Saddeek, YB (Saddeek, Yasser B.); El Mallawany, R (El Mallawany, R.); Yahia, IS (Yahia, I. S.); Dobrowolski, W (Dobrowolski, W.); Kilanski, L (Kilanski, L.); Avdonin, A (Avdonin, A.); Arciszewska, M (Arciszewska, M.)**Source:** JOURNAL OF SUPERCONDUCTIVITY AND NOVEL MAGNETISM **Volume:** 31 **Issue:** 10 **Pages:** 3079-3084 **DOI:** 10.1007/s10948-018-4812-7 **Published:** OCT 2018**Abstract:** The AC magnetic susceptibility in the range 5-130 K of the tellurite glass systems: TeO₂-MnO₂-ZnO-PbO and TeO₂-MnO₂-V₂O₅-Fe₂O₃ was measured and analyzed. The investigations of the AC magnetic susceptibility facilitated the determination of the molar susceptibility, paramagnetic magnetic susceptibility, paramagnetic Curie temperature, and magnetic entropy changes of the tellurite glasses. The results clarified that the temperature dependence of the magnetic susceptibility deviated from the Curie law and the increase of the small negative values of Curie temperature indicated negative interchange interactions between the antiferromagnetically coupled manganese ions within the present glass network. The magnetic moments evaluated from susceptibility measurements of the glasses show the predominance of the Mn²⁺ valence state than Mn³⁺ valence state of MnO₂.**Accession Number:** WOS:000444603100002**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
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Yahia, Ibrahim Sayed	G-4458-2011	
El-Mallawany, R.		0000-0003-2978-5326

ISSN: 1557-1939

eISSN: 1557-1947

Record 38 of 50**Title:** Surface optical phonon - Plasmon interaction in nanodimensional CdTe thin films**Author(s):** Mitric, J (Mitric, J.); Paunovic, N (Paunovic, N.); Mitric, M (Mitric, M.); Vasic, B (Vasic, B.); Ralevic, U (Ralevic, U.); Trajic, J (Trajic, J.); Romcevic, M (Romcevic, M.); Dobrowolski, WD (Dobrowolski, W. D.); Yahia, IS (Yahia, I. S.); Romcevic, N (Romcevic, N.)**Source:** PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES **Volume:** 104 **Pages:** 64-70 **DOI:** 10.1016/j.physe.2018.07.021 **Published:** OCT 2018**Abstract:** Structural and optical properties of CdTe thin films were investigated applying atomic force microscopy (AFM), XRD powder technique, Raman spectroscopy and far-infrared spectroscopy. CdTe thin films were prepared by using thermal evaporation technique. In the analysis of the far - infrared reflection spectra, numerical model for calculating the reflectivity coefficient for system which includes films and substrate has been applied. Effective permittivity of film mixture (CdTe and air) was modeled by Maxwell - Garnet approximation. We reveal the existence of surface optical phonon (SOP) mode and coupled plasmon-SOP modes (CPSOPM).**Accession Number:** WOS:000443990400011**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Yahia, Ibrahim Sayed	G-4458-2011	
Mitric, Jelena	AAE-8277-2019	
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ISSN: 1386-9477

eISSN: 1873-1759

Record 39 of 50**Title:** Analysis of B-8 Proton Halo Nucleus Scattered from C-12 and Ni-58 at Different Energies**Author(s):** Ibraheem, AA (Ibraheem, Awad A.); Farid, ME (El-Azab Farid, M.); Al-Hajjaji, AS (Al-Hajjaji, Arwa S.)**Source:** BRAZILIAN JOURNAL OF PHYSICS **Volume:** 48 **Issue:** 5 **Pages:** 507-512 **DOI:** 10.1007/s13538-018-0586-4 **Published:** OCT 2018**Abstract:** Angular distributions in the elastic scattering of B-8 from C-12 and Ni-58 targets at different energies have been analyzed in the framework of the double-folding (DF) optical model. The real central part of the nuclear optical potential is obtained by folding the M3Y effective interaction with the cluster density distribution of the B-8 nucleus. The experimental angular distributions have been successfully reproduced. This confirms the validity of the cluster structure of the B-8 nucleus.**Accession Number:** WOS:000442866600009

ISSN: 0103-9733

eISSN: 1678-4448

Record 40 of 50**Title:** Exploring the novel donor-nanotube archetype as an efficient third-order nonlinear optical material: asymmetric open-shell carbon nanotubes**Author(s):** Muhammad, S (Muhammad, Shabbir); Nakano, M (Nakano, Masayoshi); Al-Sehemi, AG (Al-Sehemi, Abdullah G.); Irfan, A (Irfan, Ahmad); Chaudhry, AR (Chaudhry, Aijaz Rasool); Tonami, T (Tonami, Takayoshi); Ito, S (Ito, Soichi); Kishi, R (Kishi, Ryohei); Kitagawa, Y (Kitagawa, Yasutaka)**Source:** NANOSCALE **Volume:** 10 **Issue:** 35 **DOI:** 10.1039/c8nr03009j **Published:** SEP 21 2018**Abstract:** Contrary to the enormous number of previous studies on carbon nanotubes (CNTs), herein, we realized the origin of the intrinsic open-shell

diradical character and second hyperpolarizability gamma using a broken symmetry approach. This study was inspired by our recent findings (S. Muhammad, et al., Nanoscale, 2016, 8, 17998 and Nakano, et al., J. Phys. Chem. C, 2016, 120, 1193). We performed structural modifications through a unique asymmetric donor-nanotube framework, which led to a novel paradigm of modified CNTs with tunable open-shell diradical character and remarkably superior NLO response properties. Interestingly, asymmetry and diradical character were found to be the crucial factors to modulate the second hyperpolarizability gamma. We initially performed a comparative analysis of the diradical characters and γ amplitudes of boron nitride nanotubes (BNNTs) and CNTs possessing significant ionic characters and covalent characters, respectively. The basic findings for these simple configurations were further extended to the donor-acceptor CNT paradigm, which finally led to excellent asymmetric donor-CNT configurations with remarkably larger gamma amplitudes. Furthermore, among the CNTs, finite length zigzag CNT(6,0)(3) were modified with different donor-acceptor configurations. Interestingly, for the first time, unique donor-nanotube configurations [1,4-(NH₂)(2)CNT-(6,0)(3) and 1,4-(NH₂)(2) CNT-(6,0)(5)] were found; they showed significantly robust γ amplitudes as large as 2519 x 10(3) and 4090 x 10(3) a.u. at the LC-UBLYP ($\mu = 0.33$)/6-31G* level of theory. Additionally, several molecular level insights have been obtained for these novel donor-nanotube configurations using their odd electron densities, molecular electrostatic maps, densities of states and gamma density analyses to highlight the realization of these novel materials for highly efficient optical and NLO applications.

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PubMed ID: 29872826

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Record 41 of 50

Title: Specific features of structural, electronic, optical and elastic properties of the cubic calcium pyroniobate Ca₂Nb₂O₇ crystals

Author(s): Irfan, M (Irfan, Muhammad); Azam, S (Azam, Sikander); Hussain, S (Hussain, Safdar); Khan, S (Khan, SaleemAyaz); Zaheer, A (Zaheer, Ali); Kityk, IV (Kityk, I. V.); Muhammad, S (Muhammad, Shabbir); Al-Sehemi, AG (Al-Sehemi, Abdullah G.)

Source: PHYSICA B-CONDENSED MATTER **Volume:** 545 **Pages:** 69-75 **DOI:** 10.1016/j.physb.2018.05.041 **Published:** SEP 15 2018

Abstract: Using first principles density functional theory (DFT) calculation, the structural, electronic, optical and elastic properties of cubic Ca₂Nb₂O₇ pyrochlore oxide is studied by highly accurate full potential augmented plane wave method with GGA+U approximation. The calculated lattice parameter is in good agreement with available experimental data. The electronic band structure calculations reveal that Ca₂Nb₂O₇ has direct energy band. For the understanding of optical properties of Ca₂Nb₂O₇, absorption coefficient, dielectric constant, energy loss function, reflectivity, refractive index, extension coefficient and optical conductivity are also calculated for 0-12 eV. A study of elastic properties for cubic pyrochlore oxide (Ca₂Nb₂O₇) is also conducted within a framework of DFT calculations. The stress strain method is used for the determination of elastic constants (C-11, C-12 and C-44) in cubic phase. Hence, bulk, shear and Young's modulus along with Debye temperature, elastic anisotropy factors and Poisson's ratio are calculated successfully. Furthermore, pressure dependence of transverse and longitudinal wave velocities for cubic pyrochlore oxide (Ca₂Nb₂O₇) are also calculated for the first time.

Accession Number: WOS:000449621100011

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al-sehemi, Abdullah	AAM-4039-2020	
Al-Sehemi, Abdullah	AAK-5902-2020	
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ISSN: 0921-4526

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Record 42 of 50

Title: Boron doped graphene based linear dynamic range photodiode

Author(s): Dere, A (Dere, A.); Coskun, B (Coskun, B.); Tataroglu, A (Tataroglu, A.); Al-Sehemi, AG (Al-Sehemi, Abdullah G.); Al-Ghamdi, AA (Al-Ghamdi, Ahmed A.); Alateeq, HMA (Alateeq, Hind M. A.); Qindeel, R (Qindeel, Rabia); Farooq, WA (Farooq, W. A.); Yakuphanoglu, F (Yakuphanoglu, F.)

Source: PHYSICA B-CONDENSED MATTER **Volume:** 545 **Pages:** 86-93 **DOI:** 10.1016/j.physb.2018.05.046 **Published:** SEP 15 2018

Abstract: The boron-doped graphene oxide film was prepared using drop casting/coating technique. The film was coated by hydrothermal method on p-Si substrate and thus Al/p-Si/B-doped GO/Au diode was fabricated. The structural properties of the film was investigated by SEM and EDS techniques. The optoelectronic behavior of the diode was analyzed under various solar light and frequencies. The diode indicates that the forward current is higher than that of

reverse current with a rectification ratio (RR = I-F/I-R) of 7.30×10^4 at dark and +/- 5 V. The diode electronic parameters of the diode were computed from electrical characteristics. An increase in the photocurrent of the diode with solar light intensity indicates the presence of a photoconduction mechanism. The photoconductive and photovoltaic response of the diode were analyzed using photocurrent measurements. The interface state density (N-ss) of the diode was analyzed from conductance technique. The optoelectrical results of the studied device suggest that the diode can be used in optic communications.

Accession Number: WOS:000449621100014

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Al-Sehemi, Abdullah	AAK-5902-2020	
al-sehemi, Abdullah	AAM-4039-2020	
Al-Sehemi, Abdullah	J-9967-2012	
Yakuphanoglu, Fahrettin	C-8365-2012	
Tataroglu, Adem	V-8882-2017	0000-0003-2074-574X
Coskun, Burhan		0000-0002-8242-9921
Al-Sehemi, Abdullah		0000-0002-6793-3038

ISSN: 0921-4526

eISSN: 1873-2135

Record 43 of 50

Title: Linear and Nonlinear Optics of CBD Grown Nanocrystalline F Doped CdS Thin Films for Optoelectronic Applications: An Effect of Thickness

Author(s): Khan, ZR (Khan, Z. R.); Shkir, M (Shkir, Mohd.); Ganesh, V (Ganesh, V.); Alfaify, S (Alfaify, S.); Yahia, IS (Yahia, I. S.); Zahran, HY (Zahran, H. Y.)

Source: JOURNAL OF ELECTRONIC MATERIALS **Volume:** 47 **Issue:** 9 **Pages:** 5386-5395 **DOI:** 10.1007/s11664-018-6437-9 **Published:** SEP 2018

Abstract: Fluorine (F) doped (i.e. 1 wt.%) cadmium sulfide (CdS) thin films with different thicknesses were fabricated on fluorine doped tin oxide coated glass substrates by chemical bath deposition methods. For doping of F, 1 wt.% ammonium fluoride was added into the solution. A significant influence of thicknesses on physical properties of F doped CdS thin films was observed. The thin films were investigated by various characterization techniques such as x-ray diffraction (XRD), UV-Vis-NIR, FT-Raman spectroscopy and scanning electron microscope. XRD analysis showed that the films are preferentially grown along (111) plane. The crystallites' size changed with increases the film's thickness. Films showed high transmittance in visible region. Raman spectra showed shift in first and second longitudinal phonon vibration (1LO and 2LO) with the change in thickness of the films. This shows that changing thickness leads to changes in the physical properties of films. The values of the band gaps were estimated as 2.60 eV, 2.75 eV, 2.80 eV for films of thickness 100 nm, 150 nm and 200 nm, respectively. Hence, the band gap of films increases with an increase in thickness. Refractive index, linear optical susceptibility, nonlinear optical susceptibility and nonlinear refractive index were also estimated. The higher values of nonlinear optical parameters shows good scope in nonlinear optical applications.

Accession Number: WOS:000458770800065

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Yahia, Ibrahim Sayed	G-4458-2011	
Zahran, Heba	AAR-9136-2020	
AlFaiify, S	ABF-3895-2020	0000-0002-8920-5891
GANESH, VANGA		0000-0001-8860-5503

ISSN: 0361-5235

eISSN: 1543-186X

Record 44 of 50

Title: Effect of Graphitic Carbon Nitride Nanosheets Addition on the Microstructure and Mechanical Properties of Sn-3.5Ag-0.5Cu Solder Alloy

Author(s): Zahran, HY (Zahran, H. Y.); Abd El-Rehim, AF (Abd El-Rehim, A. F.); Alfaify, S (Alfaify, S.)

Source: JOURNAL OF ELECTRONIC MATERIALS **Volume:** 47 **Issue:** 9 **Pages:** 5614-5624 **DOI:** 10.1007/s11664-018-6474-4 **Published:** SEP 2018

Abstract: The microstructure and mechanical properties of Sn-3.5Ag-0.5Cu (SAC355) solder alloy reinforced with different amounts of graphitic carbon nitride nanosheets (GCNNs) are assessed. The as-synthesized GCNNs were examined by a scanning electron microscope and X-ray diffraction techniques. A set of composite solders were fabricated by adding GCNNs with different concentrations (0 wt.%, 0.25 wt.%, 0.5 wt.%, and 1.0 wt.%) to SAC355 solder alloy. After a mechanical heat treatment, samples were immediately aged at temperatures ranging from 343 K to 403 K for 2 h followed by water quenching at 273 K. The mechanical properties of the composite solders were assessed using the indentation hardness test. The experimental results showed that the minimum creep rate values estimated from hardness data increased progressively with increasing weight percentage of GCNNs and/or aging temperature. The homogeneous distribution of GCNNs in the composite solders allows microscopic defects such as cracks to develop throughout the solders leading to higher creep rate values. The calculated values of the stress exponent and the activation energy for the creep process indicated that the creep rate controlling process depends on dislocation core diffusion in the tin matrix.

Accession Number: WOS:000458770800092

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Zahran, Heba	AAR-9136-2020	
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Yahia, Ibrahim Sayed	G-4458-2011	

ISSN: 0361-5235

eISSN: 1543-186X

Record 45 of 50

Title: Microwave-synthesis of La³⁺ doped PbI₂ nanosheets (NSs) and their characterizations for optoelectronic applications

Author(s): Shkir, M (Shkir, Mohd.); Ganesh, V (Ganesh, V.); Yahia, IS (Yahia, I. S.); AlFaify, S (AlFaify, S.)

Source: JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 29 **Issue:** 18 **Special Issue:** SI **Pages:** 15838-15846 **DOI:** 10.1007/s10854-018-9670-3 **Published:** SEP 2018

Abstract: Herein, we report the microwave-synthesis of pure and lanthanum (La³⁺) doped PbI₂ nanostructures. Single phase and good crystallinity confirmation was done using X-ray diffraction and FT-Raman spectroscopy analyses. Presence of La in the final product was proved by energy dispersive X-ray spectroscopy and homogeneous doping of La was seen in EDX elemental mapping. Vibrational modes of final products gets shifted compare to bulk values which evidently specify more relaxed nanostructure formation. The morphology was determined by scanning electron microscope analysis which was nanorods (NRs) of dimension in range of 70-100 nm of pure. However, when doped with 1% La the formation of nanosheets (NSs) are found to be more dense with well defined hexagonal morphology and the average thickness is found to be reduced which is 57 nm and size is increased. Ultra violet-visible-near infrared measurement was done and the energy gap was computed, which are in range of 2.93 to 3.26 eV. Photoluminescence emission spectra was recorded at . PL emissions positioned at 470 +/- 2 and 525 +/- 7 nm are corresponding to blue and green emissions in NSs. An enhancement in values of dielectric and electrical conductivity was observed due to doping.

Accession Number: WOS:000444200300069

Conference Title: 26th International Materials Research Congress (IMRC)

Conference Date: AUG 20-25, 2017

Conference Location: Cancun, MEXICO

Conference Sponsors: Soc Mexicana Mat, Mat Res Soc

Author Identifiers:

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AlFaify, S	ABF-3895-2020	0000-0002-8920-5891
Yahia, Ibrahim Sayed	G-4458-2011	
GANESH, VANGA		0000-0001-8860-5503

ISSN: 0957-4522

eISSN: 1573-482X

Record 46 of 50

Title: Modified Becke-Johnson calculations applied to the electronic and optical properties of Mg and Mn doped PbS

Author(s): Gassoumi, A (Gassoumi, A.); Al-Shahrani, A (Al-Shahrani, A.); Alfaify, S (Alfaify, S.); Algarni, H (Algarni, H.); Vidu, R (Vidu, R.)

Source: JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS **Volume:** 20 **Issue:** 9-10 **Pages:** 453-458 **Published:** SEP-OCT 2018

Abstract: In this paper, electronic and optical properties of magnesium (Mg) and manganese (Mn) doped lead sulfide (PbS) compounds have been investigated based on the full-potential linear augmented plane wave (FP-LAPW) method by using the modified Becke-Johnson (mBJ) method. The detailed optical studied revealed that the band gap of pure PbS was found to be similar to 0.9 eV and Mg doped PbS exhibited direct band gap energy of similar to 2eV. Further, Mn doped PbS possess a metallic behavior. The PbS compound possess a cubic rock-salt structure with the space group Fm-3m and lattice parameter $a = 5.931$ angstrom, which were used in our calculations. The optical parameters, such as dielectric constant, refractive index and reflectivity were analyzed. The results demonstrated that Mg and Mn doped PbS compounds have the potential to be used for optoelectronic applications.

Accession Number: WOS:000452505200001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
AlFaify, S	ABF-3895-2020	0000-0002-8920-5891
Vidu, Ruxandra	L-2600-2014	0000-0003-3323-9547

ISSN: 1454-4164

eISSN: 1841-7132

Record 47 of 50

Title: Quantum phase gate based on multiphoton process in multimode cavity QED

Author(s): Alqahtani, MM (Alqahtani, Moteb M.)

Source: QUANTUM INFORMATION PROCESSING **Volume:** 17 **Issue:** 9 **Article Number:** 211 **DOI:** 10.1007/s11128-018-1979-6 **Published:** SEP 2018

Abstract: We propose a scheme for implementing a two-qubit quantum phase gate in which the photonic qubits encoded on the cavity modes and a three-level V-type atom passes through the cavity. The location of the resonance is predicted from the use of the theory of multiphoton resonance. Further, we investigate the influence of variations in parameters such as the coupling strengths and detunings on the gate fidelity. We also use the wave-function and the density matrix approaches to analyze theoretically and numerically the effects of decoherence in the implementation of the gate.

Accession Number: WOS:000438919800001

ISSN: 1570-0755

eISSN: 1573-1332

Record 48 of 50

Title: Structure and transport properties of Tl₂Te₃ single crystals

Author(s): Ashraf, IM (Ashraf, I. M.); Salem, A (Salem, A.); Al-Juman, MSA (Al-Juman, M. S. Awad)

Source: RESULTS IN PHYSICS **Volume:** 10 **Pages:** 281-286 **DOI:** 10.1016/j.rinp.2018.05.044 **Published:** SEP 2018

Abstract: A special new design from melt based on the Bridgman technique has been applied to prepare Tl₂Te₃ single crystals. The grown crystals were characterized by XRD, SEM, EDAX. The electrical conductivity, Hall effect and thermoelectric power have been performed over the temperature ranges from 93 K to 448 K and 129 K to 468 K respectively. Many physical constant (such as the energy gap, the depth of the impurity level, the Hall coefficient, the conductivity type, the diffusion length, the diffusion coefficient, the scattering mechanism of the charge carriers and their concentrations, the mobility, effective mass, and the lifetime of the majority and minority carriers) have been estimated. The results show that the prepared Tl₂Te₃ single crystals can be used in the fabrication of electronic devices.

Accession Number: WOS:000443868900045

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Ebrahem, Ashraf Mahmoud	AAT-6263-2020	

ISSN: 2211-3797

Record 49 of 50

Title: New transform iterative method for solving some Klein-Gordon equations**Author(s):** Alderremy, AA (Alderremy, Aisha Abdullah); Elzaki, TM (Elzaki, Tarig M.); Chamekh, M (Chamekh, Mourad)**Source:** RESULTS IN PHYSICS **Volume:** 10 **Pages:** 655-659 **DOI:** 10.1016/j.rinp.2018.07.004 **Published:** SEP 2018

Abstract: In this study, we treat some Klein-Gordon equations (KGEs). We propose a novel iterative approach called the Elzaki iterative method (EIM). This method, which clearly depends on the choice of the initial values, is based on the new iteration method (NIM) and the Elzaki transformation. We show that the EIM could be more valid and reliable approach than the NIM. We propose an analytical approximation of a solution for KGEs for which only a few iterations are necessary to obtain a semi-analytical solution without a loss of precision.

Accession Number: WOS:000443868900100

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Alderremy, Aisha	AAC-8801-2019	

ISSN: 2211-3797

Record 50 of 50

Title: Committed effective dose to the Kuwaiti population via the dietary intake of red meat**Author(s):** Alrefae, T (Alrefae, Tareq); Nageswaran, TN (Nageswaran, Tiruvachi N.); Demir, NS (Demir, Nasser S.); Khandaker, MU (Khandaker, Mayeen Uddin); Bradley, DA (Bradley, David A.); Alkhorayef, M (Alkhorayef, Mohammed); Alzimami, KS (Alzimami, Khalid S.)**Source:** RESULTS IN PHYSICS **Volume:** 10 **Pages:** 827-831 **DOI:** 10.1016/j.rinp.2018.07.030 **Published:** SEP 2018

Abstract: Meat is a major component of the daily diet of the Kuwait population. Realizing the negative consequences of the presence of radioactive materials in foodstuffs, various types of meat (fresh and processed lamb and beef) on sale in Kuwaiti markets have been assessed. The interest is in seeking to obtain a measure of the potential radiological impact to human health that results from their consumption. High purity germanium.-ray spectrometry of the meat has revealed low activities of Ra-226 and Ra-228, key indicators of the respective U-238 and Th-232 natural decay series. While elevated activities of K-40 were observed in a number of the fresh meat samples, evidence of the anthropogenic radionuclide Cs-137 was found in one sample only. A statistically significant difference was found between the mean value of activity concentration of K-40 in fresh and processed beef samples. The total potassium concentration in the meat samples was calculated from observation of K-40 activity, values ranging between 2.6 and 17.2 g kg(-1). The annual effective dose resulting from meat consumption for a typical adult in Kuwait has been estimated to be 217 mu Sv y(-1), somewhat less than the 290 mu Sv y(-1) assessed by UNSCEAR (2008) to prevail more globally. Findings from this research are intended to underline the importance of periodic monitoring of foodstuffs in efforts towards mitigating radiological risk.

Accession Number: WOS:000443868900127

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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ISSN: 2211-3797

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Record 51 of 119**Title:** Facile one pot synthesis of novel Hg²⁺ doped PbI₂ nanostructures for optoelectronic and radiation shielding applications**Author(s):** AlFaify, S (AlFaify, S.); Shkir, M (Shkir, Mohd.); Ganesh, V (Ganesh, V.)**Source:** MATERIALS SCIENCE IN SEMICONDUCTOR PROCESSING **Volume:** 83 **Pages:** 231-238 **DOI:** 10.1016/j.mssp.2018.04.040 **Published:** AUG 15 2018**Abstract:** Facile one pot synthesis of pure and Hg²⁺ (= 0.101 nm) doped PbI₂ (Pb²⁺ = 0.133 nm) single crystalline nanoplates (NPs), nanosheets (NSs) and nanorods (NRs) were achieved through chemical route at room temperature. The single phase and high quality of the synthesized NPs, NSs and NRs was proved by X-ray diffraction and FT-Raman spectroscopic analyses. The lattice constants, crystallite size, lattice strain, dislocation density were calculated. The crystallite size was calculated to be in the range of 16-22 nm. The Hg doping in PbI₂ was approved by energy dispersive X-ray spectroscopy (EDXS) and its homogeneous distribution was confirmed by scanning electron microscopy (SEM) mapping. The morphology of pure and doped synthesized nanostructures was observed to be single crystalline NPs, NSs and NRs of nanoscale thicknesses. The optical band gap was calculated from Tauc's plot and found to be in the range of 3.27-3.20 eV. The value of dielectric constant was improved from 20 to 25 and also ac electrical conductivity due to Hg²⁺ doping. The radiation parameters such as linear absorption coefficient, half value layer, tenth value layer and mean free path were calculated and a remarkable enhancement was observed due to Hg²⁺ doping. These parameters confirm that the nanostructures are highly sensitive to Am-214 59.5KeV gamma-ray. The facilely synthesized nanostructures of PbI₂ with enhanced properties due to Hg²⁺ doping makes them more suitable for nanoelectronics and room temperature radiation detector applications.**Accession Number:** WOS:000433236200032**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
AlFaify, S	ABF-3895-2020	0000-0002-8920-5891
GANESH, VANGA		0000-0001-8860-5503

ISSN: 1369-8001**eISSN:** 1873-4081**Record 52 of 119****Title:** Microelectronic properties of the organic Schottky diode with pyronin-Y: Admittance spectroscopy, and negative capacitance**Author(s):** Yahia, IS (Yahia, I. S.); Zahran, HY (Zahran, H. Y.); Alamri, FH (Alamri, F. H.); Manthrammel, MA (Manthrammel, M. Aslam); AlFaify, S (AlFaify, S.); Ali, AM (Ali, Atif Mossad)**Source:** PHYSICA B-CONDENSED MATTER **Volume:** 543 **Pages:** 46-53 **DOI:** 10.1016/j.physb.2018.05.011 **Published:** AUG 15 2018**Abstract:** The Au/Pyronin-Y/p-Si/Al Schottky diode was designed and studied by using the DC and AC measurements. Current-voltage (I-V), capacitance-voltage (C-V) and conductance-voltage methods under different frequencies and voltage biasing were measured at room temperature. The I-V characteristics and C-V characteristics were determined by using the electrical and impedance measurements. From I-V characteristics curve, the Au/pyronin-Y/p-Si/Al Schottky diode has a rectifying behavior. The parameters of Schottky diode such as the series resistance, ideality factor, and barrier height were computed for Au/Pyronin-Y/p-Si/Al junction diode. The performance of the Au/pyronin-Y/p-Si/Al diode is attributed to the creation of the interfacial layer by the organic semiconductor dye. Admittance spectroscopy method can describe the series resistance-voltage (R-s-V) and impedance-voltage (Z-V), capacitance-voltage (C-V) and conductance-voltage (G-V) measurements at different frequencies at room temperature. This device showed a negative capacitance at higher frequencies. The origin of negative capacitance is attributed to the inductive behavior of the studied materials. From C-V analysis, different parameters were calculated and analyzed such as the doping concentration, the built-in potential, the depletion layer and the diffusing potential at zero bias. The obtained results support that the electronic properties of the silicon-based Schottky diode can be controlled by the interlayer organic layer (Pyronin-Y).**Accession Number:** WOS:000438991400008**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Yahia, Ibrahim Sayed	G-4458-2011	
Zahran, Heba	AAR-9136-2020	
AlFaify, S	ABF-3895-2020	0000-0002-8920-5891
Manthrammel, Mohamed Aslam		0000-0001-8458-2594

ISSN: 0921-4526**eISSN:** 1873-2135**Record 53 of 119****Title:** Conduction-and valence band offsets of Zn_{1-x}Mg_xSe/Zn_{1-y}Mg_ySe heterointerfaces**Author(s):** Al-Hagan, OA (Al-Hagan, O. A.); Bouarissa, N (Bouarissa, N.); Gueddime, A (Gueddim, A.); Algarni, H (Algarni, H.); Alhuwaymel, TF (Alhuwaymel, T. F.); Khan, MA (Khan, M. Ajmal)**Source:** PHYSICA B-CONDENSED MATTER **Volume:** 543 **Pages:** 54-59 **DOI:** 10.1016/j.physb.2018.05.019 **Published:** AUG 15 2018**Abstract:** Based on the model-solid theory coupled with a pseudopotential approach within the virtual crystal approximation, the conduction and valence band offsets (CBO) and (VBO) of the unstrained and strained Zn_{1-x}Mg_xSe/Zn_{1-y}Mg_ySe heterointerfaces have been investigated. The calculated elastic constants C-11 and C-12 for ZnSe and MgSe are found to agree to within 7% with experiment. Our findings showed that for electrons the CBO is negative whereas the Mg content of the overlayer (x) is lower than the Mg content of the substrate (y). Nevertheless, the reverse can be seen when x (>) y. As regards the light-and heavy holes the VBOs remain negative as far as the Mg concentration of the overlayer is lower than that of substrate layers and become positive in the opposite case. The alignment of the bands is found to be of type II (staggered) whatever is the Mg compositions of both the overlayer and the substrate layer. The relaxed and strained band-gap energies versus the composition y have been computed and the results are examined and discussed.**Accession Number:** WOS:000438991400009

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
GUEDDIM, Ahmed	AAF-6489-2019	0000-0002-4638-7269
Gueddim, Ahmed	O-1839-2016	0000-0002-4638-7269
Al-Hagan, Ola		0000-0003-0386-2418

ISSN: 0921-4526

eISSN: 1873-2135

Record 54 of 119

Title: Effect of spray pressure on optical, electrical and solar cell efficiency of novel Cu₂O thin films**Author(s):** Prabu, RD (Prabu, R. David); Valanarasu, S (Valanarasu, S.); Ganesh, V (Ganesh, V); Shkir, M (Shkir, Mohd); Kathalingam, A (Kathalingam, A.); AlFaify, S (AlFaify, S.)**Source:** SURFACE & COATINGS TECHNOLOGY **Volume:** 347 **Pages:** 164-172 **DOI:** 10.1016/j.surfcoat.2018.04.084 **Published:** AUG 15 2018

Abstract: Cu₂O thin films were deposited by nebulizer spray pyrolysis technique using different pressure rates. Structural, morphological, optical, photoluminescence, electrical and solar cell studies were done. The structural studies confirmed that the deposited Cu₂O thin films are in polycrystalline nature having cubic crystal structure matching with the standard JCPDS Card. No (77-0199). Laser Raman analysis confirmed that all peaks are correspond to Cu₂O phase. Optical analysis showed band gap values 2.26, 2.12 and 1.99 eV for pressures 1, 2 and 3 bars, respectively. Photoluminescence analysis confirmed that the emission peak obtained at 617 nm corresponds to cuprous oxide phase. Films deposited at high pressure i.e. 3 bars showed low resistivity 1.73 × 10⁽²⁾ Omega.cm. Solar cells were fabricated using the deposited Cu₂O film with ZnO as heterojunction that showed fill factor values 0.29, 0.35 and 0.39 for pressures 1, 2 and 3 bars, respectively. The power conversion efficiency (eta) was increased from 0.039 to 0.57% (about 15 times) by increasing the pressure from 1 to 3 bars.

Accession Number: WOS:000436917300019

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Valanarasu, S	AAG-4607-2021	
Kathalingam, A.	E-9804-2010	0000-0003-2303-0424
AlFaify, S	ABF-3895-2020	0000-0002-8920-5891
GANESH, VANGA		0000-0001-8860-5503
Santiago, Valanarasu		0000-0001-7315-2126

ISSN: 0257-8972

Record 55 of 119

Title: Microhardness, phase transition, acoustic wave velocities and melting temperature of Al_xGa_{1-x}Sb**Author(s):** Al-Hagan, OA (Al-Hagan, O. A.); Algarni, H (Algarni, H.); Bouarissa, N (Bouarissa, N.); Khan, MA (Khan, M. Ajmal); Alhuwaymel, TF (Alhuwaymel, T. F.)**Source:** INTERNATIONAL JOURNAL OF MODERN PHYSICS B **Volume:** 32 **Issue:** 20 **Article Number:** 1850210 **DOI:** 10.1142/S0217979218502107 **Published:** AUG 10 2018

Abstract: The band structure of Al_xGa_{1-x}Sb-x semiconducting ternary alloys and their related properties such as elastic constants, microhardness, transition pressure to the first phase, acoustic wave velocities and melting temperature have been investigated. The calculations are performed using a pseudopotential approach within the virtual crystal approximation which includes the effect of compositional disorder as an effective potential. Generally, our results are found to be in good accord with the experimental results. The composition dependence of all features of interest showed a monotonic behavior and suggests that the stiffness, hardness and structural stability becomes better in Al_xGa_{1-x}Sb-x for higher Al concentrations. The bulk sound speeds and melting temperature are found to become larger when increasing the Al content.

Accession Number: WOS:000440614900005

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Al-Hagan, Ola		0000-0003-0386-2418

ISSN: 0217-9792

eISSN: 1793-6578

Record 56 of 119

Title: Synthesis, characterization and properties of Mn-doped ZnO nanoparticles**Author(s):** Khalid, R (Khalid, Rayan); Alhazaa, AN (Alhazaa, Abdulaziz N.); Khan, MAM (Khan, M. A. Majeed)**Source:** APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING **Volume:** 124 **Issue:** 8 **Article Number:** 536 **DOI:** 10.1007/s00339-018-1934-5 **Published:** AUG 2018

Abstract: In the present study, undoped and Mn-doped ZnO nanoparticles with different Mn concentrations (4 and 6 at.%) have been prepared by polymeric precursor method. The effects of Mn content on the structural, optical, and magnetic properties of these nanoparticles were investigated in detail. Room temperature X-ray diffraction (XRD) data revealed hexagonal wurtzite structure of the samples and no other secondary phase has been noticed. The microstructural analysis confirms that the particles of Mn:ZnO are spherical in shape with size ranging between 32 and 45 nm as calculated by Scherrer's equation and transmission electron microscopy (TEM) images. UV-visible absorption spectroscopy measurements affirm a blue-shift in the band gap with increasing Mn doping in ZnO. The hysteresis loops (M-H) exhibit ferromagnetic behaviour of all samples at room temperature. Temperature-dependent resistivity measurements show semiconducting nature of the samples and reduction in the resistivity on Mn substitution.

Accession Number: WOS:000438476100001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number

Author	Web of Science ResearcherID	ORCID Number
Khan, M.	ABC-8683-2020	
ALHAZAA, ABDULAZIZ		0000-0002-6213-6662

ISSN: 0947-8396

eISSN: 1432-0630

Record 57 of 119**Title:** Construction of chaotic quantum magnets and matrix Lorenz systems S-boxes and their applications**Author(s):** Hussain, I (Hussain, Iqtadar); Anees, A (Anees, Amir); Alkhalidi, AH (Alkhalidi, Ali Hussain); Algarni, A (Algarni, Abdulmohsen); Aslam, M (Aslam, Muhammad)**Source:** CHINESE JOURNAL OF PHYSICS **Volume:** 56 **Issue:** 4 **Pages:** 1609-1621 **DOI:** 10.1016/j.cjph.2018.04.013 **Published:** AUG 2018

Abstract: When we listen regarding quantum cryptography, the first thinking that comes up to mind is, how can there be any connection between physics and cryptographic ciphers. In fact, it comes into view that is one of the hottest research in the field of cryptology to exploit physics and has been confirmed as the important objective in the protection of digital data. The topic of quantum magnets and matrix Lorenz Systems has begun to draw increasing attention in recent years. In last decade, chaotic systems have been utilized in many encryption algorithms. In this regard, Lorenz chaotic system based on differential equations achieved more recognition because of its fundamental sensitivity to initial conditions and easiness in use. This manuscript has two parts. First, we have constructed substitution boxes (S-Boxes) based on quantum magnets and matrix Lorenz chaotic system and permutation of the symmetric group S-256 and then designated an image encryption algorithm based on proposed S-boxes and Lorenz chaotic system. In cryptography, it is essential to construct secure S-Boxes to propose cryptographically strong systems. Recently, some image encryption techniques that are weak against robustness have been proposed based on chaotic S-boxes. In the first part of the manuscript, an S-Box design is proposed. Continuous-time Lorenz system is chosen as the chaotic system. The presented image encryption algorithm is based on two rounds of a novel chaotic substitution-permutation network uses proposed S-boxes for substitution purpose by iterations of the Lorenz chaotic system and special kind of permutation process to get the full cipher image. The proposed algorithms for S-box construction and image encryption give very good and coherent performance results when we analyze them with renowned analyses.

Accession Number: WOS:000442353500028**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Aslam, Muhammad	ABI-8003-2020	
hussain, Iqtadar		0000-0002-2500-4214

ISSN: 0577-9073

Record 58 of 119**Title:** High Thermoelectric Action in Vacuum Deposited Indium Alloyed Chalcogenide Thin Films: In_xSe_{100-x}**Author(s):** Sharma, P (Sharma, Pankaj); Dahshan, A (Dahshan, Alaa); Sehgal, VK (Sehgal, Vivek Kumar); Aly, KAN (Aly, Kamal Abdel-Nabi)**Source:** IEEE TRANSACTIONS ON ELECTRON DEVICES **Volume:** 65 **Issue:** 8 **Pages:** 3408-3413 **DOI:** 10.1109/TED.2018.2845413 **Published:** AUG 2018

Abstract: Chalcogenide glasses own high degree of disorder which is a significant parameter to improve the performance of thermoelectric materials. Here, we study the electrical and thermoelectric properties of vacuum deposited In_xSe_{100-x} (x = 6, 12, 18, and 24) chalcogenide thin films in the temperature range from 300 to 450 K. The values of dc conductivity have been determined and were found to increase from 0.029 x 10⁽⁻¹⁰⁾ Ω⁽⁻¹⁾ . m⁽⁻¹⁾ (x = 6) to 173.546 x 10⁽⁻¹⁰⁾ Ω⁽⁻¹⁾ . m⁽⁻¹⁾ (x = 24). Thin film samples for x = 6, 12, 18, and 24 have shown high values of the Seebeck coefficient. The obtained results for the dc conductivity and the Seebeck coefficient may lead to a high value of the power factor. Looking into the results, it is expected that x = 6, 12, 18, and 24 samples have high figure of merit and may be explored as new thermoelectric materials.

Accession Number: WOS:000439649900047**Author Identifiers:**

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Sehgal, Vivek Kumar	S-1937-2017	0000-0002-0026-2284
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Dahshan, Alaa		0000-0003-0156-4134

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Record 59 of 119**Title:** Novel report on SHG efficiency, Z-scan, laser damage threshold, photoluminescence, dielectric and surface microscopic studies of hybrid inorganic ammonium zinc sulphate hydrate single crystal**Author(s):** Ramteke, SP (Ramteke, S. P.); Baig, MI (Baig, M. I.); Shkir, M (Shkir, Mohd); Kalainathan, S (Kalainathan, S.); Shirsat, MD (Shirsat, M. D.); Muley, GG (Muley, G. G.); Anis, M (Anis, Mohd)**Source:** OPTICS AND LASER TECHNOLOGY **Volume:** 104 **Pages:** 83-89 **DOI:** 10.1016/j.optlastec.2018.02.018 **Published:** AUG 2018

Abstract: Hybrid inorganic nonlinear optical crystals find huge applications in laser assisted photonic devices therefore present communication firstly aims to investigate the dielectric, microscopic and linear nonlinear optical properties of ammonium zinc sulphate hydrate (AZSH) crystal. The inorganic AZSH complex has been synthesized and 15 x 10 x 09 mm⁽³⁾ single crystal was grown by slow solvent evaporation method. The powder and single crystal X-ray diffraction technique has been employed to evaluate the crystalline phase and determine the structural parameters of AZSH crystal. The optical transparency of AZSH crystal has been examined within the wavelength range of 200-1100 nm. The enhanced second harmonic generation efficiency of AZSH crystal is 2.53 times higher than standard KDP crystal. The laser damage threshold of AZSH crystal has been determined using the Nd:YAG laser operating at 1064 nm. The close and open aperture Z-scan studies have been performed to ascertain the nature of third order nonlinear optical (TONLO) refraction and absorption of AZSH crystal. The order of TONLO parameters n⁽²⁾, beta and chi⁽³⁾ is found to be 10⁽⁻⁹⁾ cm⁽²⁾/W, 10⁽⁻⁴⁾ cm/W, 10⁽⁻⁴⁾ esu respectively. The AZSH crystal is found to have violet colored luminescence emission centered at 370 nm. The dielectric constant and dielectric loss of AZSH crystal has been evaluated within

30 Hz to 1 MHz. The chemical etching technique has been imposed to examine the growth habitat and determine the etch pit density of AZSH crystal. (C) 2018 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000428484600012

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Record 60 of 119

Title: The tunable magnetic properties and microstructures of Co-Ni double-substituted M-type Casrla hexaferrites

Author(s): Yang, YJ (Yang, Yujie); Wang, FH (Wang, Fanhou); Shao, JX (Shao, Juxiang); Batoo, KM (Batoo, Khalid Mujasam); Huang, DH (Huang, Duohui)

Source: CHINESE JOURNAL OF PHYSICS **Volume:** 56 **Issue:** 4 **Pages:** 1789-1798 **DOI:** 10.1016/j.cjph.2018.05.009 **Published:** AUG 2018

Abstract: M-type hexaferrites with Co²⁺ and Ni²⁺ ions substituting for Fe(3+) ions (Ca_{0.30}Sr_{0.35}La_{0.35}Fe_{12.0-x}(Co_{0.5}Ni_{0.5})_xO-0.19, 0.0 ≤ x ≤ 1.0) were prepared by the traditional solid state method. X-ray diffractometer (XRD), field emission scanning electron microscopy (FE-SEM), physical property measurement system-vibrating sample magnetometer (PPMS-VSM) have been employed to study the microstructures and magnetic properties of hexaferrites. XRD patterns showed that the single magnetoplumbite phase is obtained if Co-Ni content (x) ≤ 0.4 and impurity phases are observed in the structure when Co-Ni content (x) ≥ 0.4. FE-SEM micrographs showed that the hexaferrites with hexagonal platelet-like grains is obtained. The saturation magnetization (M_s), remanent magnetization (M_r), M_r/M_s ratio, magneton number (n(B)), coercivity (H_c), magnetic anisotropy field (H_a) and first anisotropy constant (K₁) decrease with increasing Co-Ni content (x) from 0.0 to 1.0. And our reported results with tunable H_r and M_r can be used for recording applications.

Accession Number: WOS:000442353500043

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ISSN: 0577-9073

Record 61 of 119

Title: Electronic and optoelectronic properties of Al/coumarin doped Pr₂Se₃Tl₂Se/p-Si devices

Author(s): Tataroglu, A (Tataroglu, A.); Ahmedova, C (Ahmedova, C.); Barim, G (Barim, G.); Al-Sehemi, AG (Al-Sehemi, Abdullah G.); Karabulut, A (Karabulut, Abdulkarim); Al-Ghamdi, AA (Al-Ghamdi, Ahmed A.); Farooq, WA (Farooq, W. A.); Yakuphanoglu, F (Yakuphanoglu, F.)

Source: JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 29 **Issue:** 15 **Pages:** 12561-12572 **DOI:** 10.1007/s10854-018-9372-x **Published:** AUG 2018

Abstract: In this study, coumarin-doped Pr₂Se₃Tl₂Se (0.00, 0.05, 0.1, 0.3 wt% coumarin) were covered on the front side of a p-Si substrate by drop coating method and thus Al/coumarin doped Pr₂Se₃Tl₂Se/p-Si diodes were fabricated. The electronic and optoelectronic properties of the prepared diodes were investigated. The highest rectification ratio (RR = I-F/I-R) value was found to be 2.24 x 10⁵ for the diode having 0.05 wt% coumarin doping at dark and +/- 5 V. Also, the highest I-photo/I-dark photosensitivity was found to be 1327 for the diode which has 0.1 wt% coumarin doping at 100 mW/cm² and - 5 V. The photocurrent of the diodes is higher than the dark current and increases by the increase of the light intensity. These results confirm that the fabricated diodes show a strong photovoltaic behavior. The electronic parameters of the diodes, for example ideality factor and barrier height values, were calculated by the use of current-voltage characteristics. The transient measurement proves that the diodes show both photodiode and photocapacitor behaviors. The change on the conductance and capacitance by the frequency is attributed to the existence of interface states. Thus, the obtained results suggest that the prepared diodes might be used as a photosensor in the applications of optoelectronic.

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Record 62 of 119

Title: Transition metal (Mn) and rare earth (Nd) di-doped novel ZnO nanoparticles: a facile sol-gel synthesis and characterization

Author(s): Manoharan, AA (manoharan, A. Albert); Chandramohan, R (Chandramohan, R.); Kumar, KDA (Kumar, K. Deva Arun); Valanarasu, S (Valanarasu, S.); Ganesh, V (Ganesh, V.); Shkir, M (Shkir, Mohd.); Algarni, H (Algarni, H.); AlFaify, S (AlFaify, S.)

Source: JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 29 **Issue:** 15 **Pages:** 13077-13086 **DOI:** 10.1007/s10854-018-9430-4 **Published:** AUG 2018

Abstract: Undoped, Mn doped and Nd co-doped ZnO nanoparticles are synthesized through a facile sol-gel route. Characterization of the synthesized samples has been done by X-ray diffraction, scanning electron microscopy, FT-IR, diffuse reflectance spectroscopy, photoluminescence spectroscopy, hall measurement and vibrating sample magnetometry. Structural and vibrational studies shown hexagonal wurtzite structure of prepared ZnO samples. SEM images have revealed that the grains are hexagonal and spherical shapes for undoped and co-doped samples. The crystallite size was found in range of 43-34 nm. The value of optical band gap is calculated and it is found similar to 3.27 eV for undoped and decreased to 3.20 eV for Mn doped, Nd co-doped sample. This tuning in band gap is because of the fact that the impurity band of ZnO is merged with the conduction band. Photoluminescence study reveals that the intensity of the prepared samples is systematically reduced with the addition of Mn and Nd doping element. Hall effect measurements reveal that the conductivity of ZnO nanoparticles is increased with respect to temperature. The magnetic measurements indicate that the obtained nanostructures are found to be room temperature ferromagnetism (RTFM) with maximum value of saturation magnetization for Nd co-doped Mn:ZnO nanoparticles, i.e. 2.44 emu g(-1). Thus the magnetic properties of ZnO prepared by low cost sol-gel method have been enhanced by Mn doping as well as Nd co-doping which can be used for spintronic applications. In future, similar rare earth materials could be considered for enhancing the magnetic properties of nano particles.

Accession Number: WOS:000438679000063

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Record 63 of 119

Title: Effect of Pr³⁺ doping on key properties of CdO thin films deposited by spray pyrolysis using perfume atomizer

Author(s): Ravikumar, M (Ravikumar, M.); Chandramohan, R (Chandramohan, R.); Kumar, KDA (Kumar, K. Deva Arun); Valanarasu, S (Valanarasu, S.); Kathalingam, A (Kathalingam, A.); Ganesh, V (Ganesh, V.); Shkir, M (Shkir, Mohd.); AlFaify, S (AlFaify, S.); Algarni, H (Algarni, H.)

Source: JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS **Volume:** 118 **Pages:** 211-220 **DOI:** 10.1016/j.jpcs.2018.03.009 **Published:** JUL 2018

Abstract: High quality Cadmium oxide thin films doped with Praseodymium (Pr) were prepared using perfume atomizer based spray pyrolysis technique at substrate temperature near 350 degrees C. Structural analysis of films was examined by XRD and confirmed that the films are cubic in structure. All un-doped and doped films were good crystalline in nature with smooth and flat surface without significant modifications owed to doping. Optical transmittances of doped films was decrease in the visible and IR range with increasing Pr doping concentration. Band gap widened from 2.42 to 2.20 eV when doped with Pr from 0 to 5 at. %. In addition, the photoluminescence property of the films was also observed. Further, the electrical studies were performed on pure and doped samples Viz., the electrical resistivity, carrier concentration (rho) and Hall mobility (mu). It confirmed that the deposited films has good structural environments in terms of grain size, absolute stress correspond and low resistivity. Current-voltage measurements on the nanostructured Al/Pr-nCdO/p-Si/Al device showed a nonlinear electric characteristics indicating diode like behavior.

Accession Number: WOS:000430520500028

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Record 64 of 119

Title: Giant Self-Kerr Nonlinearity in the Metal Nanoparticles-Graphene Nanodisks-Quantum Dots Hybrid Systems Under Low-Intensity Light Irradiance

Author(s): Tohari, MM (Tohari, Mariam M.); Lyras, A (Lyras, Andreas); AlSalhi, MS (AlSalhi, Mohamad S.)

Source: NANOMATERIALS **Volume:** 8 **Issue:** 7 **Article Number:** 521 **DOI:** 10.3390/nano8070521 **Published:** JUL 2018

Abstract: Hybrid nanocomposites can provide a promising platform for integrated optics. Optical nonlinearity can significantly widen the range of applications of such structures. In the present paper, a theoretical investigation is carried out by solving the density matrix equations derived for a metal nanoparticles-graphene nanodisks-quantum dots hybrid system interacting with weak probe and strong control fields, in the steady state. We derive analytical expressions for linear and third-order nonlinear susceptibilities of the probe field. A giant self-Kerr nonlinear index of refraction is obtained in the optical region with relatively low light intensity. The optical absorption spectrum of the system demonstrates electromagnetically induced transparency and amplification without population inversion in the linear optical response arising from the negative real part of the polarizabilities for the plasmonic components at the energy of the localized surface plasmon resonance of the graphene nanodisks induced by the probe field. We find that the self-Kerr nonlinear optical properties of the system can be controlled by the geometrical features of the system, the size of metal nanoparticles and the strength of the control field. The controllable self-Kerr nonlinearities of hybrid nanocomposites can be employed in many interesting applications of modern integrated optics devices allowing for high nonlinearity with relatively low light intensity.

Accession Number: WOS:000442523100072

PubMed ID: 30002312

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ISSN: 2079-4991

Record 65 of 119

Title: First-principles calculations of nitrogen-doped antimony triselenide: A prospective material for solar cells and infrared optoelectronic devices

Author(s): Sajid-ur-Rehman (Sajid-ur-Rehman); Butt, FK (Butt, Faheem K.); Li, CB (Li, Chuanbo); Ul Haq, B (Ul Haq, Bakhtiar); Tariq, Z (Tariq, Zeeshan); Aleem, F (Aleem, F.)

Source: FRONTIERS OF PHYSICS **Volume:** 13 **Issue:** 3 **Article Number:** 137805 **DOI:** 10.1007/s11467-018-0790-2 **Published:** JUN 2018

Abstract: This study is focused on calculation of the electronic structure and optical properties of non-metal doped Sb₂Se₃ using the first-principles method. One and two N atoms are introduced to Sb and Se sites in a Sb₂Se₃ crystal. When one and two N atoms are introduced into the Sb₂Se₃ lattice at Sb sites, the electronic structure shows that the doping significantly modifies the bandgap of Sb₂Se₃ from 1.11 eV to 0.787 and 0.685 eV, respectively. When N atoms are introduced to Se sites, the material shows a metallic behavior. The static dielectric constants $\epsilon(1)(0)$ for Sb₁₆Se₂₄, Sb₁₅N₁Se₂₄, Sb₁₄N₂Se₂₄, Sb₁₆Se₂₃N₁, and Sb₁₆Se₂₂N₂ are 14.84, 15.54, 15.02, 18.9, and 39.29, respectively. The calculated values of the refractive index $n(0)$ for Sb₁₆Se₂₄, Sb₁₅N₁Se₂₄, Sb₁₄N₂Se₂₄, Sb₁₆Se₂₃N₁, and Sb₁₆Se₂₂N₂ are 3.83, 3.92, 3.86, 4.33, and 6.21, respectively. The optical absorbance and optical conductivity curves of the crystal for N-doping at Sb sites show a significant redshift towards the short-wave infrared spectral region as compared to N-doping at Se sites. The modulation of the static refractive index and static dielectric constant is mainly dependent on the doping level. The optical properties and bandgap narrowing effect suggest that the N-doped Sb(2)Se(3) is a promising new semiconductor and can be a replacement for GaSb due to its very similar bandgap and low cost.

Accession Number: WOS:000433426500006

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ISSN: 2095-0462

Record 66 of 119

Title: Organic semiconductor photodiode based on indigo carmine/n-Si for optoelectronic applications

Author(s): Ganesh, V (Ganesh, V.); Manthrammel, MA (Manthrammel, M. Aslam); Shkir, M (Shkir, Mohd.); Yahia, IS (Yahia, I. S.); Zahran, HY (Zahran, H. Y.); Yakuphanoglu, F (Yakuphanoglu, F.); AlFaify, S (AlFaify, S.)

Source: APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING **Volume:** 124 **Issue:** 6 **Article Number:** 424 **DOI:** 10.1007/s00339-018-1832-x **Published:** JUN 2018

Abstract: The fabrication of indigo carmine/n-Si photodiode has been done, and a robust dark and photocurrent-voltage (I-V), capacitance vs. voltage (C-V) and conductance vs. voltage (G-V) studies were done over a wide range of applied voltage and frequencies. The surface morphology was assessed by atomic force microscope (AFM), and the grain size was measured to be about 66 nm. The reverse current increased with both increasing illumination intensity and bias potential, whereas the forward current increased exponentially with bias potential. The responsivity value was also calculated. Barrier height and ideality factor of diode were estimated through a vs plot, and obtained to be 0.843 and 4.75 eV, respectively. The V-bi values are found between 0.95 and 1.2V for frequencies ranging between 100 kHz and 1 MHz. The value of R (s) is found to be lower at higher frequencies which may be due to a certain distribution of localized interface states. A strong frequency and voltage dependency were observed for interface states density N (ss) in the present indigo carmine/n-Si photodiode, and this explained the observed capacitance and resistance variation with frequency. These results suggest that the fabricated diode has the potential to be applied in optoelectronic devices.

Accession Number: WOS:000433238800028

Author Identifiers:

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ISSN: 0947-8396

eISSN: 1432-0630

Record 67 of 119

Title: On stagnation point flow of a micro polar nanofluid past a circular cylinder with velocity and thermal slip

Author(s): Abbas, N (Abbas, Nadeem); Saleem, S (Saleem, S.); Nadeem, S (Nadeem, S.); Alderremy, AA (Alderremy, A. A.); Khan, AU (Khan, A. U.)

Source: RESULTS IN PHYSICS **Volume:** 9 **Pages:** 1224-1232 **DOI:** 10.1016/j.rinp.2018.04.017 **Published:** JUN 2018

Abstract: The concerned problem is dedicated to study stagnation point flow of MHD micropolar nanomaterial fluid over a circular cylinder having sinusoidal

radius variation. Velocity jump slip phenomenon with porous medium is also taken into account. To be more specific, the physical situation of micropolar fluid in the presence of both weak and strong concentration is mathematically modeled in terms of differential equations. Here, three nanoparticles namely Titania(TiO₂), Copper (Cu) and Alumina(Al₂O₃) compared with water as base fluids are incorporated for analysis. The resulting non-linear system has been solved by Runge-Kutta-Fehlberg scheme. Numerical solutions for velocities and temperature profiles are settled for alumina-water nanofluid and deliberated through graphs and numerical tables. It is seen that the skin friction coefficients and the rate of heat transfer are maximum for copper-water nanofluid related to the alumina-water and titania-water nanofluids. Also, the precision of the present findings is certified by equating them with the previously published work.

Accession Number: WOS:000435611100162

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Nadeem, Sohail	AAA-1202-2019	0000-0002-1052-011X

ISSN: 2211-3797

Record 68 of 119

Title: Nonlinear unsteady convection on micro and nanofluids with Cattaneo-Christov heat flux

Author(s): Upadhya, SM (Upadhya, S. Mamatha); Raju, CSK (Raju, C. S. K.); Mahesha (Mahesha); Saleem, S (Saleem, S.)

Source: RESULTS IN PHYSICS **Volume:** 9 **Pages:** 779-786 **DOI:** 10.1016/j.rinp.2018.03.036 **Published:** JUN 2018

Abstract: This is a theoretical study of unsteady nonlinear convection on magnetohydrodynamic fluid in a suspension of dust and graphene nanoparticles. For boosting the heat transport phenomena we consider the Cattaneo-Christov heat flux and thermal radiation. Dispersal of graphene nanoparticles in dusty fluids finds applications in biocompatibility, bio-imaging, biosensors, detection and cancer treatment, in monitoring stem cells differentiation etc. Initially the simulation is performed by amalgamation of dust (micron size) and nanoparticles into base fluid. Primarily existing partial differential system (PDEs) is changed to ordinary differential system (ODEs) with the support of usual similarity transformations. Consequently, the highly nonlinear ODEs are solved numerically through Runge-Kutta and Shooting method. The computational results for Non-dimensional temperature and velocity profiles are offered through graphs ($\phi = 0$ and $\phi = 0.05$) cases. Additionally, the numerical values of friction factor and heat transfer rate are tabulated numerically for various physical parameters obtained. We also validated the current outcomes with previously available study and found to be extremely acceptable. From this study we conclude that in the presence of nanofluid heat transfer rate and temperature distribution is higher compared to micro fluid. (C) 2018 Published by Elsevier B.V.

Accession Number: WOS:000435611100104

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Upadhya, Mamatha S	ABH-4597-2020	

ISSN: 2211-3797

Record 69 of 119

Title: Linear triangular optimization technique and pricing scheme in residential energy management systems

Author(s): Anees, A (Anees, Amir); Hussain, I (Hussain, Iqtadar); Alkhalidi, AH (Alkhalidi, Ali Hussain); Aslam, M (Aslam, Muhammad)

Source: RESULTS IN PHYSICS **Volume:** 9 **Pages:** 858-865 **DOI:** 10.1016/j.rinp.2018.03.015 **Published:** JUN 2018

Abstract: This paper presents a new linear optimization algorithm for power scheduling of electric appliances. The proposed system is applied in a smart home community, in which community controller acts as a virtual distribution company for the end consumers. We also present a pricing scheme between community controller and its residential users based on real-time pricing and likely block rates. The results of the proposed optimization algorithm demonstrate that by applying the anticipated technique, not only end users can minimise the consumption cost, but it can also reduce the power peak to an average ratio which will be beneficial for the utilities as well. (C) 2018 The Authors. Published by Elsevier B.V.

Accession Number: WOS:000435611100115

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ISSN: 2211-3797

Record 70 of 119

Title: Modified Fourier heat flux on MHD flow over stretched cylinder filled with dust, Graphene and silver nanoparticles

Author(s): Upadhya, SM (Upadhya, S. Mamatha); Raju, CSK (Raju, C. S. K.); Saleem, S (Saleem, S.); Alderremy, AA (Alderremy, A. A.); Mahesha (Mahesha)

Source: RESULTS IN PHYSICS **Volume:** 9 **Pages:** 1377-1385 **DOI:** 10.1016/j.rinp.2018.04.038 **Published:** JUN 2018

Abstract: A Comprehensive study on laminar, magnetohydrodynamic (MHD) boundary layer flow of nanofluid (water + Silver, water + Graphene) embedded with conducting micrometer sized dust particles over a stretching cylinder with the incorporation of Cattaneo-Christov heat flux model is conducted. Appropriate similarity variables are employed to the flow governing equations and the resulting ordinary differential equations are solved by employing Runge-Kutta-Fehlberg method. The results for varied controlling parameters for both dusty nano fluid and dust phase are shown through graphs, table and discussed in detail. Authentication of the obtained results is provided by comparing with published results. Results indicate that Graphene + water dusty

nanofluid shows better heat transfer performance compared with Silver + water dusty nanofluid. Improvement in thermal relaxation boosts temperature distribution in both fluid and dust phase.

Accession Number: WOS:000435611100182

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RAJU, CHAKRAVARTHULA S K	T-8357-2019	0000-0002-8921-6566

ISSN: 2211-3797

Record 71 of 119

Title: PHYSICAL BEHAVIOR OF As-Se-Se GLASSES WITH CONSTANT COORDINATION NUMBER (NC=2.2)

Author(s): Alharbi, SR (Alharbi, S. R.); Aly, KA (Aly, K. A.); Al-Zahrani, ES (Al-Zahrani, E. S.); Dahshan, A (Dahshan, A.); Alharbi, W (Alharbi, W.)

Source: CHALCOGENIDE LETTERS **Volume:** 15 **Issue:** 6 **Pages:** 339-343 **Published:** JUN 2018

Abstract: The present work deals with the effect of S additions on glass density, molar volume, compactness and optical properties of Different compositions of $As_{0.20}Se_{0.80-x}S_x$ ($0.0 \leq x \leq 0.55$ at. %) glasses. The coordination number Se and S atoms is the same $N-Se = N-S = 2$. Therefore, the coordination number of the present glasses is constant and equal to 2.2. The glass density, compactness, the Tauc parameter root beta and the Urbach energy are decrease with the addition of S amount whereas the molar volume and the optical gap are increases. Two stoichiometric glasses were observed. The first at 25 at.% S content with Se-S and As-Se bonds and the second at 55 at.% S content with As-S and Se-S bonds. The obtained results are consistent with each others and well discussed in terms of the chemical bonds and the Mott and Davis model.

Accession Number: WOS:000434972900004

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ISSN: 1584-8663

Record 72 of 119

Title: Photoluminescence features of magnetic nano-metric metal oxides

Author(s): Rashad, M (Rashad, M.); Ali, AM (Ali, Atif Mossad); Sayyed, MI (Sayyed, M. I.); Kityk, IV (Kityk, I. V.)

Source: JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 29 **Issue:** 12 **Pages:** 10123-10128 **DOI:** 10.1007/s10854-018-9058-4 **Published:** JUN 2018

Abstract: Copper oxide (CuO) and cobalt oxide (Co₃O₄) nanoparticles (NPs) have been synthesized using microwave irradiation method. These NPs have been prepared using copper nitrate and cobalt nitrate, respectively as the starting materials. The resulted powder of these NPs were explored by X-ray diffraction (XRD), scanning electron microscopy, transmission electron microscopy (TEM), thermogravimetry and differential thermal analysis (DTA). XRD observations obtained the formation of nanostructure phase for both types of these NPs. The structural observations were helped for identifying the nano nature of these both materials. Optical properties such as photoluminescence (PL) and absorbance (A) of CuO and Co₃O₄ NPs have been studied. A resulted shift of PL with respect to absorption peak is 290 and 172 nm for CuO and Co₃O₄ NPs, respectively. Moreover, the magnetic hysteresis loop of both CuO and Co₃O₄ NPs were measured. The magnetic investigations obtained that the magnetic response with a maximum moment $M \leq 0.07$ emu/g is shown up to the maximum applied the field of 5 kOe for CuO NPs which is related to the uncompensated surface spins. On the other hand, the magnetization curve has linear shape in the field range used with the irreversible contribution for Co₃O₄ NPs.

Accession Number: WOS:000433031400044

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Record 73 of 119

Title: Evaluation of structural and optical properties of Ce³⁺ ions doped (PVA/PVP) composite films for new organic semiconductors

Author(s): Ali, FM (Ali, F. M.); Kershi, RM (Kershi, R. M.); Sayed, MA (Sayed, M. A.); AbouDeif, YM (AbouDeif, Y. M.)

Source: PHYSICA B-CONDENSED MATTER **Volume:** 538 **Pages:** 160-166 **DOI:** 10.1016/j.physb.2018.03.031 **Published:** JUN 1 2018

Abstract: Polymer blend films based on Polyvinyl alcohol (PVA)/Poly(vinylpyrrolidone) (PVP) doped with different concentration of cerium ions [(PVA/PVP)-x wt.% Ce³⁺] ($x = 3\%$, 5% , 10% and 15%) were prepared by the conventional solution casting technique. The characteristics of the prepared polymer composite films were studied using X-ray diffraction (XRD), FT-IR and UV-Vis. spectroscopy. The XRD patterns of the investigated samples revealed a clear reduction on the structural parameters such as crystallinity degree and cluster size D of the doped PVA/PVP blend films compared with the virgin one whereas there is no big difference in the d spacing of the product composite films. Significant changes in FT-IR spectra are observed which reveal an interactions between the cerium ions and PVA/PVP blends. The absorption spectra in the ultraviolet-visible region showed a wide red shift in the fundamental absorption edge of (PVA/PVP)-x wt. % Ce³⁺ composites. The optical gap E-g gradually decreased from 4.54 eV for the undoped PVA/PVP film to 3.10 eV by increasing Ce³⁺ ions content. The optical dispersion parameters have been analyzed according to Wemple-Didomenico single oscillator model. The dispersion energy E-d, the single oscillator energy E-o, the average inter-band oscillator wavelength $\lambda_{(o)}$ and the static refractive index $n(o)$ are strongly affected by cerium ions doping. Cerium ions incorporation in PVA/PVP blend films leads to a significant increase in the refractive index and decrease

in the optical gap. These results are likely of great important in varieties of applications including polymer waveguides, organic semiconductors, polymer solar cells and optoelectronics devices.

Accession Number: WOS:000430447000022

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Record 74 of 119

Title: Thermal and Spectroscopic Properties of High Dense Optical Glasses TeO₂-Bi₂O₃-WO₃ (TBW) Doped with Er₂O₃ as Laser Material

Author(s): Algarni, H (Algarni, H.); Reben, M (Reben, M.); AbouDeif, YM (AbouDeif, Y. M.); Damak, K (Damak, Kamel); Assadi, AA (Assadi, A. A.); Maalej, R (Maalej, Ramzi); Yousef, ES (Yousef, El Sayed)

Source: SCIENCE OF ADVANCED MATERIALS **Volume:** 10 **Issue:** 6 **Pages:** 818-826 **DOI:** 10.1166/sam.2018.3267 **Published:** JUN 2018

Abstract: High dense tellurite glass with system 80TeO(2)-5Bi(2)O(3)-15WO(3)-doped with (0, 2000, 10000 ppm Er₂O₃) (labeled TBW, TBW: 1000 ppm Er₂O₃ and TBW: 20000 ppm Er₂O₃) were prepared. Physical parameters such as density (rho), glass transition temperature (T-g), thermal stability (Delta T), optical energy gap and refractive index (n), of prepared glasses were evaluated. Moreover, oxygen packing density (O.p.d), molar volumes (V-m), oxygen molar volume (V-O), molar refraction (R-m), metallization criterion (M), molar polarizability (alpha(m)), the nonlinear refractive index (n(2)), two photon absorption TPA, and third order susceptibility, chi((3)), of prepared glasses have been determined. The Judd-Ofelt parameters (Omega(lambda)) (lambda = 2, 4, 6), oscillator strength type transition probabilities, spectroscopic quality factors, branching ratio and radiative lifetimes of several excited states of Er³⁺ have been estimated. The glasses with composition 80TeO(2)-5Bi(2)O(3)-15WO(3) doped with 10000 ppm Er₂O₃ has high effective emission cross section bandwidth (73.563 nm) for laser transition I-4(13/2) -> I-4(15/2) and large stimulated emission cross-section (1.04.10(-20) cm(2)). Computing physical and spectroscopic properties indicate that these glasses doped with Er³⁺ are a promising candidate for optical applications.

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Record 75 of 119

Title: Highly Sensitive Ethanol Chemical Sensor Based on Novel Ag-Doped Mesoporous alpha-Fe₂O₃ Prepared by Modified Sol-Gel Process

Author(s): Alqahtani, MM (Alqahtani, Moteb M.); Ali, AM (Ali, Atif M.); Harraz, FA (Harraz, Farid A.); Faisal, M (Faisal, M.); Ismail, AA (Ismail, Adel A.); Sayed, MA (Sayed, Mahmoud A.); Al-Assiri, MS (Al-Assiri, M. S.)

Source: NANOSCALE RESEARCH LETTERS **Volume:** 13 **Article Number:** 157 **DOI:** 10.1186/s11671-018-2572-8 **Published:** MAY 21 2018

Abstract: Mesoporous Ag/alpha-Fe₂O₃ has been synthesized via a simple sol-gel procedure in the presence of Pluronic (F-127) triblock copolymer as structure directing agent. Silver (Ag) nanoparticles were deposited onto Ag/alpha-Fe₂O₃ matrix by the photochemical reduction approach. Morphological analysis revealed the formation of Ag nanoparticles with small sizes < 20 nm onto the mesoporous structure of Ag/alpha-Fe₂O₃ possessing < 50 nm semi-spherical shape. The XRD, FTIR, Raman, UV-vis, PL, and N-2 sorption isotherm studies confirmed the high crystallinity, mesoporosity, and optical characteristics of the synthesized product. The electrochemical sensing toward liquid ethanol has been performed using the current devolved Ag/alpha-Fe₂O₃-modified glassy carbon electrode (GCE) by cyclic voltammetry (CV) and current potential (I-V) techniques, and the obtained results were compared with bare GCE or pure Ag/alpha-Fe₂O₃. Mesoporous Ag/alpha-Fe₂O₃ was found to largely enhance the sensor sensitivity and it exhibited excellent sensing characteristics during the precision detection of low concentrations of ethanol. High and reproducible sensitivity of 41.27 mu AmM⁻¹ cm⁻² at lower ethanol concentration region (0.05 to 0.8 mM) and 2.93 mu AmM⁻¹ cm⁻² at higher concentration zone (0.8 to 15 mM), with a limit of detection (LOD) of 15.4 mu M have been achieved. Investigation on reaction kinetics revealed a characteristic behavior of mixed surface and diffusion-controlled processes. Detailed sensing studies revealed also that the sensitivity toward ethanol was higher than that of methanol or isopropanol. With further effort in developing the synthesis and fabrication approaches, a proper utility for the current proposed protocol for fabricating a better sensor device performance is possible.

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PubMed ID: 29785557

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Record 76 of 119

Title: Ab-initio study of electronic, magnetic and thermoelectric behaviors of LiV₂O₄ and LiCr₂O₄ using modified Becke-Johnson (mBJ) potential

Author(s): Ali, S (Ali, Saima); Rashid, M (Rashid, Muhammad); Hassan, M (Hassan, M.); Noor, NA (Noor, N. A.); Mahmood, Q (Mahmood, Q.); Laref, A (Laref, A.);

Haq, BU (Haq, Bakhtiar Ul)

Source: PHYSICA B-CONDENSED MATTER **Volume:** 537 **Pages:** 329-335 **DOI:** 10.1016/j.physb.2018.02.039 **Published:** MAY 15 2018

Abstract: Owing to the large energy storage capacity and higher working voltage, the spinel oxides LiV₂O₄ and LiCr₂O₄, have remained under intense research attention for utilization as electrode materials in lithium-ion batteries. In this study, we explore the half-metallic nature and thermoelectric response in both LiV₂O₄ and LiCr₂O₄ spinel oxides using ab-initio density functional theory (DFT) based computations. The ground-state energies of these compounds have been studied at the optimized structural parameters in the ferromagnetic phase. In order to obtain a correct picture of the electronic structure and magnetic properties, the modified Becke-Johnson (mBJ) potential is applied to compute the electronic structures. The half-metallic behavior is confirmed by the spin-polarized electronic band structures and density of state plots. The magnetic nature is elucidated by computing the John-Teller energy, direct and indirect exchange and crystal field splitting energies. Our computations indicate strong hybridization decreasing the V/Cr site magnetic moments and increasing magnetic momenta at the nonmagnetic atomic sites. We also present the computed parameters significant for expressing the thermoelectric response, which are electrical conductivity, thermal conductivity, Seebeck coefficient and power factor. The computed properties are of immense interest owing to the potential spintronics and Li-ion battery applications of the studied spinel materials.

Accession Number: WOS:000428261200049

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Record 77 of 119

Title: Impact of copper substitution on the structural, ferroelectric and magnetic properties of tungsten bronze ceramics

Author(s): Jindal, S (Jindal, Shilpi); Devi, S (Devi, Sheela); Batoo, KM (Batoo, Khalid Mujasam); Kumar, G (Kumar, Gagan); Vasishth, A (Vasishth, Ajay)

Source: PHYSICA B-CONDENSED MATTER **Volume:** 537 **Pages:** 87-92 **DOI:** 10.1016/j.physb.2018.02.008 **Published:** MAY 15 2018

Abstract: The copper substituted tungsten bronze ceramics with generic formula Ba₅CaCuXTi₂-xNb₈O₃₀(x = 0.0, 0.02, 0.04, 0.06 and 0.08) were successfully synthesized for the first time by solid state reaction method. X-ray diffraction (XRD), Scanning electron microscopy (SEM) and energy dispersive X-ray analysis (EDAX) were utilized to examine the different structural parameters and elemental compositions. XRD study depicted the single phase tetragonal structure having space group P4bm. The crystallite size was observed to be in the range 14.4-30.23 nm. The coexistent of ferroelectricity and magnetism was established by P-E and M-H measurements. The P-E loop study indicated an increase in the coercive field (11.805-23.736 kVcm⁻¹) while the M-H study depicted a decrease in the magnetization (7.65 x 10⁻⁴-5.32 x 10⁻⁴ emu/g) with the incorporation of Cu²⁺ ions. Raman spectrum depicted that there is shift in the position of Raman modes with the substitution of copper which revealed one-mode behavior in the synthesized ceramics.

Accession Number: WOS:000428261200014

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Record 78 of 119

Title: Engineering the electronic band structures of novel cubic structured germanium monochalcogenides for thermoelectric applications

Author(s): Ul Haq, B (Ul Haq, Bakhtiar); AlFaify, S (AlFaify, S.); Ahmed, R (Ahmed, R.); Butt, FK (Butt, Faheem K.); Laref, A (Laref, A.); Goumri-Said, S (Goumri-Said, Souraya); Tahir, SA (Tahir, S. A.)

Source: JOURNAL OF APPLIED PHYSICS **Volume:** 123 **Issue:** 17 **Article Number:** 175107 **DOI:** 10.1063/1.5019986 **Published:** MAY 7 2018

Abstract: Germanium mono-chalcogenides have received considerable attention for being a promising replacement for the relatively toxic and expensive chalcogenides in renewable and sustainable energy applications. In this paper, we explore the potential of the recently discovered novel cubic structured (pi-phase) GeS and GeSe for thermoelectric applications in the framework of density functional theory coupled with Boltzmann transport theory. To examine the modifications in their physical properties, the across composition alloying of pi-GeS and pi-GeSe (such as pi-GeSi_xSe_{1-x}, for x=0, 0.25, 0.50, 0.75, and 1) has been performed that has shown important effects on the electronic band structures and effective masses of charge carriers. An increase in Se composition in pi-GeS_{1-x}Se_x has induced a downward shift in their conduction bands, resulting in the narrowing of their energy band gaps. The thermoelectric coefficients of pi-GeS_{1-x}Se_x have been accordingly influenced by the evolution of the electronic band structures and effective masses of charge carriers. pi-GeS_{1-x}Se_x features sufficiently larger values of Seebeck coefficients, power factors and figures of merit (ZTs), which experience further improvement with an increase in temperature, revealing their potential for high-temperature applications. The calculated results show that ZT values equivalent to unity can be achieved for pi-GeS_{1-x}Se_x at appropriate n-type doping levels. Our calculations for the formation enthalpies indicate that a pi-GeS_{1-x}Se_x alloying system is energetically stable and could be synthesized experimentally. These intriguing characteristics make pi-GeS_{1-x}Se_x a promising candidate for futuristic thermoelectric applications in energy harvesting devices. Published by ALP Publishing.

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ISSN: 0021-8979

eISSN: 1089-7550

Record 79 of 119**Title:** Ag-Doped ZnO Nanoparticles for Enhanced Ethanol Gas Sensing Application**Author(s):** Umar, A (Umar, Ahmad); Khan, MA (Khan, M. Ajmal); Kumar, R (Kumar, Rajesh); Algarni, H (Algarni, H.)**Source:** JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY **Volume:** 18 **Issue:** 5 **Pages:** 3557-3562 **DOI:** 10.1166/jnn.2018.14651 **Published:** MAY 2018

Abstract: Herein, we report the synthesis, characterization and ethanol gas sensing application of Ag-doped ZnO nanoparticles. The nanoparticles were synthesized through a facile hydrothermal process and characterized through various characterization techniques. The detailed characterizations confirmed that the synthesized Ag-doped ZnO nanoparticles are grown in high density with an average diameter of similar to 20+/-5 nm, possessing well-crystalline wurtzite hexagonal crystal structure and exhibiting good optical properties. The as-synthesized Ag-doped ZnO nanoparticles were further used as functional material to fabricate efficient ethanol gas sensor which exhibited excellent gas response. The detailed gas sensing experiments revealed that at an optimized temperature, i.e., 320 degrees C, the recorded gas response was 32.815 for 200 ppm concentration of ethanol gas. Finally, a plausible gas sensing mechanism was also presented in this paper.

Accession Number: WOS:000426040800065**PubMed ID:** 29442866**Author Identifiers:**

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Record 80 of 119**Title:** Metal/Carbon Hybrid Nanostructures Produced from Plasma-Enhanced Chemical Vapor Deposition over Nafion-Supported Electrochemically Deposited Cobalt Nanoparticles**Author(s):** Islam, M (Islam, Mohammad); Achour, A (Achour, Amine); Saeed, K (Saeed, Khalid); Boujtita, M (Boujtita, Mohammed); Javed, S (Javed, Sofia); Djouadi, MA (Djouadi, Mohamed Abdou)**Source:** MATERIALS **Volume:** 11 **Issue:** 5 **Article Number:** 687 **DOI:** 10.3390/ma11050687 **Published:** MAY 2018

Abstract: In this work, we report development of hybrid nanostructures of metal nanoparticles (NP) and carbon nanostructures with strong potential for catalysis, sensing, and energy applications. First, the etched silicon wafer substrates were passivated for subsequent electrochemical (EC) processing through grafting of nitro phenyl groups using para-nitrobenzene diazonium (PNBT). The X-ray photoelectron spectroscopy (XPS) and atomic force microscope (AFM) studies confirmed presence of few layers. Cobalt-based nanoparticles were produced over dip or spin coated Nafion films under different EC reduction conditions, namely CoSO₄ salt concentration (0.1 M, 1 mM), reduction time (5, 20 s), and indirect or direct EC reduction route. Extensive AFM examination revealed NP formation with different attributes (size, distribution) depending on electrochemistry conditions. While relatively large NP with >100 nm size and bimodal distribution were obtained after 20 s EC reduction in H₃BO₃ following Co²⁺ ion uptake, ultrafine NP (< 10 nm) could be produced from EC reduction in CoSO₄ and H₃BO₃ mixed solution with some tendency to form oxides. Different carbon nanostructures including few-walled or multiwalled carbon nanotubes (CNT) and carbon nanosheets were grown in a C₂H₂/NH₃ plasma using the plasma-enhanced chemical vapor deposition technique. The devised processing routes enable size controlled synthesis of cobalt nanoparticles and metal/carbon hybrid nanostructures with unique microstructural features.

Accession Number: WOS:000434711700037**PubMed ID:** 29702583**Author Identifiers:**

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eISSN: 1996-1944

Record 81 of 119**Title:** Structural, vibrational, optical, photoluminescence, thermal, dielectric, and mechanical studies on zinc (tris) thiourea sulfate single crystal: A noticeable effect of organic dye**Author(s):** Shkir, M (Shkir, Mohd); Ganesh, V (Ganesh, V); AlFaify, S (AlFaify, S.); Yahia, IS (Yahia, I. S.); Anis, M (Anis, Mohd)**Source:** CHINESE PHYSICS B **Volume:** 27 **Issue:** 5 **Article Number:** 054216 **DOI:** 10.1088/1674-1056/27/5/054216 **Published:** MAY 2018

Abstract: In this work, uranine-dyed zinc (tris) thiourea sulfate (ZTS) monocrystals, 26 mmx15 mmx10 mm in size, were synthesized by the solution method at ambient temperature. Their purity, crystallinity, lattice parameters, and functional modes were studied by x-ray diffraction, Fourier transform-infrared spectroscopy (FT-IR), and FT-Raman spectroscopy analyses. The sodium ion content of the crystals from the dye was confirmed by elemental analysis. The diffused reflectance spectral analysis of the dyed crystal revealed a characteristic absorption band at 490 nm attributed to the presence of the dye. The calculated band gaps of the non-dyed and dyed crystals were 4.53 and 4.57 eV, respectively. A green emission peak at similar to (512 +/- 4) nm was observed in the photoluminescence spectrum of the uranine-dyed crystals. A differential scanning calorimetry study confirmed that the thermal stability improved owing to the addition of the dye. Dielectric and microhardness studies were conducted to examine the significant improvements in the corresponding properties of dyed crystals. The results demonstrated the competency of the dyed ZTS crystals for applications in optoelectronic devices.

Accession Number: WOS:000432666900016

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Record 82 of 119

Title: Facile synthesis of graphene oxide/PVA nanocomposites for laser optical limiting: band gap analysis and dielectric constants

Author(s): Yahia, IS (Yahia, I. S.); Mohammed, MI (Mohammed, M. I.)

Source: JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 29 **Issue:** 10 **Pages:** 8555-8563 **DOI:** 10.1007/s10854-018-8869-7 **Published:** MAY 2018

Abstract: Casting technique was used to prepare nanocomposites of polyvinyl alcohol (PVA) and graphene oxide (GO). GO has been set up by Hummer's method and characterized by SEM and X-ray spectroscopy. Samples have been designed to contain a different weight percent of GO as follows: (0.370, 0.926, 1.852, 2.778, 3.704, 9.259 wt%) inside PVA matrix under the homogenous ultrasonic system to have a highly dispersed GO in PVA matrix. The nanocomposites were described and analyzed by utilizing different methods such as UV-Vis-NIR, dielectric studies at room temperature and optical limiting properties. It is shown that the influence of the nanofiller leads to the increase in the absorption values while diminishing the optical band gap of both direct and indirect transition. The dielectric constant (ϵ') and the dielectric loss (ϵ'') were studied within the frequency range from 3 kHz to 10 MHz and were found to be depending on the GO contents. The conduction mechanism for the studied samples can be described by the correlated barrier hopping. PVA/GO nanocomposites showed good optical limiting properties. The synthesized GO-doped PAV can be used in electronic and optoelectronic applications especially in battery electrolyte and dye-sensitized solar cells.

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Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Yahia, Ibrahim Sayed	G-4458-2011	

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Record 83 of 119

Title: Optoelectrical properties of Al/p-Si/Fe:N doped ZnO/Al diodes

Author(s): Coskun, B (Coskun, B.); Mensah-Darkwa, K (Mensah-Darkwa, K.); Soylu, M (Soylu, M.); Al-Sehemi, AG (Al-Sehemi, Abdullah G.); Dere, A (Dere, A.); Al-Ghamdi, A (Al-Ghamdi, Ahmed); Gupta, RK (Gupta, R. K.); Yakuphanoglu, F (Yakuphanoglu, F.)

Source: THIN SOLID FILMS **Volume:** 653 **Pages:** 236-248 **DOI:** 10.1016/j.tsf.2018.03.033 **Published:** MAY 1 2018

Abstract: In this work, 3% Fe doped zinc oxide (ZnO) doped by Nitrogen thin films were grown by reactive radio frequency magnetron sputtering on p-Si substrates. The structural and optical properties of the 3% Fe doped ZnO doped by Nitrogen thin films were investigated by the scanning electron microscope and spectrophotometry. The diodes with the configuration of Al/p-Si/3% Fe-ZnO: N/Al have been fabricated and it has been observed that the diodes exhibit a good rectification. The optical band gap was found to be 3.98 +/- 0.02 eV for 3% Fe doped ZnO: N thin film deposited at the N-2 flow rate of 15 sccm. The electrical parameters of the diode were determined using Cheung's and Norde's method. The capacitance-voltage and conductance-voltage characteristics of Al/p-Si/3% Fe-ZnO: N/Al structure have been investigated in the frequency range 10 kHz-1 MHz. The increase in capacitance at lower frequency is attributed to the density of interface states. It is evaluated that the prepared diodes can be used as nanoscale electronic and optoelectronic devices.

Accession Number: WOS:000429409800034

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ISSN: 0040-6090

Record 84 of 119

Title: Energy gaps, valence and conduction charge densities and optical properties of GaAs_{1-x}P_x

Author(s): Al-Hagan, OA (Al-Hagan, O. A.); Algarni, H (Algarni, H.); Bouarissa, N (Bouarissa, N.); Alhuwaymel, TF (Alhuwaymel, T. F.); Khan, MA (Khan, M. Ajmal)

Source: INTERNATIONAL JOURNAL OF MODERN PHYSICS B **Volume:** 32 **Issue:** 10 **Article Number:** 1850125 **DOI:** 10.1142/S0217979218501254 **Published:** APR 20 2018

Abstract: The electronic structure and its derived valence and conduction charge distributions along with the optical properties of zinc-blende GaAs_{1-x}P_x ternary alloys have been studied. The calculations are performed using a pseudopotential approach under the virtual crystal approximation (VCA) which

takes into account the compositional disorder effect. Our findings are found to be generally in good accord with experiment. The composition dependence of direct and indirect bandgaps showed a clear bandgap bowing. The nature of the gap is found to depend on phosphorous content. The bonding and ionicity of the material of interest have been examined in terms of the anti-symmetric gap and charge densities. The variation in the optical constants versus phosphorous concentration has been discussed. The present investigation may give a useful applications in infrared and visible spectrum light emitters.

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eISSN: 1793-6578

Record 85 of 119

Title: Linear and nonlinear optical analysis on semiorganic L-proline cadmium chloride single crystal

Author(s): Anis, M (Anis, Mohd); Baig, MI (Baig, M. I.); Hussaini, SS (Hussaini, S. S.); Shirsat, MD (Shirsat, M. D.); Shkir, M (Shkir, Mohd); Ghramh, HA (Ghramh, H. A.)

Source: CHINESE PHYSICS B **Volume:** 27 **Issue:** 4 **Article Number:** 047801 **DOI:** 10.1088/1674-1056/27/4/047801 **Published:** APR 2018

Abstract: In the current investigation, L-proline cadmium chloride monohydrate (LPCC) single crystal is grown by a slow solvent evaporation technique to identify its credibility for nonlinear optical device applications. The constituent elements of LPCC crystal are determined by the energy dispersive spectroscopic (EDS) technique. The single crystal x-ray diffraction technique is used to determine the structural dimensions of LPCC crystal. The UV-visible studies are carried out within a wavelength range of 200 nm-1100 nm to determine the optical transmittance of LPCC crystal. The linear optical parameters of LPCC crystal are evaluated using the transmittance data to discuss its importance for distinct optical devices. The Nd:YAG laser assisted Kurtz-Perry test is carried out to determine the enhancement in second harmonic generation efficiency of LPCC crystal with reference to KDP crystal. The Z-scan technique is employed to assess the third order nonlinear optical (TONLO) properties of LPCC crystal at 632.8 nm. The Z-scan data are utilized to evaluate the TONLO refraction, absorption and susceptibility of LPCC crystal. The color oriented luminescence behavior of LPCC crystal is investigated within a spectral range of 350 nm-700 nm. The dependence of dielectric constant and dielectric loss on temperature and frequency is evaluated through the dielectric measurement studies.

Accession Number: WOS:000430622400001

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Anis, Mohd		0000-0003-2106-9093

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Record 86 of 119

Title: Tailoring the linear and nonlinear optical properties of NiO thin films through Cr³⁺ doping

Author(s): Shkir, M (Shkir, Mohd.); Ganesh, V (Ganesh, V.); AlFaify, S (AlFaify, S.); Yahia, IS (Yahia, I. S.); Zahran, HY (Zahran, H. Y.)

Source: JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 29 **Issue:** 8 **Pages:** 6446-6457 **DOI:** 10.1007/s10854-018-8626-y **Published:** APR 2018

Abstract: NiO is an excellent contender for smart windows, electrochemical super capacitor and dye sensitized photocathode. Hence, thin films of NiO with different concentrations (1, 3, 5 and 7 wt%) of Cr doping has been fabricated by a facile and low cost technique. The analysis of effect of Cr concentrations on structural, vibrational, morphological, optical and nonlinear optical properties has been studied. X-ray diffraction study confirms that the fabricated films are of polycrystalline nature with cubic phase. The determination of structural parameters such as crystallite size, dislocation density, lattice strain and number of crystallites per unit area was done. The presence of Cr doping in NiO was confirmed by EDX analysis. The vibrational modes were studied by FT-Raman analysis. AFM topography was recorded for pure and Cr doped NiO films. The crystallite/grain size was found to be in the range of 36-40 nm (from X-ray) and 6-12 nm (from AFM). High optical transparency was observed from visible to near infrared region for all the deposited films which is similar to 70 to 85%. The direct and indirect optical band gap were calculated and the direct band gap is found in the range of 3.85-3.78 eV. The optical constants like linear and nonlinear refractive index, optical dielectric constant and loss, optical and electrical conductivity, third order nonlinear optical susceptibility were calculated from reflectance and absorbance data. The values of and are found to be of order of 10⁽⁻⁷⁾ and 10⁽⁻⁹⁾ esu, respectively.

Accession Number: WOS:000427715600038

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ISSN: 0957-4522

eISSN: 1573-482X

Record 87 of 119

Title: Tuning the electronic structure of graphene through alkali metal and halogen atom intercalation

Author(s): Ahmad, S (Ahmad, Sohail); Miro, P (Miro, Pere); Audiffred, M (Audiffred, Martha); Heine, T (Heine, Thomas)

Source: SOLID STATE COMMUNICATIONS **Volume:** 272 **Pages:** 22-27 **DOI:** 10.1016/j.ssc.2018.01.002 **Published:** APR 2018

Abstract: The deposition, intercalation and co-intercalation of heavy alkali metals and light halogens atoms in graphene mono-and bilayers have been studied using first principles density-functional calculations. Both the deposition and the intercalation of alkali metals gives rise to n-type doping due to the formation of Mthorn-C-pairs. The cointercalation of a 1:1 ratio of alkali metals and halogens derives into the formation of ionic pairs among the intercalated species, unaltering the electronic structure of the layered material.

Accession Number: WOS:000425845300005

Author Identifiers:

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Heine, Thomas	H-5446-2011	0000-0003-2379-6251

ISSN: 0038-1098

eISSN: 1879-2766

Record 88 of 119

Title: LUMINESCENCE PROPERTIES OF ZINC NIOBIUM TELLURIUM GLASSES DOPED THULIUM OXIDE

Author(s): Abou Deif, YM (Abou Deif, Y. M.); Alqahtani, MM (Alqahtani, M. M.); Emara, AM (Emara, A. M.); Algarni, H (Algarni, H.); Yousef, ES (Yousef, E. S.)

Source: CHALCOGENIDE LETTERS **Volume:** 15 **Issue:** 4 **Pages:** 219-226 **Published:** APR 2018

Abstract: In this paper, the tellurite glasses $76.4\text{Te}(\text{O}_2)-12\text{Nb}(\text{O}_5)-12.6\text{ZnO}$ doped with 3000ppm Tm_2O_3 ions were prepared by conventional melt quenching method. The optical properties of the glasses were estimated by measuring UV-Vis-NIR spectroscopy in the range from 200 to 2500 nm and linear refractive indices (n) at different wavelength was estimated. From the absorption edge studies, the value of optical band gap (E_{opt}) was determined. Moreover, the nonlinear refractive index ($n^{(2)}$), third-order nonlinear susceptibility ($\chi^{(3)}$), and nonlinear absorption coefficient, ($/g=b/$), were observed. It is noticed that ($n^{(2)}$), $\chi^{(3)}$ and $/g=b/$ increase by decreasing the value of optical band gap (E_{opt}). The classical McCumber theory was used to evaluate the emission cross-sections for the $F-3(4) > H-3(6)$ transition at a wavelength of around $2/g=m//m$. Gain cross-section for the Tm^{3+} laser transition $F-3(4) \rightarrow H-3(6)$ was obtained. These glasses have the effective emission cross section bandwidth (108 nm) and large stimulated emission cross-section ($28.3 \times 10^{-21} \text{cm}^2$). Spectroscopic properties indicate that these glasses doped with Tm^{3+} are a promising candidate for optical applications and may be suitable for optical fibre lasers and amplifiers. Furthermore, the structures of these glasses were analyzed by Raman spectroscopy.

Accession Number: WOS:000432452600005

Author Identifiers:

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ISSN: 1584-8663

Record 89 of 119

Title: Effects of inclined magnetic field on mixed convection in a nanofluid filled double lid-driven cavity with volumetric heat generation or absorption using finite element method

Author(s): Hussain, S (Hussain, Shafqat); Oztop, HF (Oztop, Hakan F.); Mehmood, K (Mehmood, Khalid); Abu-Hamdeh, N (Abu-Hamdeh, Nidal)

Source: CHINESE JOURNAL OF PHYSICS **Volume:** 56 **Issue:** 2 **Pages:** 484-501 **DOI:** 10.1016/j.cjph.2018.02.002 **Published:** APR 2018

Abstract: A computational analysis has been performed on mixed convection in a double sided lid-driven cavity in the presence of volumetric heat generation or absorption. Effects of inclined magnetic field are also studied. The governing parameters are solved via Galerkin weighted residual finite element method in space and the Crank-Nicolson in time. Governing parameters are nanoparticle volume fraction ($0.0 \leq \phi \leq 0.04$), Richardson number ($0.01 \leq \text{Ri} \leq 10$), internal heat generation or absorption parameter ($-10 \leq q \leq 10$), inclination angle of magnetic field ($0 \text{ degrees} \leq \gamma \leq 90 \text{ degrees}$) and Hartmann number ($0 \leq \text{Ha} \leq 100$). It is observed that the highest heat transfer is obtained in case of the maximum value of heat absorption. As a further finding, heat transfer decreases with increasing of Hartmann number and increases with increasing of nanoparticle volume fraction.

Accession Number: WOS:000429822100004

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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ISSN: 0577-9073

Record 90 of 119

Title: Evaluation of the structural, optical and electrical properties of AZO thin films prepared by chemical bath deposition for optoelectronics

Author(s): Kumar, KDA (Kumar, K. Deva Arun); Valanarasu, S (Valanarasu, S.); Rosario, SR (Rosario, S. Rex); Ganesh, V (Ganesh, V.); Shkir, M (Shkir, Mohd.); Sreelatha, CJ (Sreelatha, C. J.); AlFaify, S (AlFaify, S.)

Source: SOLID STATE SCIENCES **Volume:** 78 **Pages:** 58-68 **DOI:** 10.1016/j.solidstatesciences.2018.02.003 **Published:** APR 2018

Abstract: Aluminum doped zinc oxide (AZO) thin films for electrode applications were deposited on glass substrates using chemical bath deposition (CBD) method. The influence of deposition time on the structural, morphological, and opto-electrical properties of AZO films were investigated. Structural studies confirmed that all the deposited films were hexagonal wurtzite structure with polycrystalline nature and exhibited (002) preferential orientation. There is no other impurity phases were detected for different deposition time. Surface morphological images shows the spherically shaped grains are uniformly arranged on to the entire film surface. The EDS spectrum confirms the presence of Zn, O and Al elements in deposited AZO film. The observed optical transmittance is high (87%) in the visible region, and the calculated band gap value is 3.27 eV. In this study, the transmittance value is decreased with increasing deposition time. The room temperature PL spectrum exposed that AZO thin film deposited at (60 min) has good optical quality with less defect

density. The minimum electrical resistivity and maximum carrier concentration values were observed as 8.53×10^{-3} (Ω cm) and 3.53×10^{18} cm⁻³ for 60 min deposited film, respectively. The obtained figure of merit (ϕ) value 3.05×10^{-3} (Ω /sq)⁻¹ is suggested for an optoelectronic device. (c) 2018 Elsevier Masson SAS. All rights reserved.

Accession Number: WOS:000428290700008

Author Identifiers:

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ISSN: 1293-2558

eISSN: 1873-3085

Record 91 of 119

Title: Effect of the different concentrations of ZnO:Mn incorporation on the microstructure and dielectric properties of epoxy nanocomposites

Author(s): Bouzidi, A (Bouzidi, A.); Omri, K (Omri, K.); Jilani, W (Jilani, W.); Guermazi, H (Guermazi, H.); Yahia, IS (Yahia, I. S.)

Source: JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 29 **Issue:** 7 **Pages:** 5908-5917 **DOI:** 10.1007/s10854-018-8563-9 **Published:** APR 2018

Abstract: The Mn:ZnO/epoxy nanocomposites (MZO-EP-NCs) resin samples are prepared using the ultrasonication method. This work deals with the systematic investigation of microstructural, optical and electrical properties of MZO fillers incorporating to the epoxy resin. These samples are characterized by scanning electron microscopy (SEM), X-ray diffraction and UV-Vis spectroscopy. SEM micrographs revealed that the as-prepared MZO nanocrystals are presented in the spherical clusters. X-ray diffraction indicates that the MZO-EP-NCs samples exhibit the presence of MZO nanocrystals peaks. Optical analyses showed a decrease in the band gap energy with increasing the MZO concentrations and a high UV-absorption of MZO-EP-NCs due to the light scattering due to the incorporating MZO particles in the epoxy. Such changes can be described by the shift of HOMO and LUMO band's transition in the studied samples. Our results support the correlation between structure and optical properties of the mentioned nanocomposites. At high electromagnetic waves, the dielectric permittivities are decreased linearly with the addition of MZO clusters compared to neat epoxy. The obtained optical parameters supporting the improvement of the UV shielding properties of MZO-EP-NCs samples.

Accession Number: WOS:000427680400076

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ISSN: 0957-4522

eISSN: 1573-482X

Record 92 of 119

Title: Graphene Oxide/Poly(3-hexylthiophene) Nanocomposite Thin-Film Phototransistor for Logic Circuit Applications

Author(s): Mansouri, S (Mansouri, S.); Coskun, B (Coskun, B.); El Mir, L (El Mir, L.); Al-Sehemi, AG (Al-Sehemi, Abdullah G.); Al-Ghamdi, A (Al-Ghamdi, Ahmed); Yakuphanoglu, F (Yakuphanoglu, F.)

Source: JOURNAL OF ELECTRONIC MATERIALS **Volume:** 47 **Issue:** 4 **Pages:** 2461-2467 **DOI:** 10.1007/s11664-018-6081-4 **Published:** APR 2018

Abstract: Graphene is a sheet-structured material that lacks a forbidden band, being a good candidate for use in radiofrequency applications. We have elaborated graphene-oxide-doped poly(3-hexylthiophene) nanocomposite to increase the interlayer distance and thereby open a large bandgap for use in the field of logic circuits. Graphene oxide/poly(3-hexylthiophene) (GO/P3HT) nanocomposite thin-film transistors (TFTs) were fabricated on silicon oxide substrate by spin coating method. The current-voltage (I-V) characteristics of TFTs with various P3HT compositions were studied in the dark and under light illumination. The photocurrent, charge carrier mobility, subthreshold voltage, density of interface states, density of occupied states, and I (ON)/I (OFF) ratio of the devices strongly depended on the P3HT weight ratio in the composite. The effects of white-light illumination on the electrical parameters of the transistors were investigated. The results indicated that GO/P3HT nanocomposite thin-film transistors have high potential for use in radiofrequency applications, and their feasibility for use in digital applications has been demonstrated.

Accession Number: WOS:000426586000035

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ISSN: 0361-5235

eISSN: 1543-186X

Record 93 of 119

Title: Dynamic load mitigation using dissipative elastic metamaterials with multiple Maxwell-type oscillators

Author(s): Alamri, S (Alamri, SAGR); Li, B (Li, Bing); Tan, KT (Tan, K. T.)

Source: JOURNAL OF APPLIED PHYSICS **Volume:** 123 **Issue:** 9 **Article Number:** 095111 **DOI:** 10.1063/1.5015001 **Published:** MAR 7 2018

Abstract: Dissipative elastic metamaterials have attracted increased attention in recent times. This paper presents the development of a dissipative elastic metamaterial with multiple Maxwell-type resonators for stress wave attenuation. The mechanism of the dissipation effect on the vibration characteristics is systematically investigated by mass-spring-damper models with single and dual resonators. Based on the parameter optimization, it is revealed that a broadband wave attenuation region (stopping band) can be obtained by properly utilizing interactions from resonant motions and viscoelastic effects of the Maxwell-type oscillators. The relevant numerical verifications are conducted for various cases, and excellent agreement between the numerical and theoretical frequency response functions is shown. The design of this dissipative metamaterial system is further applied for dynamic load mitigation and blast wave attenuation. Moreover, the transient response in the continuum model is designed and analyzed for more robust design. By virtue of the bandgap merging effect induced by the Maxwell-type damper, the transient blast wave can be almost completely suppressed in the low frequency range. A significantly improved performance of the proposed dissipative metamaterials for stress wave mitigation is verified in both time and frequency domains. Published by AIP Publishing.

Accession Number: WOS:000427104500047

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ISSN: 0021-8979

eISSN: 1089-7550

Record 94 of 119

Title: Direct Observation of Ultrafast Exciton Dissociation in Lead Iodide Perovskite by 2D Electronic Spectroscopy

Author(s): Jha, A (Jha, Ajay); Duan, HG (Duan, Hong-Guang); Tiwari, V (Tiwari, Vandana); Nayak, PK (Nayak, Pabitra K.); Snaith, HJ (Snaith, Henry J.); Thorwart, M (Thorwart, Michael); Miller, RJD (Miller, R. J. Dwayne)

Source: ACS PHOTONICS **Volume:** 5 **Issue:** 3 **Pages:** 852-860 **DOI:** 10.1021/acsp Photonics.7b01025 **Published:** MAR 2018

Abstract: The unprecedented success of hybrid organic-inorganic lead halide perovskites in photovoltaics motivates fundamental research to unravel the underlying microscopic mechanism for photoinduced charge generation. Recent studies suggest that most photoexcitations in perovskites are free charge carriers, although the contribution of the electron-hole pairs (i.e., excitons) at room temperature has been a matter of debate. We have employed ultrafast two-dimensional (2D) electronic spectroscopy to directly probe the elementary optical excitation of CH₃NH₃PbI₃ thin films with similar to 16 fs temporal resolution. We distinctly capture the ultrafast dissociation of excitons to the charge carriers at room temperature and at 180 K. Interestingly, we also observe that the coherent oscillations of the off-diagonal signals in the 2D electronic spectra live for similar to 50 fs at room temperature. The entropy-driven dissociation of excitons to charge carriers happens within the electronic dephasing time scale and is favored by the low exciton binding energy, which we determine to be similar to 12 meV at room temperature. This ultrafast dissociation of excitons to charge carriers can be one of the important contributions to the high efficiency of perovskite-based photovoltaics.

Accession Number: WOS:000428356400027

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Thorwart, Michael	H-1721-2011	0000-0002-5837-0835

ISSN: 2330-4022

Record 95 of 119

Title: Modified solvothermal synthesis of cobalt ferrite (CoFe₂O₄) magnetic nanoparticles photocatalysts for degradation of methylene blue with H₂O₂/visible light

Author(s): Kalam, A (Kalam, Abul); Al-Sehemi, AG (Al-Sehemi, Abdullah G.); Assiri, M (Assiri, Mohammed); Du, GH (Du, Gaohui); Ahmad, T (Ahmad, Tokeer); Ahmad, I (Ahmad, Irfan); Pannipara, M (Pannipara, M.)

Source: RESULTS IN PHYSICS **Volume:** 8 **Pages:** 1046-1053 **DOI:** 10.1016/j.rinp.2018.01.045 **Published:** MAR 2018

Abstract: Different grads of magnetic nano-scaled cobalt ferrites (CoFe₂O₄) photocatalysts were synthesized by modified Solvothermal (MST) process with and without polysaccharide. The indigenously synthesized photocatalysts were characterized by means of X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), high-resolution transmission electron microscopy (HRTEM), thermo gravimetric analysis (TGA), Fourier transform infrared (FT-IR), UV-visible (UV-vis) spectroscopy and N₂ adsorption-desorption isotherm method. The Fourier transform infrared spectroscopy study showed the Fe-O stretching vibration 590-619 cm⁻¹, confirming the formation of metal oxide. The crystallite size of the synthesized photocatalysts was found in the range between 20.0 and 30.0 nm. The surface area of obtained magnetic nanoparticles is found to be reasonably high in the range of 63.0-76.0 m²/g. The results shown that only MST-2 is the most active catalyst for photo-Fenton like scheme for fast photodegradation action of methylene blue dye, this is possible due to optical band gap estimated of 2.65 eV. Captivatingly the percentage of degradation efficiency increases up to 80% after 140 min by using MST-2 photocatalyst. Photocatalytic degradation of methylene blue (MB) dye under visible light irradiation with cobalt ferrite magnetic nanoparticles followed first order kinetic constant and rate constant of MST-2 is almost 2.0 times greater than MST-1 photocatalyst. (C) 2018 The Authors. Published by Elsevier B.V.

Accession Number: WOS:000428027700144

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ISSN: 2211-3797

Record 96 of 119**Title:** Thermally induced optical nonlinearity and optical power limiting action of 2,4,5-trimethoxy-4'-nitrochalcone under CW laser regime**Author(s):** Fadhul, ZSMMM (Fadhul, Zainab S. M. M. M.); Ali, EAHF (Ali, Eman A. H. F.); Maidur, SR (Maidur, Shivaraj R.); Patil, PS (Patil, Parutagouda Shankaragouda); Shkir, M (Shkir, M.); Henari, FZ (Henari, Fryad Z.)**Source:** JOURNAL OF NONLINEAR OPTICAL PHYSICS & MATERIALS **Volume:** 27 **Issue:** 1 **Article Number:** 1850012 **DOI:** 10.1142/S0218863518500121 **Published:** MAR 2018

Abstract: In the present work, we report the results of thermally induced third-order nonlinear optical (NLO) properties of 2,4,5-trimethoxy-4'-nitrochalcone (abbreviated as 2,4,5TMNC) investigated by Z-scan technique using continuous wave (CW) Argon ion laser at a wavelength of 488 nm with adjusted power ranging from 2.5 mW to 20 mW. The experiments were performed by varying the concentration of the molecules in solution. The sample demonstrated strong reverse saturable absorption (RSA) and self-defocusing effect (negative nonlinear refractive index). The estimated values of the NLO absorption coefficient (β), nonlinear refraction ($n(2)$) and absolute nonlinear susceptibility $\chi^{(3)}$ are found to be of the order of $10(-5)$ m/W, $10(-11)$ m²/W and $10(-5)$ esu, respectively. The magnitude of the nonlinear absorption coefficient (β) was found to increase with concentration. The linear absorption spectrum of 2,4,5TMNC was measured using UV-Vis-NIR spectrometer. The optical band gap (E_g) value of title chalcone is obtained from the tauc's plot of $(\alpha h\nu)^2$ versus $h\nu$. The optical limiting performance of 2,4,5TMNC is also investigated for device application. In addition to the above, the computation studies are also carried out to attain the ground state molecular geometry which is found in close to experimental results. Time-Dependent-Density Function Theory (TD-DFT) was used to determine the UV-Vis spectrum at B3LYP/6-31G* level of theory and found to be comparable with experimental data. The HOMO-LUMO energy gap was also determined and discussed. The results promote this chalcone derivative as a promising candidate for optical limiting and optical switching applications.

Accession Number: WOS:000430947300012**Author Identifiers:**

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ISSN: 0218-8635

eISSN: 1793-6624

Record 97 of 119**Title:** A first principles study of key electronic, optical, second and third order nonlinear optical properties of 3-(4-chlorophenyl)-1-(pyridin-3-yl) prop-2-en-1-one: a novel D-pi-A type chalcone derivative**Author(s):** Shkir, M (Shkir, Mohd); AlFaify, S (AlFaify, S.); Arora, M (Arora, M.); Ganesh, V (Ganesh, V.); Abbas, H (Abbas, Haider); Yahia, IS (Yahia, I. S.)**Source:** JOURNAL OF COMPUTATIONAL ELECTRONICS **Volume:** 17 **Issue:** 1 **Pages:** 9-20 **DOI:** 10.1007/s10825-017-1050-3 **Published:** MAR 2018

Abstract: In this work we assess the significant electrooptic properties of a novel chalcone derivative 3-(4-chlorophenyl)-1-(pyridin-3-yl) prop-2-en-1-one using a computational approach. The ground-state molecular geometry was optimized, and geometrical parameters and vibrational modes are established and found to be in strong correlation with experimental results. The excitation energy is observed to be 326 nm (3.8 eV), calculated at the TD/B3LYP/6-31G level (stands for time dependent/Becke's three Lee-Yang-Parr/basis set). Additionally, a unique insight was gained on a number of properties of the molecular levels such as the HOMO-LUMO gap (i.e.) and electrostatic potential maps. The potential applications of the 3-(4-chlorophenyl)-1-(pyridin-3-yl)prop-2-en-1-one (CPP) molecule in nonlinear optics are confirmed by second and third harmonic generation studies at five different characteristic wavelengths. The static and dynamic polarizability are found to be many-fold higher than that of urea. The second and third harmonic generation values of the titled molecule are found to be 56 and 158 times higher than standard urea molecule, respectively, computed at same wavelength (i.e. 1064.13 nm). From these studies it is clear that the material possesses superior properties and could be applied in optoelectronic device fabrications.

Accession Number: WOS:000425761200002**Author Identifiers:**

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ISSN: 1569-8025

Record 98 of 119**Title:** Synthesis, Optical and Photoluminescence Properties of Cu-Doped ZnO Nano-Fibers Thin Films: Nonlinear Optics**Author(s):** Ganesh, V (Ganesh, V.); Salem, GF (Salem, G. F.); Yahia, IS (Yahia, I. S.); Yakuphanoglu, F (Yakuphanoglu, F.)**Source:** JOURNAL OF ELECTRONIC MATERIALS **Volume:** 47 **Issue:** 3 **Pages:** 1798-1805 **DOI:** 10.1007/s11664-017-5950-6 **Published:** MAR 2018

Abstract: Different concentrations of copper-doped zinc oxide thin films were coated on a glass substrate by sol-gel/spin-coating technique. The structural properties of pure and Cu-doped ZnO films were characterized by different techniques, i.e., atomic force microscopy (AFM), photoluminescence and UV-Vis-NIR spectroscopy. The AFM study revealed that pure and doped ZnO films are formed as nano-fibers with a granular structure. The photoluminescence spectra of these films showed a strong ultraviolet emission peak centered at 392 nm and a strong blue emission peak centered at 450 nm. The optical band gap of the pure and copper-doped ZnO thin films calculated from optical transmission spectra (3.29-3.23 eV) were found to be increasing with increasing copper doping concentration. The refractive index dispersion curve of pure and Cu-doped ZnO film obeyed the single-oscillator model. The optical

dispersion parameters such as E-o, E-d , and $n(\infty)$ (2) were calculated. Further, the nonlinear refractive index and nonlinear optical susceptibility were also calculated and interpreted.

Accession Number: WOS:000424341700008

Author Identifiers:

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GANESH, VANGA		0000-0001-8860-5503

ISSN: 0361-5235

eISSN: 1543-186X

Record 99 of 119

Title: Exploring single-layered SnSe honeycomb polymorphs for optoelectronic and photovoltaic applications

Author(s): Ul Haq, B (Ul Haq, Bakhtiar); AlFaify, S (AlFaify, S.); Ahmed, R (Ahmed, R.); Butt, FK (Butt, Faheem K.); Laref, A (Laref, A.); Shkir, M (Shkir, Mohd.)

Source: PHYSICAL REVIEW B **Volume:** 97 **Issue:** 7 **Article Number:** 075438 **DOI:** 10.1103/PhysRevB.97.075438 **Published:** FEB 23 2018

Abstract: Single-layered tin selenide that shares the same structure with phosphorene and possesses intriguing optoelectronic properties has received great interest as a two-dimensional material beyond graphene and phosphorene. Herein, we explore the optoelectronic response of the newly discovered stable honeycomb derivatives (such as alpha, beta, gamma, delta, and epsilon) of single-layered SnSe in the framework of density functional theory. The alpha, beta, gamma, and delta derivatives of a SnSe monolayer have been found to exhibit an indirect band gap, however, the dispersion of their band-gap edges demonstrates multiple direct band gaps at a relatively high energy. The epsilon-SnSe, however, features an intrinsic direct band gap at the high-symmetry Gamma point. Their energy band gaps (0.53, 2.32, 1.52, 1.56, and 1.76 eV for alpha-, beta-, gamma-, delta-, and epsilon-SnSe, respectively), calculated at the level of the Tran-Blaha modified Becke-Johnson approach, mostly fall right in the visible range of the electromagnetic spectrum and are in good agreement with the available literature. The optical spectra of these two-dimensional (2D) SnSe polymorphs (besides beta-SnSe) are highly anisotropic and possess strictly different optical band gaps along independent diagonal components. They show high absorption in the visible and UV ranges. Similarly, the reflectivity, refraction, and optical conductivities inherit strong anisotropy from the dielectric functions as well and are highly visible-UV polarized along the cartesian coordinates, showing them to be suitable for optical filters, polarizers, and shields against UV radiation. Our investigations suggest these single-layered SnSe allotropes as a promising 2D material for next-generation nanoscale optoelectronic and photovoltaic applications beyond graphene and phosphorene.

Accession Number: WOS:000426015300007

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Butt, Faheem	N-5904-2019	0000-0001-8424-3437
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ISSN: 2469-9950

eISSN: 2469-9969

Record 100 of 119

Title: Optical phonon modes and polaron related parameters in $GaxIn_{1-x}P$

Author(s): Bouarissa, N (Bouarissa, N.); Algarni, H (Algarni, H.); Al-Hagan, OA (Al-Hagan, O. A.); Khan, MA (Khan, M. A.); Alhuwaymel, TF (Alhuwaymel, T. F.)

Source: PHYSICA B-CONDENSED MATTER **Volume:** 531 **Pages:** 144-148 **DOI:** 10.1016/j.physb.2017.12.046 **Published:** FEB 15 2018

Abstract: Based on a pseudopotential approach under the virtual crystal approximation that includes the effect of compositional disorder, the optical lattice vibration frequencies and polaron related parameters in zinc-blende $GaxIn_{1-x}P$ have been studied. Our findings showed generally reasonably good accord with data in the literature. Other case, our results are predictions. The composition dependence of longitudinal optical (LO) and transverse optical (TO) phonon modes, LO-TO splittings, Frohlich coupling parameter, Debye temperature of LO phonon frequency, and polaron effective mass has been analyzed and discussed. While a non-monotonic behavior has been noticed for the LO and TO phonon frequencies versus Ga concentration x, a monotonic behavior has been observed for the rest of the features of interest. The information derived from this investigation may be useful for optoelectronic technological applications.

Accession Number: WOS:000424809500023

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Al-Hagan, Ola		0000-0003-0386-2418

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**Record 101 of 119**

Title: An effect of temperature on structural, optical, photoluminescence and electrical properties of copper oxide thin films deposited by nebulizer spray pyrolysis technique

Author(s): Prabu, RD (Prabu, R. David); Valanarasu, S (Valanarasu, S.); Ganesh, V (Ganesh, V.); Shkir, M (Shkir, Mohd); AlFaify, S (AlFaify, S.); Kathalingam, A (Kathalingam, A.); Srikumar, SR (Srikumar, S. R.); Chandramohan, R (Chandramohan, R.)

Source: MATERIALS SCIENCE IN SEMICONDUCTOR PROCESSING **Volume:** 74 **Pages:** 129-135 **DOI:** 10.1016/j.mssp.2017.10.023 **Published:** FEB 2018

Abstract: In this work, copper oxide thin films were deposited on glass substrate by nebulizer spray pyrolysis technique with different temperatures (i.e. 250-320 degrees C). All the deposited films were characterized by X-ray diffraction (XRD), atomic force microscopy (AFM), Laser Raman, UV-Vis, Photoluminescence and Hall Effect measurements for the Structural, morphological, vibrational, optical and electrical properties. The XRD studies confirmed that the films deposited with different temperatures from 250 to 300 degrees C possess single cubic crystal structure phase of cuprous oxide (Cu₂O) whereas the films deposited at 310 and 320 degrees C were found to have a mixed phase of CuO and Cu₂O. When the temperature reaches above 310 degrees C the Cu₂O phase become unstable and started to convert as CuO. Laser Raman studies confirmed that the observed peaks at 109, 148, 219, 416, 515 and 635 cm⁻¹ are belong to Cu₂O phase deposited at 250 and 280 degrees C. However, the films deposited at 310 degrees C and 320 degrees C having additional peaks at 273, 327 and 619 cm⁻¹ which conforms the presence of mixed (CuO and Cu₂O) phase. The AFM studies shows that the deposited films has uniformly distributed with homogeneity and the particles extended all over the surface. Optical measurement showed that the band gap of deposited thin films in the range of 2.44-1.97 for 250-320 degrees C, respectively. A single and strong emission peak at similar to 617 nm is observed in PL spectra, which conforms the copper oxide film. Hall Effect measurements showed that all the films are of p-type conductivity with resistivity (ρ) of $4.61 \times 10^{(2)} \Omega \text{ cm}$, carrier concentration (n) of $13.53 \times 10^{(15)} \text{ cm}^{-(3)}$ and mobility of $1.0 \text{ cm}^{(2)}/\text{vs}$ at 320 degrees C temperature. The low activation energy of 0.012 eV were observed for the film deposited at 320 degrees C.

Accession Number: WOS:000415924400019

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ISSN: 1369-8001

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Record 102 of 119

Title: Optical parameters of Ge₁₅Sb₅Se₈₀ and Ge₁₅Sb₅Te₈₀ from ellipsometric measurements

Author(s): Abdel-Wahab, F (Abdel-Wahab, F.); Ashraf, IM (Ashraf, I. M.); Alomairy, SE (Alomairy, S. E.)

Source: PHYSICA B-CONDENSED MATTER **Volume:** 530 **Pages:** 300-306 **DOI:** 10.1016/j.physb.2017.11.087 **Published:** FEB 1 2018

Abstract: The optical properties of Ge₁₅Sb₅Se₈₀ (GSS) and Ge₁₅Sb₅Te₈₀ (GST) films prepared by thermal evaporation method were investigated in the photon energy range from 0.9 eV to 5 eV by using a variable-angle spectroscopic ellipsometer. Combinations of multiple Gaussian, and Tauc - Lorentz or Cody-Lorentz dispersion functions are used to fit the experimental data. The models' parameters (Lorentz oscillator amplitude, resonance energy, oscillator width, optical band gap, and Urbach energy) of both GSS and GST films were calculated. Refractive indices and extinction coefficients of the films were determined. Analysis of the absorption coefficient shows that the optical absorption edge of GSS and GST films to be 1.6 eV and 0.89 eV, respectively. Manca's relation based on mean bond energy and the bond statistics of chemically ordered model (COM) and random covalent network model (CRNM) is applied for the estimation of the optical band gap (E_g) of the investigated films. A good agreement between experimental and calculated E_g is obtained.

Accession Number: WOS:000423768100046

Author Identifiers:

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Ebrahem, Ashraf Mahmoud	AAT-6263-2020	

ISSN: 0921-4526

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Record 103 of 119

Title: Microstructure and magnetic characterization of the Sm-CoMn co-substituted SrCaM hexagonal ferrites

Author(s): Yang, YJ (Yang Yujie); Wang, FH (Wang Fanhou); Shao, JX (Shao Juxiang); Batoo, KM (Batoo, Khalid Mujasam); Rehman, KMU (Rehman, Khalid Mehmood Ur); Huang, DH (Huang Duohui)

Source: CHINESE JOURNAL OF PHYSICS **Volume:** 56 **Issue:** 1 **Pages:** 108-116 **DOI:** 10.1016/j.cjph.2017.11.017 **Published:** FEB 2018

Abstract: A series of Sm-CoMn substituted hexagonal ferrites with chemical composition of Sr_{0.85-x}Ca_{0.15}S_mxFe_{12-y}(Co_{0.5}Mn_{0.5})_yO₁₉ (0.00 ≤ x ≤ 0.60, (0.00 ≤ y ≤ 0.50) were synthesized by the solid-state reaction method. Microstructure and magnetic properties of the hexaferrites have been investigated by the X-ray diffraction, field emission scanning electron microscopy and a permanent magnetic measuring system. A single magnetoplumbite phase is exhibited in the hexaferrites with the substitution of Sm (0.00 ≤ x ≤ 0.12) and CoMn (0.00 ≤ y ≤ 0.10) contents. For the hexaferrites containing Sm (x ≥ 0.24) and CoMn (y ≥ 0.20), impurity phases are observed in the structure. The FESEM micrographs exhibit that the hexaferrites with different Sm-CoMn contents have formed hexagonal structures and the grain size of the hexaferrites remains unchanged with increasing Sm-CoMn content. The remanence (B_r), H_k/H_{cj} ratios, and maximum energy product [(BH)_{max}] decrease with increasing Sm-CoMn content (0.00 ≤ x ≤ 0.60, (0.00 ≤ y ≤ 0.50). Intrinsic

coercivity (H-cj) and magnetic induction coercivity (H-cb) increase with increasing Sm-CoMn content ($0.00 \leq x \leq 0.12$, $0.00 \leq y \leq 0.10$), and then decrease with increasing Sm-CoMn content ($0.12 \leq x \leq 0.36$, $0.10 \leq y \leq 0.30$), while for the hexaferrites with Sm ($x \geq 0.36$) and CoMn ($y \geq 0.30$), with increasing Sm-CoMn content, H-cj increases and H-cb decreases.

Accession Number: WOS:000427505300013

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ISSN: 0577-9073

Record 104 of 119

Title: Interdependence between electrical and magnetic properties of polycrystalline cobalt-substituted tungsten bronze multiferroic ceramics

Author(s): Jindal, S (Jindal, Shilpi); Devi, S (Devi, Sheela); Vasishth, A (Vasishth, Ajay); Batoo, KM (Batoo, Khalid Mujasam); Kumar, G (Kumar, Gagan)

Source: JOURNAL OF ADVANCED DIELECTRICS **Volume:** 8 **Issue:** 1 **Article Number:** UNSP 1850002 **DOI:** 10.1142/S2010135X18500029 **Published:** FEB 2018

Abstract: Polycrystalline cobalt-substituted tungsten bronze ferroelectric ceramics with chemical composition $\text{Ba}_5\text{CaTi}_2\text{-xCoxNb}_8\text{O}_{30}$ ($x = 0.00, 0.02, 0.04$ and 0.08) were synthesized by solid state reaction technique. X-ray diffraction (XRD) technique was used to confirm the phase formation and it revealed the formation of single phase tetragonal structure with space group P4bm. The surface morphology of the samples was studied by using the scanning electron microscopy (SEM) technique. The dielectric properties such as dielectric constant and dielectric loss have been investigated as a function of temperature and frequency. The P-E and M-H studies confirmed the coexistent of ferroelectricity and magnetism at room temperature. The P-E loop study indicated an increase in the coercive field while the M-H study depicted a decrease in the magnetization with the incorporation of cobalt ions.

Accession Number: WOS:000427079000004

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ISSN: 2010-135X

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Record 105 of 119

Title: Effect of replacement of selenium by indium on the thermal stability and crystallization kinetics of quaternary $\text{Se}_{90-x}\text{-Zn}_5\text{-Te}_5\text{-In}_x$ glassy alloys

Author(s): Soraya, MM (Soraya, M. M.); Shaaban, ER (Shaaban, E. R.); Awad, MA (Awad, M. A.); Hassan, HS (Hassan, H. Shokry); Eman, MI (Eman, M. I.); Algarni, H (Algarni, H.)

Source: APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING **Volume:** 124 **Issue:** 2 **Article Number:** 197 **DOI:** 10.1007/s00339-018-1603-8 **Published:** FEB 2018

Abstract: This paper reports the effect of replacement of selenium by indium on the thermal stability and crystallization kinetics of $\text{Se}_{90-x}\text{-Zn}_5\text{-Te}_5\text{-In}_x$ ($x = 0, 2, 4, 6, 8, 10$) glassy alloys. Assessment of the thermal stability of these glassy alloys was achieved using various simple quantitative methods based on the characteristic temperatures of DSC curves. In this case, $k(\text{gl})$ may be more suitable for estimating the glass thermal stability in the above composition range. The kinetic parameter $K-r(T)$ is added to the stability criteria. The results of all thermal stability parameters confirm that the thermal stability increases with increasing indium at expense of selenium in $\text{Se}_{90-x}\text{-Zn}_5\text{-Te}_5\text{-In}_x$ glassy alloys. These results have been discussed in terms of cohesive energy and average heat of atomization. Finally, according to the average values of Avrami indices, $n = 2$ for the crystallization peaks means volume nucleation and two-dimensional growth for all the compositions.

Accession Number: WOS:000424515500102

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Mohamed, Soraya	ABD-8268-2020	0000-0003-1549-523X

ISSN: 0947-8396

eISSN: 1432-0630

Record 106 of 119

Title: Structural, optical and AFM characterization of PVA:La³⁺ polymer films

Author(s): Ali, FM (Ali, F. M.); Maiz, F (Maiz, F.)

Source: PHYSICA B-CONDENSED MATTER **Volume:** 530 **Pages:** 19-23 **DOI:** 10.1016/j.physb.2017.10.124 **Published:** FEB 1 2018

Abstract: In this paper the structural and optical properties of pure Polyvinyl alcohol (PVA) and La³⁺-doped PVA films in the concentration range of 4%, 12% and 20% weight percent of Lanthanum were prepared by the conventional casting technique. X-ray diffraction pattern and atomic force microscopy studies of the investigated samples reveal their semi-crystalline nature. It is found that, absorption coefficient and cluster size of lanthanum: PVA composite increase with increasing salt concentration. However, the optical energy gap shows a slight decreasing trend.

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Record 107 of 119

Title: Sextic and decatic anharmonic oscillator potentials: Polynomial solutions

Author(s): Maiz, F (Maiz, F.); Alqahtani, MM (Alqahtani, Moteb M.); Al Sdran, N (Al Sdran, N.); Ghnaim, I (Ghnaim, I.)

Source: PHYSICA B-CONDENSED MATTER **Volume:** 530 **Pages:** 101-105 **DOI:** 10.1016/j.physb.2017.11.010 **Published:** FEB 1 2018

Abstract: We seek the possible polynomial solutions of the Schrodinger equation for the sextic and decatic potentials. Under certain conditions on the parameters of the potentials, we show that these potentials are exactly solvable. We evaluate the first four eigenstates for both potentials. We derive general expressions of the energy levels, for high energy levels, eigenvalues are a function of potentials' parameters and the eigenfunction's zeros.

Accession Number: WOS:000423768100017

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Record 108 of 119

Title: Effect of Precursors on Key Opto-electrical Properties of Successive Ion Layer Adsorption and Reaction-Prepared Al:ZnO Thin Films

Author(s): Kumar, KDA (Kumar, K. Deva Arun); Valanarasu, S (Valanarasu, S.); Ganesh, V (Ganesh, V.); Shkir, M (Shkir, Mohd); Kathalingam, A (Kathalingam, A.); Alfaify, S (Alfaify, S.)

Source: JOURNAL OF ELECTRONIC MATERIALS **Volume:** 47 **Issue:** 2 **Pages:** 1335-1343 **DOI:** 10.1007/s11664-017-5920-z **Published:** FEB 2018

Abstract: Aluminum-doped zinc oxide (Al:ZnO) thin films were deposited on glass substrates by successive ion layer adsorption and reaction (SILAR) method using different precursors. This inexpensive SILAR method involves dipping of substrate sequentially in zinc solution, de-ionized water and ethylene glycol in multiple cycles. Prepared films were investigated by x-ray diffraction (XRD), scanning electron microscope (SEM), atomic force microscope (AFM), optical absorption, photoluminescence (PL), Raman spectroscopy and electrical studies. XRD study confirmed incorporation of aluminum in ZnO lattice with a polycrystalline hexagonal wurtzite structure of the films. The crystallite size determined by the Scherrer equation showed an increase from 28 nm to 35 nm for samples S1 to S4, respectively. SEM study showed smooth morphology with homogeneous distribution of particles. From the AFM images, the surface roughness was found to change according to precursors. For the optical analysis, the zinc chloride precursor showed high optical transmittance of about 90% in the visible range with a band gap value 3.15 eV. The room-temperature PL spectra exhibited a stronger violet emission peak at 420 nm for all the prepared samples. The Raman spectra showed a peak around 435 cm^{-1} which could be assigned to non-polar optical phonons (E-2-high) mode AZO films of a ZnO wurtzite structure. Hall effect measurements showed n-type conductivity with low resistivity (ρ) and high carrier concentrations (n) of $2.39 \times 10^{(-3)}$ $\Omega\text{-cm}$ and $8.96 \times 10^{(20)}$ cm^{-3} , respectively, for the film deposited using zinc chloride as precursor. The above properties make the prepared AZO film to be regarded as a very promising electrode material for fabrication of optoelectronic devices.

Accession Number: WOS:000419791800056

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Record 109 of 119

Title: Effect of microwave power on morphology of AgO thin film grown using microwave plasma CVD

Author(s): Ansari, AR (Ansari, Akhalakur Rahman); Imran, M (Imran, Mohd); Yahia, IS (Yahia, I. S.); Abdel-Wahab, MS (Abdel-Wahab, Mohamed Shaaban); Alshahrie, A (Alshahrie, Ahmed); Khan, AH (Khan, Afzal Husain); Sharma, C (Sharma, Chandan)

Source: INTERNATIONAL JOURNAL OF SURFACE SCIENCE AND ENGINEERING **Volume:** 12 **Issue:** 1 **Pages:** 1-12 **DOI:** 10.1504/IJSURFSE.2017.10009320 **Published:** 2018

Abstract: In this study, pure silver (Ag) thin film of 8 nm was deposited onto glass substrate by using radio frequency (RF) sputtering technique and was then exposed to microwave assisted oxygen plasma generated by microwave plasma CVD. The oxidation of Ag into AgO thin film was studied using varying microwave power. The influence of microwave power on morphology and size of oxide film was investigated. The crystal structure, crystal size, chemical composition, morphologies and optical properties of oxidised silver thin film (AgO) was characterised by using x-ray powder diffraction (XRD), field emission scanning electron microscopy (FESEM), Raman spectroscopy and UV-vis spectroscopy. Morphological characterisation of these films reveals a systematic change from metallic silver (Ag) to silver oxide (AgO). The size of AgO thin film was calculated using Scherrer equation and was observed to be 11 nm, 12 nm and 13.5 nm at 400 W, 800 W and 1200 W respectively. A considerable change in UV-vis spectra was observed with increase in annealing temperature.

Accession Number: WOS:000427424000001

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Ansari, Akhalakur Rahman	J-4244-2017	
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ISSN: 1749-785X

eISSN: 1749-7868

Record 110 of 119**Title:** Ruthenium(II) Complex Based Photodiode for Organic Electronic Applications**Author(s):** Tataroglu, A (Tataroglu, A.); Ocaya, R (Ocaya, R.); Dere, A (Dere, A.); Dayan, O (Dayan, O.); Serbetci, Z (Serbetci, Z.); Al-Sehemi, AG (Al-Sehemi, Abdullah G.); Soyulu, M (Soyulu, M.); Al-Ghamdi, AA (Al-Ghamdi, Ahmed A.); Yakuphanoglu, F (Yakuphanoglu, F.)**Source:** JOURNAL OF ELECTRONIC MATERIALS **Volume:** 47 **Issue:** 1 **Pages:** 828-833 **DOI:** 10.1007/s11664-017-5882-1 **Published:** JAN 2018

Abstract: In this study, the electrical and photoresponse properties of a photovoltaic device with Ruthenium(II) complex interfacial thin film were investigated. Heteroleptic Ru(II) complex including bidentate and tridentate ligands thin film was coated on n-Si substrate by the spin coating technique. From current-voltage (I-V) measurements of an Au/Ru(II)/n-Si photodiode, it is observed that the reverse bias current under light is higher than that of the current in the dark. This indicates that the photodiode exhibits a photoconducting characteristic. The transient measurements such as photocurrent, phot capacitance and photoconductance were performed under various illumination conditions. These measurements indicate that the photodiode has a high photoresponsivity. The electrical parameters such as barrier height (I broken vertical bar(b)), ideality factor (n) and series resistance (R (s)) of the photodiode were determined from the analysis of I-V characteristics. Moreover, the capacitance/conductance-voltage characteristics of the photodiode highly depend on both voltage and frequency. Results show that the heterojunction can be used for various optoelectronic applications.

Accession Number: WOS:000418580800098**Author Identifiers:**

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Record 111 of 119**Title:** Elastic constants and mechanical stability of $\text{In}_x\text{Al}_{1-x}\text{As}_y\text{Sb}_{1-y}$ lattice-matched**Author(s):** Algarni, H (Algarni, H.); Al-Hagan, OA (Al-Hagan, O. A.); Bouarissa, N (Bouarissa, N.); Alhuwaymel, TF (Alhuwaymel, T. F.); Khan, MA (Khan, M. Ajmal)**Source:** PHILOSOPHICAL MAGAZINE **Volume:** 98 **Issue:** 28 **Pages:** 2582-2594 **DOI:** 10.1080/14786435.2018.1494862 **Part:** A **Published:** 2018

Abstract: Based on a pseudopotential approach under the virtual crystal approximation, the elastic modulus of $\text{In}_x\text{Al}_{1-x}\text{As}_y\text{Sb}_{1-y}$ quaternaries lattice-matched to InP, GaSb and InAs substrates has been investigated. Our findings show a reasonably good accord with experiment. The dependence of the elastic features of interest on the indium concentration x shows a monotonic behaviour when $\text{In}_x\text{Al}_{1-x}\text{As}_y\text{Sb}_{1-y}$ is lattice-matched to InP substrate. In that case, the elastic constants have larger values and the material system of interest becomes less harder and its rigidity becomes weaker. The mechanical stability criteria is verified in terms of elastic constants and shows that $\text{In}_x\text{Al}_{1-x}\text{As}_y\text{Sb}_{1-y}$ is mechanically stable for each x and substrate being considered here. The change in indium content x and the substrate is found to have no much effect on both the Poisson ratio and machinability. The present study showed that a proper choice of the indium composition x and substrate may provide more diverse opportunities as regards the elastic modulus of $\text{In}_x\text{Al}_{1-x}\text{As}_y\text{Sb}_{1-y}$.

Accession Number: WOS:000442728700003**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Al-Hagan, Ola		0000-0003-0386-2418

ISSN: 1478-6435

eISSN: 1478-6443

Record 112 of 119**Title:** Theoretical Study of the Structure and Stability of $\text{He-K-2}(+)(X-2 \text{Sigma}(+)(g))$ van der Waals Complex**Author(s):** Ghanmi, C (Ghanmi, C.); Al Qarni, HJ (Al Qarni, H. J.); Al-Hagan, O (Al-Hagan, O.); Berriche, H (Berriche, H.)**Edited by:** AlKamli A; Souadi GO; Hakami J; Can N; Mahdy A; Mahgoub M; Mujahid ZUI**Source:** SIXTH SAUDI INTERNATIONAL MEETING ON FRONTIERS OF PHYSICS 2018 (SIMFP2018) **Book Series:** AIP Conference Proceedings **Volume:** 1976 **Article Number:** 020026 **DOI:** 10.1063/1.5042393 **Published:** 2018

Abstract: We studied theoretically the structure and stability of the Helium atom interacting with the diatomic system $\text{K-2}(+)(X-2 \text{Sigma}(+)(g))$. The calculations carried out using an accurate ab initio calculation based on the pseudo-potential approach and for an extensive range of the remaining two Jacobi coordinates, R and θ . The pseudo-potential method has reduced the number of active electrons of the $\text{He-K-2}(+)(X-2 \text{Sigma}(+)(g))$ van der Waals complex to only one electron. The potential energy surfaces determined and used to extract the spectroscopic data related to the stability of the $\text{He-K-2}(+)(X-2 \text{Sigma}(+)(g))$ van der Waals complex. The results show that the $\text{He-K-2}(+)(X-2 \text{Sigma}(+)(g))$ van der Waals complex is more stable in the linear geometry and the Helium atom does not perturb the stretching mode of $\text{K-2}(+)(X-2 \text{Sigma}(+)(g))$.

Accession Number: WOS:000437006400026**Conference Title:** 6th Saudi International Meeting on Frontiers of Physics (SIMFP)**Conference Date:** FEB 27-MAR 01, 2018

Conference Location: Jazan Univ, Jazan, SAUDI ARABIA

Conference Host: Jazan Univ

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ISSN: 0094-243X

ISBN: 978-0-7354-1685-7

Record 113 of 119

Title: Theoretical Investigation of the Electronic Properties of the Dication BeB₂⁺

Author(s): Ghanmi, C (Ghanmi, Chedli); Alshamrani, R (Alshamrani, Razan); Farjallah, M (Farjallah, Mohamed); Berriche, H (Berriche, Hamid)

Edited by: AlKamli A; Souadi GO; Hakami J; Can N; Mahdy A; Mahgoub M; Mujahid ZUI

Source: SIXTH SAUDI INTERNATIONAL MEETING ON FRONTIERS OF PHYSICS 2018 (SIMFP2018) **Book Series:** AIP Conference Proceedings **Volume:** 1976 **Article Number:** 020017 **DOI:** 10.1063/1.5042384 **Published:** 2018

Abstract: The electronic properties of the dication BeB₂⁺ have been studied using an ab initio approach based on the use of non-empirical pseudopotentials and parameterized l dependent polarization potentials. The potential energy curves and their spectroscopic constants for the ground and the low lying electronic states of (2)Sigma(+) symmetry have been determined. Results show that the 1-2(2)Sigma(+) and 4-5(2)Sigma(+) states are repulsive, while the 3(2)Sigma(+) and 6-9(2)Sigma(+) are metastable states. Some avoided crossings between the (2)Sigma(+) states have been localized and analysed. Furthermore, the transition dipole moments from the ground state to the higher states of (2)Sigma(+) and (2)Pi symmetries have been computed.

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Conference Title: 6th Saudi International Meeting on Frontiers of Physics (SIMFP)

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Conference Location: Jazan Univ, Jazan, SAUDI ARABIA

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Record 114 of 119

Title: Analysis of Alpha Particles Scattered from S-32 at 386 MeV

Author(s): Ibraheem, AA (Ibraheem, Awad A.); Algahatani, F (Algahatani, F.)

Edited by: AlKamli A; Souadi GO; Hakami J; Can N; Mahdy A; Mahgoub M; Mujahid ZUI

Source: SIXTH SAUDI INTERNATIONAL MEETING ON FRONTIERS OF PHYSICS 2018 (SIMFP2018) **Book Series:** AIP Conference Proceedings **Volume:** 1976 **Article Number:** 020022 **DOI:** 10.1063/1.5042389 **Published:** 2018

Abstract: The elastic scattering data of alpha particles from (32)S at incident energy of 386 MeV have been reanalyzed. Both imaginary phenomenological Woods Saxon (WS) form and real double folding (DF) optical model based on DDM3Y interaction with and without renormalization factor by adding the dynamic polarized potential are used. A new forms for the cluster density is employed for the first time. A comparison between our results with available data in literatures measured for angular distributions of the differential cross sections has been presented. We reproduced the data successfully to validate our method of calculation.

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Conference Title: 6th Saudi International Meeting on Frontiers of Physics (SIMFP)

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Record 115 of 119

Title: Scattering of Neutron-halo nucleus He-6 around the Coulomb barrier Using Microscopic Model

Author(s): Ibraheem, AA (Ibraheem, Awad A.); Amri, HAL (Amri, Huda A. L.)

Edited by: AlKamli A; Souadi GO; Hakami J; Can N; Mahdy A; Mahgoub M; Mujahid ZUI

Source: SIXTH SAUDI INTERNATIONAL MEETING ON FRONTIERS OF PHYSICS 2018 (SIMFP2018) **Book Series:** AIP Conference Proceedings **Volume:** 1976 **Article Number:** 020021 **DOI:** 10.1063/1.5042388 **Published:** 2018

Abstract: In this work, we analyzed the elastic scattering cross sections of He-6 scattered from C-12, Ni-58, Sn-120, and Pb-208 targets at four energies above the Coulomb barrier (30, 21.7, 20.5 and 22 MeV respectively). Moreover, we analyzed the inelastic scattering of He-6 projectiles from C-12 target at 30 MeV. These analyses are performed in the framework of optical model potential (OMP). The real part of the OMP is obtained using the folding model. We studied the effect of the iso-spin degree of freedom in the scattering data. For this reason, we used the DDM3Y effective nucleon-nucleon interaction with the iso-scalar and the iso-vector components. In addition, different forms of the matter density of projectile are used. The obtained potentials are used to analyze the scattering data. The obtained results are compared with the corresponding measured data as well as those obtained from the phenomenological Woods Saxon potential. The obtained differential scattering cross sections and the total reaction cross sections are successfully reproduced using our derived potentials.

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Record 116 of 119**Title:** Sextic and Decatic Anharmonic Oscillator Potentials Including Odd Power Terms: Polynomial Solutions**Author(s):** Maiz, F (Maiz, F.); Alqahtani, MM (Alqahtani, Moteb M.); Ghnaim, I (Ghnaim, I)**Edited by:** AlKamli A; Souadi GO; Hakami J; Can N; Mahdy A; Mahgoub M; Mujahid ZUI**Source:** SIXTH SAUDI INTERNATIONAL MEETING ON FRONTIERS OF PHYSICS 2018 (SIMFP2018) **Book Series:** AIP Conference Proceedings **Volume:** 1976 **Article Number:** 020034 **DOI:** 10.1063/1.5042401 **Published:** 2018**Abstract:** We study the sextic and decatic potentials energy including the odd power terms, and explore possible polynomial solutions for Schrodinger equation. Moreover, we proved that generals sextic and decatic potentials are exactly solvable under certain conditions on the potential's parameters; these conditions connect the potential's parameters to each other and to wave function's zeros. We compare achieved results with those evaluated by numerical methods. Finally, we derive general expressions of the energy levels and evaluate the first eigenstates for both potentials.**Accession Number:** WOS:000437006400034**Conference Title:** 6th Saudi International Meeting on Frontiers of Physics (SIMFP)**Conference Date:** FEB 27-MAR 01, 2018**Conference Location:** Jazan Univ, Jazan, SAUDI ARABIA**Conference Host:** Jazan Univ

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Record 117 of 119**Title:** Singularity of the Exact QCD beta-Function**Author(s):** Souadi, GO (Souadi, G. O.); Crewther, RJ (Crewther, R. J.)**Edited by:** AlKamli A; Souadi GO; Hakami J; Can N; Mahdy A; Mahgoub M; Mujahid ZUI**Source:** SIXTH SAUDI INTERNATIONAL MEETING ON FRONTIERS OF PHYSICS 2018 (SIMFP2018) **Book Series:** AIP Conference Proceedings **Volume:** 1976 **Article Number:** 020002 **DOI:** 10.1063/1.5042369 **Published:** 2018**Abstract:** Rytov and Sannino suggested an exact expression for the QCD beta -function. However, it has a space-like pole at a finite value of the coupling constant. The pole makes the exact beta(RS)-function undefined for some values of the running coupling alpha between the origin and a fixed point alpha(FP). Thus, we use the property of renormalization scheme dependence to obtain a non-singular form for the exact beta(RS)-function. The modified exact (beta) over bar (RS)-function has an infrared fixed point even for a small number of quark flavors.**Accession Number:** WOS:000437006400002**Conference Title:** 6th Saudi International Meeting on Frontiers of Physics (SIMFP)**Conference Date:** FEB 27-MAR 01, 2018**Conference Location:** Jazan Univ, Jazan, SAUDI ARABIA**Conference Host:** Jazan Univ

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Record 118 of 119**Title:** Effect of different solvents on the key structural, optical and electronic properties of sol-gel dip coated AZO nanostructured thin films for optoelectronic applications**Author(s):** Kumar, KDA (Kumar, K. Deva Arun); Ganesh, V (Ganesh, V.); Shkir, M (Shkir, Mohd.); AlFaify, S (AlFaify, S.); Valanarasu, S (Valanarasu, S.)**Source:** JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 29 **Issue:** 2 **Pages:** 887-897 **DOI:** 10.1007/s10854-017-7985-0 **Published:** JAN 2018**Abstract:** Transparent conducting aluminum (i. e. 2 at.%) doped zinc oxide (AZO) thin films were prepared on glass substrates by sol-gel dip coating technique using different solvents. This inexpensive dip coating method involves dipping of substrate consecutively in zinc solution and tube furnace for required cycles. Prepared films were investigated by XRD, SEM, PL, Raman spectroscopy optical and electrical studies. From the XRD studies, it confirmed the incorporation of aluminum in ZnO lattice. The prepared samples are polycrystalline nature, and these films reveal hexagonal wurtzite arrangement with (002) direction. The structural parameters such as crystallite size, dislocation density, micro strain, texture coefficient and lattice constant were investigated. SEM study showed well defined smooth and uniformed ganglia shaped grains are regularly distributed on to the entire glass substrate without any pinholes and cracks, and the average grain size is 75 nm. From the optical studies, the observed highest transmittance is 93% in the visible range and the band gap - (E-g) is 3.26 eV. Room temperature PL spectra exhibited strong UV emission peak located at 386 nm for all the films. The electrical properties of the AZO thin films were studied by Hall-Effect measurements and found as n-type conductivity with high carrier concentrations (n), $2.76 \times 10^{19} \text{ cm}^{-3}$ and low resistivity (ρ), $7.56 \times 10^{-3} \text{ Ohm cm}$ for the film deposited using methanol as solvent.**Accession Number:** WOS:000433466100001**Author Identifiers:**

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Record 119 of 119

Title: Strained noble metal di chalcogenides PtX₂ (X = S, Se) mono-layer: Ab initio study of electronic and lattice dynamic properties

Author(s): Ahmad, S (Ahmad, Sohail)

Source: PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES **Volume:** 95 **Pages:** 139-143 **DOI:** 10.1016/j.physe.2017.09.016 **Published:** JAN 2018

Abstract: Electronic properties of noble metal dichalcogenides PtX₂ (X = S, Se) mono-layers have been studied using plane wave pseudopotential method based on density functional theory. The band gap is observed to be as 1.94 eV (1.37 eV) in case of PtS₂ (PtSe₂) mono-layer which is found to be in close agreement with previous known results. A further variation in band gap is observed in both the two mono-layers on applying biaxial tensile as well as compressional strain. Phonon spectrum of these mono-layers and its strained structure reflects its dynamical stability.

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