SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

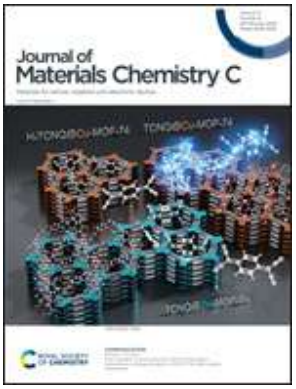
Journal Name: Journal of Materials Chemistry **IF: 6.4**

Title: Morphological evolution of individual microrods to self-assembled 3D hierarchical flower architectures of CuBixIn1−xSe2 for photo response applications

Author: Priyadarshini P., Senapati S., Mohapatra A., Pradhan M., Alagarasan D., Naik R.

Details: Volume 12, Issue 8, Pages 2879 – 2893, 15 January 2024

Abstract: $CuInSe_2$ and $CuInGaSe_2$ are extremely promising materials for solar cell applications, wherein bandgap shrinkage is highly desirable for manufacturing transparent/semitransparent layers. In this work, this shrinkage was achieved by replacing In with Bi, and the change in current-voltage responses for photodetector applications was further studied. $CuBi_xIn_{1-x}Se_2$ microrod (MR) flowers (x = 0, 0.2, 0.4, 0.6, and 0.8) were synthesized via microwave synthesis using different Bi/In concentrations. The variation in the composition of Bi/In caused alteration in structural, morphological, and optical behaviors. $CuInSe_2$ showed a polycrystalline nature, while Bi incorporation led to the appearance of a Bi_2Se_3 phase. Raman peaks corresponding to different vibrational bonds shifted with change in Bi/In content, indicating that the composition variation induced structural transformation inside the matrix. Morphological analysis showed a transition from MRs to MR-based flowers with the introduction of bismuth. Optical absorption was enhanced with an increase in Bi content due to a change in the MR size, forming a flower-like architecture. This reduced the optical bandgap by increasing defects and disorders in the forbidden gap. At 532 nm excitation, broad photoluminescence band emission was observed for all samples. Each spectrum showed three deconvoluted peaks, which were attributed to a transition among localized states over the forbidden gap region. The MRs demonstrated good photo response towards white light. Their photocurrent reduced from the μA to the nA range with varying compositions. The observed optical and electrical properties of the MRs are most suitable for various optoelectronic device applications.



URL: https://pubs.rsc.org/en/content/articlelanding/2024/tc/d3tc03250g

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

Journal Name: Journal of Alloys and Compound **IF: 6.2**

Title: Optimization of (Ba1−xCax)(Ti0.9Sn0.1)O3 ceramics in X-band using Machine Learning

Author: Dikshit A.P., Das D., Samal R.R., Parashar K., Mishra C., Parashar S.K.S.

Details: Volume 982, April 2024, Article Number 173797

Abstract: Developing efficient electromagnetic interference shielding materials has become significantly important in present times. This paper reports a series of (Ba1−xCax)(Ti0.9Sn0.1)O3 (BCTS) (x=0,0.01,0.05,0.1) ceramics synthesized by conventional method which were studied for electromagnetic interference shielding (EMI) applications in X-band (8–12.4 GHz). EMI shielding properties and all S parameters (S11 & S12) of BCTS ceramic pellets were measured in the frequency range (8–12.4 GHz) using a Vector Network Analyser (VNA). The BCTS ceramic pellets for x = 0.05 showed maximum total effective shielding of 46 dB indicating good shielding behaviour for high-frequency applications. However, the development of lead-free ceramics with different concentrations usually requires iterative experiments resulting in, longer development cycles and higher costs. To address this, we used a machine learning (ML) strategy to predict the EMI shielding for different concentrations and experimentally verify the concentration predicted to give the best EMI shielding. The ML model predicted BCTS ceramics with concentration (x = 0.06, 0.07, 0.08, and 0.09) to have higher shielding values. On experimental verification, a shielding value of 58 dB was obtained for x = 0.08, which was significantly higher than what was obtained experimentally before applying the ML approach. Our results show the potential of using ML in accelerating the process of optimal material development, reducing the need for repeated experimental measures significantly.

URL: https://www.sciencedirect.com/science/article/pii/S0925838824003839?via%3Dihub

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

Journal Name: Journal of Alloys and Compound **IF: 6.2**

Title: Tailoring optical properties of hydrothermally synthesized SnMnSe nanocubes for optoelectronic and dielectric application

Author: Abinash Parida , Subrata Senapati , Gopal K. Pradhan & Ramakanta Naik

Details: Volume 970 , January 2024

Abstract: In the current paper, we investigate the optical and dielectric properties of the SnMnSe nanocubes. The $Sn_{0.5+x}Mn_{0.5-x}Se$ (x = 0.375, 0.250, 0.125, 0) samples are prepared by simple hydrothermal method with the variation of the Sn and Mn concentration. The X-ray diffraction study shows that all the prepared samples are polycrystalline in nature. The average crystallite size increases along with the dislocation density and the average strain value with the increase in the Mn concentration. The morphology shows the formation of nanocubes. The average size of the cubes increases with the increase of Mn content. The reflectance data demonstrate the decreasing order of absorption edges with the increase of Mn content in the sample. The variation of the absorption edges with Mn content tends to decrease the optical bandgap by creating more disorder and defects between the gap region. Broad orange-red photoluminescence emission is observed for all the samples with 532 nm excitation. The electrical study of the sample shows high resistance values. The dielectric behavior as a function of frequency and temperature is investigated, and parameters like dielectric constant, AC conductivity, impedance spectroscopy, and electric modulus are deeply analyzed. The dielectric properties are useful for energy storage applications. All the above optical and dielectric properties of the SnMnSe matrix have potential use in the field of optoelectronics and dielectric applications.

URL: https://www.sciencedirect.com/science/article/pii/S0925838823038239?via%3Dihub

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

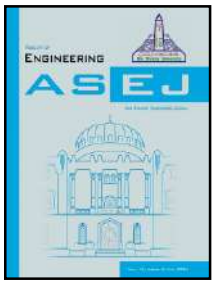
Journal Name: Ain Shams Engineering Journal **IF: 6**

Title: Optimal strategies for green investment, sharing contract and advertisement effort in a supply chain coordination problem

Author: Saha S., Alrasheedi A.F., Khan M.A.-A., Manna A.K.

Details: Volume 15, Issue 4, April 2024

Abstract: The global environment is experiencing increasingly rapid pollution due to the presence of harmful products generated by human activities, the emissions from vehicular traffic, and the release of carbon dioxide from industrial sources. To save this beautiful earth as well as human beings, it is necessary to reduce pollution by producing eco-friendly products and reducing reckless carbon emissions from industry. Furthermore, advertising serves as a very efficacious strategy for promoting sustainable green products and encouraging customer engagement. In response to the current circumstances, a supply chain model including a manufacturer, a retailer, and customers is devised, incorporating investments in green practices and advertising. This study examines the relationship between client demand and three key factors: marketing effort, the product's green level, and the selling price. In addition, a sharing contract policy between the manufacturer and the retailer on green investment costs is applied in this model. The main focus of this study is to find the optimal values of advertisement effort, the product's green level, the manufacturer's wholesale price, the retailer's selling price and the sharing percentage of green investment that maximize the profits of the retailer and manufacturer, as well as the integrated supply chain system of the proposed model. In order to demonstrate the practical significance of the concept, a numerical example is solved and then a comparative analysis is conducted. Moreover, sensitivity studies are performed to assess the impact of different model parameters on decision factors and profitability. In conclusion, this study provides management insights and offers some closing observations, along with suggestions for future research directions. The findings indicate that the implementation of a sharing contract policy yields more earnings to the participants in the supply chain compared to a decentralized situation. The centralized strategy in supply chain management (SCM) results in higher joint earnings for the manufacturer and the retailer compared to the decentralized and sharing contract policies.



URL: https://www.sciencedirect.com/science/article/pii/S2090447923004847?via%3Dihub

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

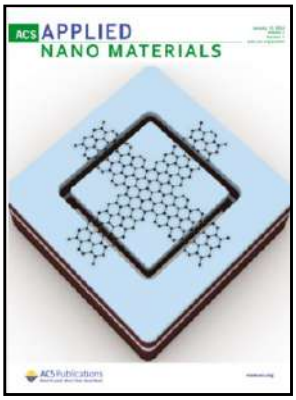
Journal Name: ACS Applied Nano Materials **IF: 5.9**

Title: No-Stirring Synthesis of sub-50 nm Hollow Silver Nanoshells with Dimethylglyoxime-Induced Plasmons in Visible and Second NIR Windows for Biomedical Applications

Author: Dadhich B.K., Gupta P., Ballav S., Bhushan B., Datta P.K., Priyam A.

Details: Volume 7, Issue 1, Pages 1212 – 1221, 12 January 2024

Abstract: A unique no-stirring synthesis has been developed to obtain highly monodisperse hollow silver nanoshells (HAgNSs) with plasmons in the second near-IR (NIR-II) window. The method also introduces dimethylglyoxime (DMG) as a quadrupole-supporting agent. The quadrupole surface plasmon resonance (Q-SPR) was found to be highly intense and tunable from 450 to 558 nm. Two types of dipolar resonances, symmetric dipole surface plasmon resonance (SD-SPR) and antisymmetric dipole surface plasmon resonance (AD-SPR), are also observed. The AD-SPR peaks remain constant at 333 nm while the SD-SPR peaks are tuned gradually from 780 to 850 → 920 → 1000 → 1150 nm. They were accordingly named HAgNS-780, HAgNS-850, HAgNS-920, HAgNS-1000, and HAgNS-1150, and their outer diameters were found to be 53 ± 4, 49 ± 3, 54 ± 3, 62 ± 5, and 39 ± 3 nm, respectively. The corresponding aspect ratios (outer diameter/shell thickness) were 3.31, 3.37, 3.48, 4.13, and 5.2, respectively. A correlation between the tunability of SD-SPR, AD-SPR, and Q-SPR and aspect ratio has been established. The shape and size parameters were utilized for the simulation of the extinction spectra by the discrete dipole approximation (DDA) method. Second derivative FTIR analysis reveals the peculiar binding mode of DMG to the HAgNS which is the genesis of Q-SPR in such smaller-sized nanoshells. The further red shift of Q-SPR and SD-SPR was observed with the addition of folic acid (FA). It also imparts greater aqueous solubility, colloidal stability, and biocompatibility, making them suitable for biomedical applications.



URL: https://pubs.acs.org/doi/10.1021/acsanm.3c05191

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

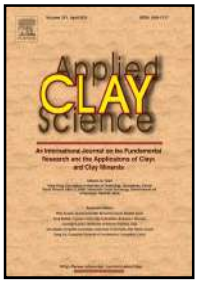
Journal Name: Applied Clay Science **IF: 5.6**

Title: Structural defect-induced white light emission from synthetic Zn-rich trioctahedral smectite

Author: Soren, Dhani; Mehena, Gayatree; Behera, J. N.; Pattojoshi, Puspalata; Deheri, Pratap Kumar

Details: Volume 251, April 2024, Article Number 107317

Abstract: In this research work, AlIII substituted by MgII and ZnII atoms in smectites (Sm) of the formula [Na0.7Mg2.5-xZnxLi0.3Si4O10(OH)2] were synthesized. Its structural and intrinsically highly photoluminescent (PL) properties were reported. The complex distributions of MgII and ZnII atoms were observed in both octahedral and tetrahedral sites in the synthesized Sm (as evident with XRD, XPS, and ESR studies). The visible white light emission was observed when excited with UV light (250 nm). The observed strong photoluminescence (PL) was attributed to the electronic transition from oxygen vacancy to acceptor atoms induced by isomorphous substitution in both tetrahedral and octahedral sites (MgAl′,MgSi′′,ZnAl′,ZnSi′′). With introduction of ZnII atom, there was an increase in MgAl′andMgSi′′defects energy levels that resulted in bathochromic shifts in VO··→MgAl′′, VO··→MgSi′′ and VO··→VO emission lines. Moreover, two additional emission lines in blue and red-light regions were observed due to two new ZnAl′,ZnSi′′ defect centers that led to VO··→ZnAl′ and VO··→ZnSi′′ electronic transitions.



URL: https://www.sciencedirect.com/science/article/pii/S0169131724000656?via%3Dihub

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

Journal Name: Nanomedicine **IF: 5.5**

Title: Near infrared-responsive quinacrine-gold hybrid nanoparticles deregulate HSP-70/P300-mediated H3K14 acetylation in ER/PR+ breast cancer stem cells

Author: Dash S.R.; Das C.; Das B.; Jena A.B.; Paul S.; Sinha S.; Tripathy J.; Kundu C.N.

Details: Volume 19, Issue 7, 1 March 2024

Abstract: Aim: This study aimed to determine if quinacrine-gold hybrid nanoparticles (QAuNPs) + near-infrared (NIR) deregulate HSP-70/P300 complex-mediated H3K14 acetylation in estrogen receptor/progesterone receptor (ER/PR+) breast cancer stem cells (CSCs). Materials & methods: Various cells and mouse-based systems were used as models. Results: QAuNP + NIR treatment reduced the nuclear translocation of HSP-70, affected the histone acetyltransferase activity of P300 and specifically decreased H3K14 acetylation in ER/PR+ breast CSCs. Finally, HSP-70 knockdown showed a reduction in P300 histone acetyltransferase activity, decreased H3K14 acetylation and inhibited activation of the TGF-β gene. Conclusion: This study revealed that QAuNP + NIR irradiation inhibits oncogenic activation of the TGF-β gene by decreasing H3K14 acetylation mediated through the HSP-70/P300 nuclear complex in ER/PR+ breast CSCs.

URL: https://www.futuremedicine.com/doi/10.2217/nnm-2023-0269

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

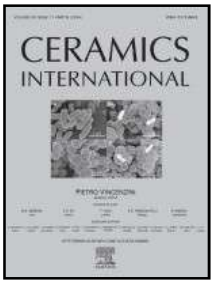
Journal Name: Ceramics International **IF: 5.2**

Title: Dielectric, electric, and magnetic response of modified bismuth ferrite-based double perovskites for NTC-thermistor application

Author: Sahoo S., Mishra S., Sahoo L., Parida B.N., Biswal L., Parida R.K.

Details: Volume 50, Issue 11, June 2024.

Abstract: Owing to the variation of the characteristics due to the cationic substitution of diverse elements at both A and B sites, the new polycrystalline double perovskite BaBiFeMnO6, synthesized via a cost-efficient solid-state reaction route. Initial structural refinement by Rietveld analysis reveals material crystallised in dual phases i.e. monoclinic and orthorhombic. The respective cell parameters for monoclinic as well as orthorhombic phases are a = 5.5881 Å, b = 5.6541 Å, c = 7.9186 Å with cell angles α = γ = 900 and β = 89.90810 and a = 5.4807Å, b = 5.3583Å, c = 7.4045Å and refined angles are α = β = γ = 900 respectively. The microstructural interpretation of the present sample reflects a non-uniform distribution of the grains with an average grain size of 2.97 µm with a mean crystalline size of 342.65 nm. The Fourier-Transform Infrared Spectroscopy (FTIR) graph indicated that the sample belongs to the perovskite family. The impedance measurement was carried out in a selected frequency and an assigned temperature range to investigate the electrical features of the material which suggested the non-Debye type relaxation and negative temperature coefficient of resistance (NTCR). Furthermore, the thermistor constant (β) and temperature coefficient of resistance (TCR) contributed to investigating the NTCR characteristic of the sample under NTC-type thermistor applications. The room temperature dielectric constant is 1707.67 with a minimal tangent loss of 0.7069 at 100Hz frequency has been estimated by fitting the dielectric data by utilizing the Havrilliak-Negami function. The polarization (P) induced due to the maximum applied electric field of 1.287 kV is studied from the hysteresis loop plotted between them. The hysteresis loop indicates the ferroelectric property of the material with a lossy nature. The room temperature remnant magnetization (2Mr) of 0.4424 emu/g and coercivity (2Hc) of 6.2 kOe have been estimated from the M □ H loop. The potentiality of the material to be used as a viable candidate in various energy storage devices and supercapacitors is suggested by all of the characterisations in conjunction with the high value of εr i.e. □80000 at 300 °C for the lower frequency.



URL: https://www.sciencedirect.com/science/article/pii/S0272884224010654?via%3Dihub

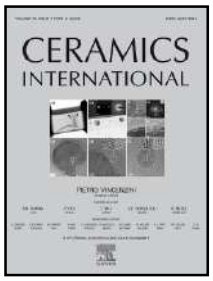
Journal Name: Ceramics International **IF: 5.2**

Title: Structural, relaxor behavior, and energy storage performance of BaTiO3-Bi (Mg2/3Nb1/3)O3 solid solutions for potential MLCC application

Author: Sahoo, S.; Badapanda, T.; Kumar, D.; Rout, S. K.; Mohanty, S.; Ray, J.; Tripathy, Satya N.

Details: Volume 49,Issue 23 Part A, December 2023, Pages 37700-37711

Abstract: In the discussed work, (1-x) BaTiO3 (BT)-x Bi(Mg2/3Nb1/3)O3 (BMN) solid-combinations have been synthesized via the solid-state process; and both corresponding dielectric and ferroelectric behavior have been learned for possible Multilayer Ceramic Capacitor (MLCC) applications. The phase confirmation has been identified utilizing X-ray diffraction; and Rietveld refinement technique has been used for structural analysis that unveils the formation of pure perovskite structure of the prepared ceramics. Rietveld refinement results reveal the structural changeover from tetragonal to pseudo-cubic for x≥0.125. Raman spectroscopy measurements confirm the structural phase changes and lattice modifications due to the chemical substitutions. Microstructural analysis has been done with the help of electron micrograph. Dielectric performance of the synthesized (1-x)BaTiO3(BT)-xBi(Mg2/3Nb1/3)O3(BMN) solid solutions has been examined within a temperature range of 173K–473K at different applied frequencies. A broad phase transition and relaxor character is detected from dielectric investigation. The relaxor behavior has been quantified by the Vogel-Fulcher fitting. The thermal stability of the prepared samples was calculated by means of standard formula of Temperature Coefficient of Capacitance (TCC). Hysteresis loop was undertaken to identify the ferroelectric properties and energy storage capacity. Among all the compositions, x = 0.10 shows good thermal stability, an elevated recoverable energy density; and a remarkable efficiency that makes it suitable for MLCC applications.



URL: https://www.sciencedirect.com/science/article/pii/S0272884223027190?via%3Dihub

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

Journal Name: Polymer Composites **IF: 5.2**

Title: Fabrication of Multiwalled Carbon Nanotubes (MWCNT) and Reduced Graphene Oxide (rGO)-based thermoplastic polyurethane and polypyrrole nanocomposites for electromagnetic wave absorption application with a low reflection

Author: Acharya Swatee, Swain Lopa Mudra, Samal Ritu Roumya, Parashar S. K. S, Sahoo Bibhu Pras

Details: 22 December 2023

Abstract: Electromagnetic radiation (EMR) pollution is a serious concern in today's environment, causing problems not just for electronic gadgets but also for living society. The goal of this research is to fabricate thermoplastic polyurethane (TPU) and polypyrrole (PPy)-based 95:5 blend nanocomposites using a simple solvent casting method at such a low concentration of rGO and MWCNT (0.3, 0.4, 0.5 php) (parts per hundred polymers), for electromagnetic wave (EMW) absorption applications. The chemical interaction between the different phases and morphology of the nanocomposites is characterized by Raman spectroscopy, X-ray diffraction (XRD), and field emission scanning electron microscopy (FESEM) techniques. The material properties, such as dielectric and magnetic properties, are analyzed in X-band frequency (8.2–12.4 GHz). The total shielding effectiveness of (SETot) 0.5 rGO system is found to be 27 dB, whereas, for corresponding MWCNT nanocomposites, it is 26 dB. Interestingly, in 0.5 rGO nanocomposites, absorption shielding effectiveness (SEAbs) is approximately 25 dB, and reflection shielding effectiveness (SERef) is less than 2 dB, which indicates the absorption of 70% of the electromagnetic wave, and the rest gets reflected. Apart from that, the rGO-based nanocomposites possess a greater extent of thermal stability than the corresponding MWCNT-based nanocomposites.

URL: https://4spepublications.onlinelibrary.wiley.com/doi/10.1002/pc.28027?af=R

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

Journal Name: Scientific Reports **IF: 4.6**

Title: Stronger EPR-steering criterion based on inferred Schrödinger–Robertson uncertainty relation

Author: Naik L.P., Das R.M., Panigrahi P.K.

Details: Volume 14, Issue 1, December 2024

Abstract: Steering is one of the three in-equivalent forms of nonlocal correlations intermediate between Bell nonlocality and entanglement. Schrödinger–Robertson uncertainty relation (SRUR), has been widely used to detect entanglement and steering. However, the steering criterion in earlier works, based on SRUR, did not involve complete inferred-variance uncertainty relation. In this paper, by considering the local hidden state model and Reid's formalism, we derive a complete inferred-variance EPR-steering criterion based on SRUR in the bipartite scenario. Furthermore, we check the effectiveness of our steering criterion with discrete variable bipartite two-qubit and two-qutrit isotropic states.

URL: https://www.nature.com/articles/s41598-023-50029-z

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

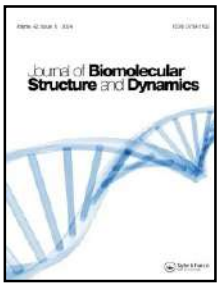
Journal Name: Journal of Biomolecular Structure and Dynamics **IF: 4.4**

Title: In silico screening of phytoconstituents as potential anti-inflammatory agents targeting NF-κB p65: an approach to promote burn wound healing

Author: Pattnaik S., Murmu S., Prasad Rath B., Singh M.K., Kumar S., Mohanty C.

Details: 2024

Abstract: Chronic burn wounds are frequently characterised by a prolonged and dysregulated inflammatory phase that is mediated by over-activation of NF-κB p65. Synthetic wound healing drugs used for treatment of inflammation are primarily associated with several shortcomings which reduce their therapeutic index. In this scenario, phytoconstituents that exhibit multifaceted biological activities including anti-inflammatory effects have emerged as a promising therapeutic alternative. However, identification and isolation of phytoconstituents from medicinal herbs is a cumbersome method that is linked to profound uncertainty. Hence, present study aimed to identify prospective phytoconstituents as inhibitors of RHD of NF-κB p65 by utilizing in silico approach. Virtual screening of 2821 phytoconstituents was performed against protein model. Out of 2821 phytoconstituents, 162 phytoconstituents displayed a higher binding affinity (≤ −8.0 kcal/mol). These 162 phytoconstituents were subjected to ADMET predictions, and 15 of them were found to satisfy Lipinski's rule of five and showed favorable pharmacokinetic properties. Among these 15 phytoconstituents, 5 phytoconstituents with high docking scores i.e. silibinin, bismurrayaquinone A, withafastuosin B, yuccagenin, (+)-catechin 3-gallate were selected for molecular dynamics (MD) simulation analysis. Results of MD simulation indicated that withafastuosin B, (+)-catechin 3-gallate and yuccagenin produced a compact and stable complex with protein without significant variations in conformation. Relative binding energy analysis of best hit molecules indicate that withafastuosin B, and (+)-catechin 3-gallate exhibit high binding affinity with target protein among other lead molecules. Findings of study suggest that these phytoconstituents could serve as promising anti-inflammatory agents for treatment of burn wounds by inhibiting the RHD of NF-κB p65.



URL: https://www.tandfonline.com/doi/full/10.1080/07391102.2024.2306199

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

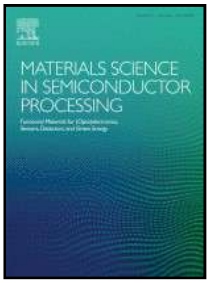
Journal Name: Materials Science in Semiconductor Processing **IF: 4.1**

Title: Synthesis of 3D rice-like BiOCl battery-type electrode material and evaluation of their electrochemical performance in a symmetrical super capacitor device configuration

Author: Thakur Y.S., Acharya A.D., Sharma S., Amisha, Bisoyi S., Bhawna, Manhas S.S.

Details: Volume 177, July 2024

Abstract: 3D porous rice-like BiOCl nanostructure was prepared via solvothermal technique with sodium chlorate as a surfactant which serves as electrode material for the supercapacitor applications. The prepared nanoparticles supported on nickel foam textile exhibit high battery-type charge storage ability in a 3 M KOH aqueous electrolyte solution. The dominance of the battery-type charge storage mechanism of the BiOCl electrode was confirmed through the CV study. Furthermore, the GCD study revealed a good specific capacity of 501 C/g at 0.5 A/g current density and cycle stability of 80% over 2500 cycles. In the presence of a 3 M KOH electrolyte, a symmetric supercapacitor device was constructed with two identical 3D rice-like BiOCl electrodes. This configuration unveiled an impressive energy density of 21.8 Wh/kg at 772.5 W/kg power density. To illustrate its practical viability, two BiOCl/BiOCl symmetric devices were connected in series, successfully powering a red LED for approximately 50 s with high light intensity. This underscores the practical potential of the 3D rice-like BiOCl electrode in energy storage systems. In order to maximize the potential of BiOCl material in the future, the focus could be shifted towards mitigating the challenge of potential drop. This hurdle could be tackled by fabricating nanocomposites of BiOCl incorporated with conductive polymers and graphene oxide, thus elevating its overall performance.



URL: https://www.sciencedirect.com/science/article/pii/S1369800124002725?via%3Dihub

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

Journal Name: Energy Technology **IF: 3.8**

Title: Innovative Synthesis of Zeolitic Imidazolate Framework by a Stovetop Kitchen Pressure Cook Pot for Triboelectric Nanogenerator

Author: Dhal, Bikash Chandra; Hajra, Sugato; Priyadarshini, Anulipsa; Panda, Swati; Vivekananthan, Venkateswaran; Swain, Jaykishon; Swain, Subrat; Das, Niharika; Samantray, Raghabendra; Kim, Hoe Joon; Sahu, Rojalin

Details: March 2024

Abstract: This study presents a novel approach utilizing solvothermal techniques to synthesize zeolitic imidazolate framework (ZIF-4) particles. Various properties of the ZIF-4 particles are investigated to shed light on the structural and morphological characteristics. These ZIF-4 particles act as a positive triboelectric layer in the fabrication of a triboelectric nanogenerator (TENG) designed for powering electronic devices. The solvothermal-assisted synthesis ensures the controlled and efficient production of ZIF-4, optimizing its characteristics for enhanced performance in the TENG. The generated TENG, based on ZIF-4 particles, determines promising capabilities in converting mechanical energy into electrical power. The highest power of TENG is obtained to be 18 μW at a load resistance of 50 MΩ. This work contributes major insights to the search for sustainable and effective power solutions for electronic gadgets. It emphasizes the potential of ZIF-4 as a crucial triboelectric material, demonstrating its importance in the advancement of TENGs.

URL: https://onlinelibrary.wiley.com/doi/10.1002/ente.202400099

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

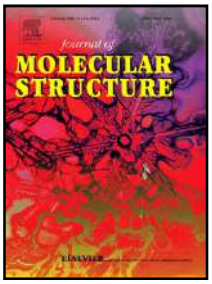
Journal Name: Journal of Molecular Structure **IF: 3.8**

Title: Exploration of structural, relaxor behavior and energy storage performance of Bi(Mg2/3Ta1/3)O3 modified BaTiO3

Author: Sahoo S., Badapanda T., Kumar D., Rout S.K., Ray J., Tripathy S.N.

Details: Volume 1308, July 2024, Article number 138006

Abstract: The effect of Bi(Mg2/3Ta1/3)O3 (BMT) on the structural, dielectric, and ferroelectric performance of BaTiO3 (BT) has been discussed in the manuscript. The (1-x)BaTiO3-xBi(Mg2/3Ta1/3)O3(0.05≤x≤0.15) compounds are prepared using the mixed oxide route. X-ray diffraction spectroscopy is used to analyze the structure, followed by Rietveld refinement of the XRD patterns and Raman spectroscopy. The structural analysis emphasizes that the compound holds tetragonal symmetry (P4mm) until x = 0.075 and is transferred to pseudo-cubic symmetry for x ≥ 0.10. FE-SEM images have been employed to examine the impact of BMT on the grain size of the BT ceramics. The dielectric characteristics of the (1-x)BT-xBMT solid solutions have been tested throughout a temperature span ranging from 213 K to 473 K at various applied frequencies that indicate the existence of a diffuse phase transition with relaxor behavior. The relaxor nature is further quantified using Vogel-Fultcher fitting. The temperature stability of the permittivity is examined by calculating the Temperature Coefficient of Capacitance (TCC) values. The ferroelectric performance and the energy storage capabilities of the solid solutions have been studied using P-E loops in various electric fields and frequencies. The stability of the hysteresis and energy storage performance with frequency and temperature response was verified. The fatigue endurance was also studied for the optimum composition. The leakage current measurements were carried out for all the compositions. Based on the dielectric, ferroelectric, and energy storage performance, the composition x=0.125 was found to be most suitable for MLCC application.



URL: https://www.sciencedirect.com/science/article/abs/pii/S0022286024005283?via%3Dihub

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

Journal Name: Physical Chemistry Chemical Physics **IF: 3.3**

Title: Laser power and high-temperature dependent Raman studies of layered bismuth and copper-based oxytellurides for optoelectronic applications

Author: Kumar, Prabhukrupa C.; Senapati, Subrata; Pradhan, Monalisa; Pradhan, Gopal K.; Naik, Ramakanta

Details: Volume 26, Issue 15, April 2024

Abstract: Layered metal oxychalcogenide materials have gained significant attention in recent years due to their numerous applications in various emerging fields. The bismuth (Bi) based ternary and quaternary oxychalcogenide materials have become popular due to their excellent potential in optoelectronic, thermoelectric, and semiconducting applications. Adding copper (Cu) to these building matrices has enhanced their usefulness in various ways. In this work, Bi and Cu-based ternary and quaternary layered oxytellurides are synthesized using a unique, rarely used “microwave (MW) assisted method,” and their temperature and laser power-dependent Raman measurements are carried out. All the samples are prepared at the same MW power and at a fixed irradiation time. Crystallographic studies show that the good crystallinity of the synthesized materials matches well with the phases reported previously. Nanosheet-like morphology was observed for all the prepared samples. The optical properties and band gap energies of these materials were obtained using the diffuse reflectance spectroscopy technique, which are in the range of 1.15–2.52 eV. The photoluminescence spectrum shows broad peaks around orange-red regions, indicating the potential applicability of these materials in various optoelectronic applications. The effect of high temperature and laser power on the Raman spectra of the oxytellurides is demonstrated, where the appearance of different vibrational modes along with a redshift in peak positions with the increase in temperature and power is observed.

URL: https://pubs.rsc.org/en/content/articlelanding/2024/cp/d4cp00562g

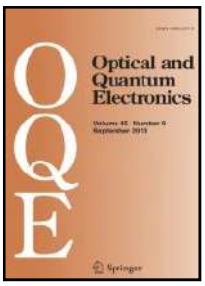
Journal Name: Optical and Quantum Electronics **IF: 3**

Title: New wave dynamics of the time-fractional Kaup–Kupershmidt model of seventh-order arises in shallow water waves

Author: Tripathy A., Sahoo S.

Details: Volume 56, Issue, March 2024, Article Number 472

Abstract: In this paper, a new variety of solitary wave patterns to the time-fractional seventh-order Kaup–Kupershmidt equation is studied. This model is important because of its nonlinear effects on the propagation of different water waves. For this study, we have considered the beta-fractional derivative form of the model. To derive the required exact solutions, we have used two analytical methods, specifically the new Kudryashov (nK) and modified Khater (mK) methods. Different types of wave patterns are produced from the solutions for distinct fractional and unidentified parameter values. These solutions include bright, two-soliton propagation, combined bright-dark, w-shaped pattern, combined dark-bright, m-shape wave, l-shaped bright wave, w-shaped periodic, u-shaped wave-form, and grey-type w-shaped periodic wave solutions. These dynamics of different wave natures are analyzed thoroughly by the graphical depiction of the solutions. Additionally, the characteristics of water waves and their many application areas can benefit greatly from these solutions such as surface waves in deep water, the dynamics of liquid-vapour interfaces, and many more. These solutions help us to understand how nonlinearity can affect the system during wave propagation. The novel aspect of this work is that the investigated model of the beta fractional form has never been solved before.



URL: https://link.springer.com/article/10.1007/s11082-023-05901-7

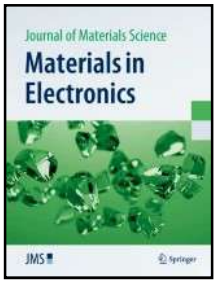
Journal Name: Journal of Materials Science-Materials in Electronics **IF: 2.8**

Title: Design of dual-band rectangular strip patch antenna on Bi0.5Na0.5TiO3 substrate

Author: Samal, Ritu Roumya; Das, Dibyaranjan; Dikhsit, Arpita Priyadarsini; Parashar, Kajal; Parashar, S. K. S.

Details: Volume 35, Issue 7, Article number 482

Abstract: Recently, ceramic patch antennas have been intensively researched for mobile communication systems. This work shows the unique use of Bi0.5Na0.5TiO3 (BNT) ceramic in microstrip patch antenna substrates for 8–12 GHz operation. The synthesized ferroelectric perovskite-based substrate of thickness t = 1.02 mm was utilized to produce the simulated antenna. The relevant electromagnetic parameters of permittivity, permeability, dielectric loss, magnetic loss, and miniaturization factor were studied. Characterization procedures are used to analyze the synthesized sample's crystal structure, local vibration, surface morphology, and elemental analysis. The rectangular-based split ring microstrip patch antenna's reflection loss, return loss, and radiation pattern were calculated using CST Microwave Studio v. 2019. The best yield result of simulation is − 55 dB which corresponds to the fabricated result of about − 25 dB for substrate thickness of t = 1.02 mm. The uniqueness of the synthesized sample has been modified parametrically by modifying its thickness for t = 0.9 mm, t = 1 mm, and t = 1.02 mm among which t = 1.02 mm thickness of the substrate is optimal for optimum results



URL: https://link.springer.com/article/10.1007/s10854-024-12271-7

Journal Name: Optimization **IF: 2.2**

Title: On inverse variational-hemivariational inequalities and its regularization

Author: Mahalik K., Nahak C.

Details: February 2024

Abstract: In this article, we propose the inverse variational-hemivariational inequalities problems (IVHIP) and its Tikhonov regularization theory. We establish the existence results for IVHIP and its regularized problems. Moreover, we also discuss the nonemptiness, boundedness and the asymptotic analysis of regularized solutions. Furthermore, we also investigate the existence results of the regularized solutions on the unbounded constrained through the coercive conditions. Several examples are given to support the new findings.

URL: https://www.tandfonline.com/doi/full/10.1080/02331934.2024.2313689

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

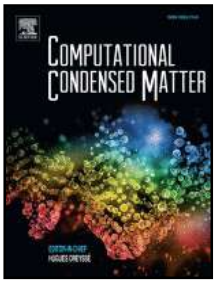
Journal Name: Computational Condensed Matter **IF: 2.1**

Title: Metal-insulator transition and G-type antiferromagnetism in CaNbO3 perovskite: Insight from DFT+U study

Author: Priyambada A., Deep R., Parida P.

Details: Volume 39, June 2024, Article number e00893

Abstract: In this work, we have investigated the ground state electronic and magnetic properties of CaNbO3 perovskite using the density functional theory, along with the Hubbard corrections. The study of structural, electronic, and magnetic properties was carried out using semi-empirical parameters. The structural properties reveal that Nb-O bond lengths are unequal in all directions, and ∠O-Nb-O bond angles are not equal to 90°, which makes NbO6 octahedra distorted. The electronic behavior of the compound, considering the strong correlation effect, shows a metal–insulator transition. The reason for this transition is found to be Jahn–Teller distortion. The stable magnetic state of the compound is obtained to be a G-type antiferromagnetic, using various U values.



URL: https://www.sciencedirect.com/science/article/pii/S2352214324000157?via%3Dihub

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

Journal Name: Solid State Communications **IF: 2.1**

Title: Iron(II)-induced defect luminescence and deconvolution of ferromagnetic and paramagnetic behaviour in Zn(1-x)FexO (x = 0.01, 0.03, 0.05) nanoparticles

Author: Dash S., Dadhich B.K., Patra S.K., Priyam A., Kavita S., Bhushan B.

Details: Volume 385, July 2024

Abstract: Zn(1-x)FexO (x = 0.00, 0.01, 0.03, 0.05) nanoparticles (NPs) were prepared by co-precipitation method and the wurtzite phase was confirmed by x-ray diffraction (XRD). The average crystallite size changes from 36 nm to 26 → 23→22 nm as the Fe-doping level varies from 0 to 1% → 3% → 5 % and the lattice strain increases concomitantly. The pristine ZnO NPs exhibit well-defined peak at 370 nm in the UV–vis absorption spectra which gets broadened on Fe-doping. The photoluminescence (PL) spectra of the pristine ZnO NPs shows a dominant excitonic peak at 390 nm. On Fe(II)-doping, new PL peaks at 449, 490 and 525 nm appear that are attributed to Zn-interstitials (Zni), oxygen vacancies (VO) and Zn vacancies (VZn), respectively. For all the Fe-doped ZnO NPs, M vs H plots have a complex non-saturating appearance indicating combination of ferromagnetic (FM) and paramagnetic (PM) behaviors. The subtraction of PM contribution revealed the FM curves with saturation magnetization (Ms). On going from 1% to 5% Fe-doping, the Ms values increase substantially by 39 times (0.00361 → 0.1398 emu/g) whereas the paramagnetic susceptibility, χP, increased 35 times (0.28 × 10−6 → 9.72 × 10−6 emu g−1 Oe−1)

URL: https://www.sciencedirect.com/science/article/pii/S0038109824000772?via%3Dihub

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

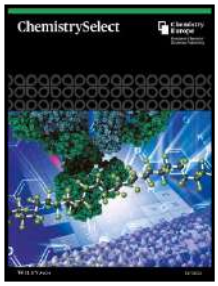
Journal Name: Chemistry Select **IF: 2.1**

Title: Effortless Fabrication of Bi2O3-Co3O4 Nanocomposite Catalyst: Harnessing Photocatalytic Power for Efficient Cationic Dye Degradation

Author: Pradhan, Debapriya; Nayak, Nibedita; Kanar, Monalisha; Dash, Suresh Kumar

Details: Volume 9, Issue 13, April 2024, Article Number e202400217

Abstract: A cost-effective and simple co-precipitation approach was used to create an efficient photocatalyst Co3O4-Bi2O3 with identical stoichiometry (1 : 1 of both Co3O4 and Bi2O3). XRD, FTIR, TEM, SEM-EDS, XPS, UV-DRS, PL, BET, and TGA were used to characterize the produced material's structural and optical properties. The presence of a single phase spinel structure with a distinctive plane (311) was verified by the XRD peak of 2 at 36.9° for Co3O4-Bi2O3. The SEM pictures revealed clustered consolidated spheres, suggesting particle homogeneity and high interconnectedness. The HR-TEM and SAED pictures revealed an average crystallite size of 28 nm for the Co3O4-Bi2O3 heterojunction. The UV-DRS spectral data demonstrated a 2.1 eV reduction in band gap energy for Co3O4-Bi2O3 (whereas Co3O4 is 2.4 eV and Bi2O3 is 2.7 eV). Under solar light irradiation, pristine Co3O4, Bi2O3, and Co3O4-Bi2O3 composites were investigated for photocatalytic degradation of Methylene Blue (MB) and Malachite green (MG) dyes. By adjusting factors such as pH, starting dye concentration, catalyst dosage, and agitation duration, the optimal efficiency was determined. The acquired results showed Co3O4-Bi2O3 's superior activity over both precursors. The composite obtained maximal degradation of 98 % (at pH=11) and 97 % (at pH=9) for MB and MG, respectively. The enhanced photo degradation activity of Co3O4-Bi2O3 can be due to larger visible light absorption, increased surface area, and decreased h+/e− recombination. The reactive species trapping study was performed to determine the importance of superoxide and hydroxyl radicals during photo degradation. Dye degradation was governed by a pseudo-first-order kinetic model. The reusability and stability of Co3O4-Bi2O3 were confirmed by utilizing the same material for five consecutive runs with both MB and MG dyes. Mass spectra analysis provided insights into the successful degradation of dyes, elucidating intermediate products. The synthesized Co3O4-Bi2O3 nanocomposite offers unrivalled advantages in terms of structural and optical properties, superior photocatalytic activity, and remarkable stability, making it a promising candidate for efficient dye degradation applications without the formation of toxic by-products.



URL: https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/slct.202400217

SCHOLARLY PUBLICATIONS
School of Applied Sciences
KIIT Deemed to be University

Journal Name: International Journal of System Assurance Engineering and Management **IF: 2**

Title: A fuzzy mathematical model to solve multi-objective trapezoidal fuzzy fractional programming problems

Author: Maharana S., Nayak S.

Details: April 2024

Abstract: Decision making problems with ambiguous data often arise in numerous practical fields which can be formulated as optimization models in fuzzy environment. This paper develops a new mathematical model using a proposed methodology to efficiently solve a multi-objective linear fuzzy fractional programming problem in trapezoidal fuzzy environment and generate a set of nondominated solutions. The concept of fuzzy cuts with different degrees of satisfaction is implemented which transforms the fuzzy optimization into an equivalent interval valued optimization. Subsequently, interval valued linear functions approximate the fuzzy valued fractional functions based on Taylor's series expansion. Finally, a proposed concept using weighting sum approach with varying weight vectors is utilized to design a mathematical model which generates the set of nondominated solutions. Two numerical examples including an existing problem and an additional practical problem in the field of production are solved for the illustration of the proposed model. The results of the numerical problems are comparatively discussed with graphical analysis to justify the feasibility and applicability of the proposed model.

URL: https://link.springer.com/article/10.1007/s13198-024-02298-8