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NATIONAL INSTITUTE OF TECHNOLOGY, UTTARAKHAND

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आज़ादी का अमृत महोत्सव

NCRAPS 2023

5th National Conference on Recent Advancement in Physical Sciences (NCRAPS-2023)

(DECEMBER 19-20, 2023)

HYBRID MODE

Jointly Organized by :

Department of Chemistry, Department of Physics & Department of Mathematics

NATIONAL INSTITUTE OF TECHNOLOGY, UTTARAKHAND

PATRON

Prof. Lalit Kumar Awasthi,
Director, NIT Uttarakhand

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उत्तराखण्ड
National Institute of Technology,
Uttarakhand

MESSAGE

National Institute of Technology Uttarakhand (NITUK) is honored to host the fifth "*National Conference on Recent Advancements in Physical Sciences*" (NCRAPS-2023) being jointly organized by the Department of Chemistry, Physics and Mathematics, NITUK during December 19-20, 2023 through hybrid mode. NCRAPS-2023 is the fifth consecutive version and very unique platform to promote the advancements in the physical sciences and engineering. Let me congratulate to organizing committees of NCRAPS-2023 for carrying out the series of NCRAPS every year. It is appreciable that last four versions of the conference have been a huge success. The selected papers of first two versions of conferences were published in Journal of Physics Conference series, IOP Publishing whereas the papers for the latter two versions of NCRAPS are published in AIP Conference Proceeding, AIP Publishing.

I am happy to know that exceeding 100 extended abstract/papers have been received and followed by peer reviewing more than 90 abstract/papers have been selected based on quality of works and good standard of the conference which will be presented in NCRAPS-2023 and the selected papers will be published in *AIP Conference Proceedings.* I wish to congratulate team NITUK for their quality efforts which enabled excellent participation.

On behalf of NITUK family, I extend my warm welcome to all the eminent guests, speakers, delegates and participants. I wish a grand success to NCRAPS-2023 in its endeavor of promoting the advancement in Physical Sciences.

Prof. Lalit Kumar Awasthi,
Director, NIT Uttarakhand

CONTENTS

PREFACE

The 5th National Conference on "*Recent Advancements in Physical Sciences*" (**NCRAPS-2023**) is being jointly organized by Departments of Chemistry, Physics and Mathematics, NIT Uttarakhand during December 19-20, 2023 *via* hybrid mode. The 1st version of NCRAPS was conducted on December 19-20, 2019 at satellite campus, MNIT Jaipur while 2nd, 3rd and 4th versions of the conference were organized during December 19-20, 2020, December 19-20, 2021 and December 19-20, 2022 *via* virtual mode. The past four versions of NCRAPS have been a grand success. The selected papers of first two versions of conferences were published in J. Physics Conference series, IOP Publishing whereas the papers for the latter two versions of NCRAPS have been published in AIP Conference Proceeding, AIP Publishing.

NCRAPS-2023 has been deliberated to showcase the research accomplishments and to enrich the educational experience in Physical Sciences and Engineering with focus on emerging multidisciplinary research areas *viz*. Biophysics, Nanotechnology & Materials Science, Fluid Mechanics & Biomechanics, Applied Mathematics & Analysis, Optical Sensors/Devices, Modelling and Simulation of Molecules as well as Advanced Materials, etc. The details of the conference can be accessed at https://ncraps23.nituk.ac.in. **NCRAPS-2023** aims to comprise various most recent and innovative results from physical sciences and engineering that will be discussed by the learned experts from each subject to bring interdisciplinary junctions amongst the participants. We feel ecstatic to witness that the conference has received a huge response from participants all across the country along with their valuable views on diverse issues.

The conference organizing committee has invited 02 plenary speakers, 03 keynote speakers and 12 other invited experts to deliver their lectures. The 02 plenary speakers and 03 keynote speakers shall cover the different areas of the conference i.e. **1.** Dr. Kaustabh Kumar Maiti (CSIR-NIIST, Trivandrum) will be talking on *"Advancement of Surface-Enhanced Raman Spectroscopy in Cancer Management"*, **2.** Prof. S. K. Tomar (VC JC Bose University, Faridabad) will be discussing about "*Rayleigh-Type Surface Waves In Nonlocal Micropolar Thermoelastic Half-Space Containing Void Pores*", **3.** Prof. PVSN Murthy (IIT Kharagpur) will be talking on *"Solute dispersion in a non-Newtonian (Ellis) fluid flow in a circular tube*" **4.** Prof. G. P. Raja Sekhar (IIT Kharagpur) will speak on *"Physical Insights On Hydrodynamics of Swimming Micro-Organisms"*, **5.** Prof. Manish K. Kasayap (JNU, New Delhi) will deliver a talk on *"Investigation Of Novel 2d Magnetic Van Der Waals Heterostructures; A Dry Lab Approach" alongwith 12 invited lectures viz. Prof. Anantharaman (IIT Kanpur), Prof. Manoj Antil (Baba Mastnath University, Rohtak), Prof. Praveen Bhatt (Baba Mastnath University, Rohtak), Dr. R. Sivaraj (NIT Jalandhar), Dr. Hanumesh Vaidya (Vijayanagara Sri Krishnadevaraya University, Ballari), Dr. Ashok Kumar (HNB Garhwal University), Dr. Saral Kumar Gupta (Banasthali University), Dr. Amit Pratap Singh (NIT Delhi), Dr. Satyananda Panda (NIT Calicut), Dr. Jay Singh (BHU, Varanasi), Dr. Bhaskaran (HNB Garhwal University, Srinagar) and Dr. Nidhi Tyagi (Amity University Punjab) shall cover a vide interdisciplinary areas.*

The conference has received a total number of 120 extended abstract/paper submissions which were peer reviewed and around 110 abstracts have been accepted for oral presentation. The abstracts have been split between three technical sessions in conference broad subject areas of Chemistry, Mathematics, Physics and Engineering. The participants across the country enabled the **NCRAPS-2023** of a national scope. The two-day conference with nearly 110 oral presentations shall create the heart of the conference and provided ample opportunity for discussion during the conference. The organizing committee will stringently examine the best research accomplishments out of 110 shortlisted abstracts and the work selected in second round will be processed to the full paper publication in Institute of Physics (IOP) as conference proceedings.

As conference chairs/secretaries, we have many people to thank and would like to put the appreciation of their contributions on record. In this regard, the largest burden fell upon the experienced shoulders of Plenary Speakers, Keynote Speakers, Invited Speakers, Session Chairs and our technical reviewers along with substantial assistance received from active student volunteers. Therefore, these are the foremost in the list of people to be thanked.

We also thank to all the authors who have submitted their papers to this conference. It was both a privilege and a great responsibility to oversee the reviewing of submitted papers. We sincerely thank to our Chief Guest, the Director and Patron of the conference, Prof. Lalit Kumar Awasthi and Guest of Honor, Dr. Kaustabh Kumar Maiti, for their motivation, encouragement, financial support to the conference and helping us to make this event successful.

Thank You
Conference Chair(s)/Secretaries
NCRAPS-2023

NATIONAL ADVISORY COMMITTEE

1 Dr. G P Raja Sekhar, Indian Institute of Technology Kharagpur
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TECHNICAL PROGRAM

5th National Conference on Recent Advancement in Physical Sciences (NCRAPS-2023)
PROGRAM SCHEDULE
(DAY 01; DECEMBER 19, 2023)

Time /Session	Event				
10:00 AM-10:35 AM	INAUGURATION link: https://meet.google.com/stg-mzvk-rpm				
SESSION A	Lecture Name	Speakers	Title of the Lecture		Session Chair
10:35 AM-11:20 AM	Plenary Address	Dr. Kaustabh Kumar Maiti	Advancement of Surface-Enhanced Raman Spectroscopy in Cancer Management		Dr. Rakesh Kumar Mishra
11:20 AM-11:30 AM	High Tea				
SESSION B	Session B1, Session Chair: Dr. Avinash Chaturvedi, Dr. Ashish Pathak https://meet.google.com/wib-vmrw-scc			Session B2, Session Chair: Prof. Ram Sagar Mishra, Prof. M. D. Pandey https://meet.google.com/jcx-ibxp-qwt	
	Lecture Name	Speakers	Title of the Lecture	Speakers	Title of the Lecture
11:30 AM-11:50 AM	Invited Lecture	Dr. R. Sivaraj	Convective Flows of Nanofluids In Cavities And Applications	Dr. Nidhi Naithani	Asymmetric Thiazolo[5,4-D]thiazole Derivative as solvFluorochromic Dye for Acid Vapour Sensing
11:50 AM-12:10 PM		Dr. Ashok Kumar	Non-Darcy Mixed Convective Flow In Vertical Pipe And Its Stability	Prof. G. Anantharaman	Multifunctional MOFs for Water harvesting, Sensing and Catalysis
12:10 PM-12:30 PM		Dr. Satyananda Panda	Process Paramater Identification In Thin Film Flows Driven By A Stretching Surface	Dr. Amit Pratap Singh	Post-Functionalized Ordered Mesoporous Materials: Application In Catalysis And Sensing
12:30 PM-12:50 PM				Dr. Saral Kumar Gupta	Micro-analysis in Science and Engineering: Field Emission Scanning Electron Microscopy (FESEM)
12:50 PM-02:00 PM	LUNCH				
SESSION C	TECHNICAL PRESENTATIONS				
	Session C1 https://meet.google.com/wib-vmrw-scc		Session C2 https://meet.google.com/jcx-ibxp-qwt		Session C3 https://meet.google.com/ucv-nocn-mzi
02:00 PM-04:30 PM	Session Chairs Dr. Ganesh Chandra Nandi, Dr. Mukesh Choudhary		Session Chairs Dr. Praveen Gupta, Dr. Aanand		Session Chairs Dr. Amit Singh, Dr. Rajesh Prasad
	CHEM- 01, 02, 04, 05, 06, 07, 08,10, 11, 12, 13, 14, 15, 16, 17, 18		MATH-01, 02, 03, 04, 05, 06, 07, 09, 10, 11, 12, 13, 14, 15, 40, 41		MATH-08, 16, 17, 18, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32
SESSION D	link: https://meet.google.com/stg-mzvk-rpm				
	Lecture Name	Speakers	Title of the lecture		Session Chair
04:30 PM-05:10 PM	Keynote Address	Prof. PVSN Murthy	Solute dispersion in a non-Newtonian (Ellis) fluid flow in a circular tube		Dr. Alok Kumar Pandey
05:10 PM-05:50 PM		Prof. G. P. Raja Sekhar	Physical Insights On Hydrodynamics Of Swimming Micro-Organisms		
05:50 PM-06:10 PM	Invited Lecture	Dr. Juginder Kumar	Stability analysis of double-diffusive electro-convection in couple stress anisotropic fluid-saturated rotating porous layer		Dr. Dharmendra Tripathi

5th National Conference on Recent Advancement in Physical Sciences (NCRAPS-2023)
PROGRAM SCHEDULE
(DAY 02; DECEMBER 20,2023)

Time (Hrs.)	Event				
SESSION E 10:00 AM-11:25AM	link: https://meet.google.com/stg-mzvk-rpm				
	Lecture Name	Speaker	Title of the lecture		Session Chair
10:00 AM- 10:40 AM	Keynote Address	Prof. Manish K. Kasayap	Investigation Of Novel 2d Magnetic Van Der Waals Heterostructures; A Dry Lab Approach		Dr. Jagrati Sahariya
SESSION F	SESSION F1, Session Chair: Dr. Jagrati Sahariya, Dr. Kusum Sharma https://meet.google.com/wib-vmrw-scc			SESSION F2, Session Chair: Dr. Rakesh Kumar Mishra, Dr. R P Pandey https://meet.google.com/jcx-ibxp-qwt	
	Lecture Name	Speaker	Title of the lecture	Speaker	Title of the lecture
10:40 AM-11:00 AM	Invited Lecture	Prof. Praveen Bhatt	Introduction of Vedic Atomic Physics	Dr. Bhaskaran	Experimental and Quantum Chemical Studies of Ionic Liquids as Green Corrosion Inhibitors
11:00 AM-11:20 AM		Prof. Manoj Antil	Golden Ratio and Applications of Mathematics In Real Life	Dr. Jay Singh	Potential of Nanomaterials Revolutionizing Biosensors in Clinical Applications" along with a short biography
11:20 AM-11:30 AM	Tea Break				
SESSION G	TECHNICAL PRESENTATIONS				
	Session G1 https://meet.google.com/wib-vmrw-scc		Session G2 https://meet.google.com/jcx-ibxp-qwt		Session G3 https://meet.google.com/ucv-nocn-mzi
11:30 AM - 01:00 PM	Session Chairs: Dr. Manoj Mishra, Prof. Praveen Bhatt		Session Chairs: Dr. Sudesh Kumar Prajapati, Dr. Anand Sharma		Session Chairs: Prof. Manoj Kumar Antil, Dr. Akmal Hussain
	PHY-01, 02, 03, 04, 07, 09, 10, 11, 12		ENG-01, 02, 03, 04, 05, 06, 07, 08, 09		MATH- 21, 33, 34, 35, 36, 37, 38, 39, 42, 43
01:00 PM-02:00 PM	LUNCH				
SESSION H	TECHNICAL PRESENTATIONS				
	Session H1 https://meet.google.com/wib-vmrw-scc		Session H2 https://meet.google.com/jcx-ibxp-qwt		Session H3 https://meet.google.com/ucv-nocn-mzi
02:00 PM-03:40 PM	Session Chairs Dr. Jay Singh, Dr. Brajraj Singh		Session Chairs Dr. Manisha Gupta, Dr. Piyush Sinha		Session Chairs Dr. Ravindra Pandey, Dr. Harshita Sachdeva
	PHY-05, 06, 08, 13, 14, 15, 16, 17, 18, 19, 26, 27, 28, 33		PHY-20, 21, 22, 23, 24, 25, 29, 30, 31, 32, 34, 35, 36, 37		CHY-03, 09, 19, 20, 21, 22
SESSION I	link: https://meet.google.com/stg-mzvk-rpm				
	Lecture Name	Speaker	Title of the lecture		Session Chair
3:40 PM-04:25 PM	Plenary Address	Prof. S. K. Tomar	Rayleigh-Type Surface Waves In Nonlocal Micropolar Thermoelastic Half-Space Containing Void Pores		Dr. Rajshekkhar Chaudhary
04:30 PM-5:00 PM	Valedictory Function				

PLENARY LECTURES

Dr Kaustabh Kumar Maiti

Sr. Principal Scientist, CSTD, Organic Chemistry Section, CSIR-National Institute of Interdisciplinary Science and Technology (NIIST), Industrial Estate P.O., Pappanamcode, Trivandrum 695019, India, E-mail: kkmaiti@niist.res.in

Kaustabh Kumar Maiti studied Chemistry at the University of Calcutta, and received his B.Sc. in 1991, M.Sc. in 1993, and Ph.D. in 2001. He started his professional journey in leading pharmaceutical R&D in India (Alembic Ltd and Sun Pharmaceuticals Industries Ltd). Subsequently, he did postdoctoral research at POSTECH, South Korea, Complex Carbohydrate Research Centre (CCRC), University of Georgia, USA, and later engaged as a Research Scientist at Singapore Bioimaging Consortium (SBIC), A*STAR, Singapore. In 2012, he was appointed as a Senior Scientist at CSIR-NIIST, Thiruvananthapuram, India, and subsequently promoted to Sr. Principal Scientist and Professor, AcSIR, in April 2020. His current research focuses on molecular diagnostics based on the SERS modality, Targeted drug delivery system, and the development of new phytochemical entities from natural products. He has published nearly 100 scientific papers and filed 14 patents so far.

ADVANCEMENT OF SURFACE-ENHANCED RAMAN SPECTROSCOPY IN CANCER MANAGEMENT

ABSTRACT

Surface-enhanced Raman scattering (SERS) was investigated as a highly sensitive spectroscopic modality where the signal intensity of molecular vibration is enhanced up to 10^8 –10^{14} folds compared to simple Raman spectra. Multiplexing capability of Raman fingerprints, molecular specificity, high sensitivity, and capability to fish out complex biological compositions at the molecular level augmented SERS as a potential diagnostic modality in biology and medicine. While assessing all the merits of classical Raman spectroscopy, SERS provides a more sensitive and selective detection and quantification platform. Non-invasive, chemically specific, and spatially resolved analysis facilitates the exploration of SERS-based nanoprobes in cancer management i.e., diagnostic and theranostic applications with improved clinical outcomes compared to the currently available so-called state-of-the-art technologies. Adequate knowledge of the mechanism and properties of SERS-based nanoparticle probes is inevitable in utilizing the full potential of this modality for biomedical applications. The safety and efficiency of metal nanoparticles and Raman reporters must be critically evaluated for the successful translation of SERS into clinics. Exploration of a sensitive diagnostic nanoprobe, especially with the aim of point-of-care treatment, is another challenging task for early and accurate detection of cancer biomarkers, which facilitates efficacious therapy by reducing mortality and morbidity. Recently, we have fabricated programmable nanoparticles that feature a label-free SERS-based detection and grading of cervical cancer. We also developed SERS-nanoprobes which are conjugated with target-specific antibodies for the multiplex detection of breast and lung cancer biomarkers, which furnished a semi-quantitative evaluation of biomarkers through both modalities. In another approach, we have developed a gold nanorod (GNR)--based therapeutic nanoprobe for targeting metastatic melanoma by combining PTT, PDT, and chemotherapy along with SERS imaging for better treatment and an effective follow-up therapeutic response. We believe that this proof-of-concept will provide a blueprint for the diagnosis and differential staging of cancer into various histological subtypes based on the differential

expression of the antigens. Recently, we are progressing SERS with artificial intelligence (AI) screening/prevalence of multiple cancers from clinical blood samples. Therefore, SERS techniques are being explored as an upcoming molecular diagnostic modality, ranging from simple detection platforms to complicated clinical applications.

References

1. *K.K Maiti et.al.*, **Nano Today**, 2012; 7, 85-93
2. *A N Ramya & K.K Maiti et.al*., **Nanomedicine**., 2015;10(4), 561–571
3. *G Saranya and K. K. Maiti et.al.*, **ACS Applied Materials and Interfaces**, 2018, 10 (45), pp 38807–38818
4. *P. T. Sujai, & K K Maiti** **ACS Applied Biomaterials**, 2019, 2 (1), pp 588–600
5. *M. M. Joseph & K K Maiti et.al.*, **Biomaterials,** 2018, 140-181.

Prof. S. K. TOMAR

Department of Mathematics, Panjab University, Chandigarh

Dr. Tomar is a Professor of Mathematics at Panjab University, Chandigarh. Presently, he is the Vice Chancellor of J. C. Bose University of Science and Technology, YMCA, Faridabad, Haryana (Formerly known as YMCA University of Science and Technology). Prior to joining this university, he remained at the positions of Dean of University Instruction, Dean Research, Dean Student Welfare and Director, Human Resource Development Center at Panjab University, Chandigarh. He is also nominated member of the Senate of Panjab University and elected Vice-President of All India Association of Vice-Chancellors and Academicians, New Delhi. His current areas of research include Applied Mathematics, Continuum Mechanics and Numerical Methods. He is also an elected fellow of National Academy of Science, India (NASI) and is a recipient of P L Bhatnagar Award lecture of Indian Mathematical Society. He is a widely travelled person and has visited several countries under research collaborations. He has also been honored with the prestigious IAPS Fellowship Award for his exceptional contributions to the field of Mathematics by the International Academy of Physical Sciences (IAPS), Prayagraj. In order to sensitize science education among the children and to all other corners of the society, he initiated Chandigarh Vigyan Parishad in the year 2016 which is a part of Vigyan Bharti at national level. Prof. Tomar has 129 publications in the journals of international repute and delivered over 151 lectures in the country and abroad on the different topics of his research. He has guided 9 students for their Ph. D. degree. He is widely travelled person and has visited several countries under research collaborations.

RAYLEIGH-TYPE SURFACE WAVES IN NONLOCAL MICROPOLAR THERMOELASTIC HALF-SPACE CONTAINING VOID PORES

ABSTRACT

Propagation of Rayleigh-type surface waves is investigated in a half-space composed of nonlocal micropolar thermoelastic material containing void pores. Dispersion relation is derived for a mechanically stress-free and thermally insulated boundary surface of the half-space. The dispersive behavior of Rayleigh-type waves is found to be different in low and high frequency ranges due to the presence of voids and nonlocality. The particle motion during the propagation of waves is found to follow elliptical path. Numerical computations are performed for a particular medium to analyze the characteristics of propagating Rayleigh-type waves in detail. The computational results are displayed graphically and explained. Comparison between the phase speed and corresponding attenuation coefficient in various reduced half-spaces is also shown graphically. The effect of various parameters on the characteristics of waves is also studied.

KEY NOTE LECTURES

Prof. P.V.S.N. Murthy

Department of Mathematics, Indian Institute of Technology, Kharagpur

P. V. S. N. Murthy, currently working as a Professor in the Department of Mathematics, Indian Institute of Technology Kharagpur. He completed his Ph.D. in Fluid mechanics from Department of Mathematics, Indian Institute of Technology Kanpur. He has served as the Member, National Coordinating Team, SPARC, Ministry of Education, Government of India during 2020-2023 and he is the Local Institute Coordinator, SPARC, IIT Kharagpur. He has also ser ved as the secretary of the Indian Society for Theoretical and Applied Mechanics (ISTAM) for two terms (2006-2009; 2012-2015). He was the President of the Indian Society for Theoretical and Applied Mechanics (ISTAM) for the session 2018-2019. He was a reviewer, Shanti Swarup Bhatnagar prize for Science and Technology, CSIR, HRDG, India. Also, evaluated several projects for the international funding agencies such as Indo French IFCPAR/CEFIPRA project, Austrian Science Fund and National Research Foundation, South Africa. Visited the School of Mechanical Engineering, Fluid Dynamics Laboratory, Institute of Nature and Environmental Technology, Kanazawa University, JAPAN in July 2015, the School of Naval Architecture, Ocean and Civil Engineering, Shanghai Jiaotong University (SJTU), CHINA in July 2015, Department of Mathematics, Statistics and Computer Science, University of Kwazulu-Natal, Pietermaritzburg, South Africa, in both July and December 2012, the Department of Mechanical Engineering, Hong Kong University, Hong Kong, June 2007, Florida Institute of Technology, Florida, USA, June 2004 and Pohang University of Science and Technology (POSTEC) Seoul, South Korea, February 2003. He has more than 120 research papers in the leading journals such as Journal of Fluid Mechanics, Proceedings of the Royal Society, Physics of Fluids, International Journal of Heat and Mass Transfer, Transactions of ASME-Journal of Heat Transfer, Transport in Porous Media, etc.

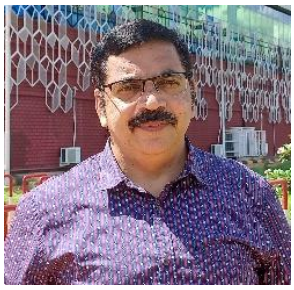
SOLUTE DISPERSION IN A NON-NEWTONIAN (ELLIS) FLUID FLOW IN A CIRCULAR TUBE

ABSTRACT

The unsteady dispersion of solute in a pulsatile Ellis fluid flow in a circular tube is considered to investigate the role of skewness and kurtosis on the concentration distribution using the Aris method of moments. Ellis fluid is a 2 parameter non-Newtonian flow model consisting of the shear stress at which apparent viscosity has dropped to half its zero shear value $\tau_{1/2}$, degree of shear thinning behaviour a. The flow is taken to be pulsating fluid flow. Due to the pressure pulsation, a non-dimensional number called the Womersley frequency parameter α^2 arises in the mathematical modelling. Firstly, the time-dependent velocity profile is obtained analytically considering this parameter (α^2 < 1) as the perturbation parameter. Also, an analytical solution for the concentration distribution in the circular tube is obtained for the unsteady and pulsatile flow for α << 1. The solute dispersion is understood through the standard exchange, convection, and dispersion coefficients which account for estimating the axial mean concentration of the solute. Along with the variations in the mean concentration distribution of the solute in the tube, significant variations in the skewness and kurtosis coefficients against various values of the flow governing parameters, such as the shear stress at which apparent viscosity has dropped to half its zero shear value $\tau_{1/2}$, degree of shear thinning behaviour a, the wall absorption parameter β, the Womersley frequency parameter α, and the amplitude of the fluctuating pressure component e are presented graphically. We explore in detail all the time variations of these five moments versus flow-regulating factors. As a result of the inclusion of the skewness and kurtosis, a deflection and reduction in the axial mean concentration distribution of a solute in the circular tube is noticed. Also, the significance of the skewness and kurtosis is analysed that indicated a deviation from Gaussianity for small time. This also lead to a decrease in the peak of the mean concentration profile at a initial regions of the injection of the solute into the tube. The dispersion process in oxygenators and the cardiovascular system can be studied using this dispersion model in non-Newtonian pulsatile flow.

Prof. G P Raja Sekhar

Department of Mathematics, Indian Institute of Technology, Kharagpur



Prof. Raja Sekhar has more than 25 years of teaching and Research. He has been recipient of several prestigious Awards and fellowship, to name a few are, INSA (Indian National Science Academy) Young Scientist Award, JSPS (Japan Society for Promotion of Science) Fellowship, Alexander von Humboldt Fellowship. Prof. Raja Sekhar is a fellow of Fellow of National Academy of Sciences, Prayagraj, Andhra Pradesh Akademi of Sciences, West Bengal Academy of Science and Technology. He was awarded the JBS Gold Medal by *Indian Academy of Mathematical Modeling and Simulation in the year 2018. Recently, Prof. Raja Sekhar was awarded the Mathematician of the year by Ponnala Trust Instituted at National Institute of Technology Warangal. Prof. Raja Sekhar has held several administrative positions at IIT Kharagpur. He held the position of Organizing Chairman, GATE 2014; Chairman, Career Development Center,* Convenor, All IIT Placement Committee (AIPC), Dean (Planning and Coordination), *Dean of Faculty of Sciences at IIT Kharagpur. Prof. Raja Sekhar has visited several countries for research collaboration. To name a few, UK, Poland, Germany, Romania, Japan etc. He has more than 120 research articles published in reputed International journals and supervised 14 Ph.Ds. At present he is serving as Associate Editor of Journal of Engineering Mathematics; Managing Editor of Diff. Eqns. And Dyn. Systems; Member, Editorial Board, Journal of Indian Math. Soc.*

PHYSICAL INSIGHTS ON HYDRODYNAMICS OF SWIMMING MICRO-ORGANISMS

ABSTRACT

Microorganisms follow various strategies to swim in a viscous medium. From the modelling perspective, theoretical works concentrated on the active systems. On the other hand, droplets are also used in different microfluidic devices involving encapsulation of biological cells. In order to understand the swimming of ciliated microorganisms, this talk briefs our study on low Reynolds number locomotion of a spherical viscous droplet under the combined influence of an inhomogeneous surfactant and non-isothermal temperature fields. Then we move on to rigid slip-stick swimmer where the propulsive slip-velocity is concentrated around annular patch which imitates the distinctive surface activity of the microorganisms.

Prof. Manish K. Kashyap

Renewable Energy Laboratory, School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110067, India

Prof. Manish K. Kashyap is a Professor in the School of physical Sciences of the Jawaharlal Nehru University, India. Before this, he has worked as **Associate and Assistant Professor of Physics** (Nov 2007 – Dec 2020) at Department of Physics, Kurukshetra University, Kurukshetra. He completed his **Ph.D.** degree from **IIT Roorkee** under the supervision of **Prof. Sushil Auluck** and **Prof. Tashi Nautiyal** and one Post-Doctorate from Ames Laboratory, USA during August 2016 to July 2017 **under** the supervision of **Prof. Bruce Harmon on UGC-Raman Fellowship.** His current areas of research includes Theoretical Condensed Matter Physics, Materials Science, Plasma Physics, Accelerator Physics, [**Research Interests:** 2D materials/heterostructures for magnetism and photovoltaics, Hybrid Halide Perovskites for solar cells, Rare earth/Transition Metal based materials for permanent magnets, DMS and Heusler Alloys for Spintronics, Plasma instabilities in ECR ion sources, Interaction of heavy ion with plasma, Density functional theory (DFT) Simulations]. He has a large volume of impactful publications (> 100) in various International Journals and conference proceedings. He has been awarded **2 times** by **Gold Medalists** in B.Sc. and M.Sc. Physics degrees for being university topper at Kurukshetra University, Kurukshetra in 2001 and 2003, respectively. He has guided 8 Ph.D. students and 1 postdoc till date and Currently 7 Ph.D. students are working under the guidance. He has successfully **c**ompleted 3 research projects from UGC, DST-SERB(EMR), DST Haryana, and 1 project from IKS Scheme, AICTE is still going on with him,

INVESTIGATION OF NOVEL 2D MAGNETIC VAN DER WAALS HETEROSTRUCTURES; A DRY LAB APPROACH

ABSTRACT

2D van der Waals heterostructures are of prime interest on both experimental and theoretical fronts in present scenario due to various technological applications. These heterostructures consist of the layers of different 2D materials and are arranged in a same way as Lego bricks are stacked in a specific order. The grapheme based heterostructures in which one layer is represented by graphene and the second layer to any other 2D-material is the latest attention in this area. The density functional theory (DFT) is a computational method based on the principles of quantum mechanics which can predict the ground state properties of existing as well as unknown materials. In this talk, the basic principle of DFT and its capability for predicting the electronic band structure of the materials will be addressed. The recent DFT results of our research group for novel 2D magnetic van der Waals heterostructures having one layer made up of graphene will also be explained.

INVITED LECTURES

Dr. R. Sivaraj

Department of Mathematics, Dr B R Ambedkar National Institute of Technology Jalandhar, Punjab, India

Dr R Sivaraj has more than 10 years of teaching and research experience and presently, he is working as an Associate Professor in the Department of Mathematics, Dr B R Ambedkar National Institute of Technology, Jalandhar, Punjab, India. He worked as a Postdoctoral Fellow in the Department of Mathematics, United Arab Emirates University, United Arab Emirates. He worked at Guangdong University of Technology, Guangzhou, China under a Faculty Exchange Programme. He has received the Royal Society Commonwealth Science Conference Fellow on Grant from Royal Society of London. He has received a Travel Grant form CSIR India to participate in a conference at Turkey. He is the Joint Secretary for the Academia for Advanced Research in Mathematics Society (AARM). He has published 60 manuscripts which includes several Q1/Q2 journals, SCI, SCIE, and SCOPUS journals. He has guided 4 PhD scholars. He has received the VIT research award for 9 consecutive years. His H-Index is 22 with more than 1300 citations as per SCOPUS. He has visited several universities/institutes around the world to deliver invited talks. He has served as a Guest Editor for several journals and book series. He has published a book in Chapman and Hall/CRC, New York. He has organized several international conferences and workshops to promote research in India and UAE. He has evaluated several PhD theses and served in various academic committees at various institutes.

CONVECTIVE FLOWS OF NANOFLUIDS IN CAVITIES AND APPLICATIONS

ABSTRACT

Natural convective flow occurs due to the combined effects of thermal expansion and buoyancy. Natural convection finds applications in nuclear reactors, stellar physics, solar ponds, cooling of molten metals, and fluid flows around shrouded heat-dissipation fins. The nanofluids are prepared by suspending the nano-sized particles into base-fluids such as water, ethylene glycol, oil. The nanoparticles are synthesized from metals/oxides/carbides/carbon nanotubes. Nanofluids are very useful in various applications including heat exchanger, domestic refrigerator, vehicle thermal management hybrid-powered engines microelectronics, and pharmaceutical processes. The convective flows of nanofluids in cavities is widely used to analyse the fluid flow and heat transfer in various engineering and industrial situations. Now-a-days, the accuracy of the results which are obtained using CFD techniques is highly increased. The impact of all the controlling parameters of the physical problems can be thoroughly analysed in various combinations and so the CFD techniques reduces the number of trails to set experiments and get the optimum results as well as it saves time, cost, and efforts. With this motivation, this talk showcases some theoretical and experimental studies on convective flows of nanofluids in cavities and applications.

Dr. Ashok kumar

Department of Mathematics, H. N. B. Garhwal University (A Central University) Srinagar

Dr. Ashok Kumar is a Associate Professor in the Mathematics Department of the H. N. B. Garhwal University (A Central University) Srinagar, India. He completed his M.Sc. & Ph.D. from the Department of Mathematics, IIT Roorkee. He has more than 12 year teaching and research experiences. He worked as an assistant professor in Government College of Uttar Pradesh and NIT Jalandhar. He is working in the field of Computational Fluid Dynamics and Numerical Solution of ODE & PDE. He has completed major and minor projects of SERB and UGC respectively. A project under MATRICS scheme of SERB is going on. Five students completed their Ph.D. under his supervision and 05 students are pursuing their Ph.D. under his guidance right now.

NON-DARCY MIXED CONVECTIVE FLOW IN VERTICAL PIPE AND ITS STABILITY

ABSTRACT

A non-isothermal flow in a linearly heated vertical pipe filled with porous medium is a fundamental and attractive problem in fluid dynamics due to its wide range of practical interests in sciences and engineering. The instability mechanism of non-isothermal flow is a field of active and ongoing research. The Darcy-Brinkman-extended model is considered here to characterize the flow in porous medium and a linear theory of hydrodynamics is used for the prediction of flow transition between laminar to turbulent. The Chebyshev spectral collocation method is used to solve numerically the set of linear disturbance equations of stability. The impact of different controlling parameters on the stability boundary and the disturbance field variables are analyzed.

Prof. Satyananda Panda

Department of Mathematics, National Institute of Technology Calicut

Dr. Satyananda Panda, currently working as a Professor in the Department of Mathematics, National Institute of Technology Calicut. He earned his Ph.D. in Industrial Mathematics from the Technical University of Kaiserslautern, Germany. His research areas include Mathematical Modeling, Fluid Mechanics, Asymptotic Analysis, and Scientific Computing. He has many publications in the reputed journals.

PROCESS PARAMATER IDENTIFICATION IN THIN FILM FLOWS DRIVEN BY A STRETCHING SURFACE

ABSTRACT

The flow of a thin liquid film over a heated stretching surface is considered. Due to a potential non-uniform temperature distribution on the stretching sheet, a temperature gradient occurs in the fluid which produces surface tension gradient at the free surface of the thin film. As a result, the free surface deforms and these deformations are advected by the flow in the stretching direction. This talk will focus on the inverse problem of reconstructing the sheet temperature distribution and the sheet stretch rate from observed free surface variations. Using the model based on lubrication approximation we show that after algebraic manipulation of a discrete form of the governing equations, it is possible to reconstruct either the unknown temperature field on the sheet and hence the resulting heat transfer or the stretching rate of the underlying surface. We illustrate the proposed methodology and test its applicability on a range of test problems.

Dr. Nidhi Naithani

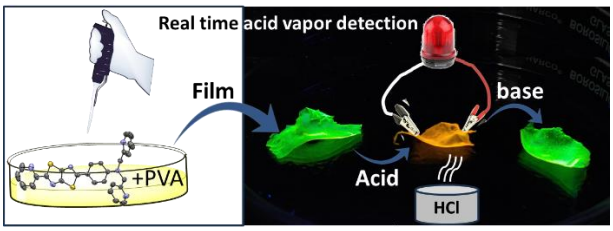
Amity School of Chemical Sciences (ASCS), Amity University Punjab

Dr. Nidhi Naithani is **c**urrently working as an Assistant Professor at Amity University Punjab, Mohali, prior to which she was working as a women scientist (WOS-A) on a DST funded project at Institute of Nano Science and Technology, Mohali and Nehru postdoctoral fellow at CSIR-National Institute for Interdisciplinary Science and Technology (NIIST), Thiruvananthapuram. She has carried out Ph. D. (Chemistry), M. Tech. (Advanced Chemical Analysis) and M.Sc (Chemistry) from Indian Institute of Technology Roorkee, Roorkee. She has several years of experience in synthesizing chromophore functionalized metal complexes, their nano/ polymeric materials and studying their *in-vitro* activity such as ROS generation and their application in sensing as well as PDT. She has published 27 research papers in peer reviewed international journal of high repute.

ASYMMETRIC THIAZOLO[5,4-D]THIAZOLE DERIVATIVE AS SOLVFLUOROCHROMIC DYE FOR ACID VAPOUR SENSING

ABSTRACT

Exposure or inhalation of strong acid, eg HCl, vapours lead to gastrointestinal complications, inflammation in the respiratory tract, failure of circulatory system ultimately leading to death. Despite these concerns, HCl is widely employed in various industries such as textile, plasma etching and semiconductor manufacturing etc and is unavoidable for various manufacturing processes. Therefore, detection and sensing of HCl gas leakage is vital to ensure the safety of the industry personnel and the entire ecosystem. Herein, the talk mainly focuses on photophysically attractive, asymmetric and multifunctional TTz derivative and its polymeric film which exhibits strong solvatofluorochromism with mega Stokes shifts and selectively detects acid vapours at very low pH. Furthermore, cost-effective electronic prototype using thin film was demonstrated to exhibit reversible visual fluorescence switching upon acid exposure which was used to fabricate a device for real-time detection of HCl vapours.



Prof. G. Anantharaman

Department of Chemistry, Indian Institute of Technology, Kanpur

Dr. Anantharaman completed Ph.D. at the University of Goettingen, Germany, under the supervision of Professor H. W. Roesky. He joined the Institute in the year 2004. Subsequently, he rose to different levels from Lecturer, Assistant Professor (2007), Associate Professor (2016), to Professor in 2021. He has served at various academic and institute levels, notably as a member and convener of the department postgraduate committee and as a member and chairman of the Senate Library Committee. Apart from these, he has been a "*Subject expert for appointment of Guest/permanent Faculty*" at Invertis University, Bareilly- UP, India, and M. M. M. University of Technology, Gorakhpur; Member of "*the expert committee for M. Sc syllabus*," "*Board of studies*", at M. M. M. University of Technology and "*Research Degree Committee (RDC)*" of Chemistry/Applied Chemistry discipline, Dr. A.P.J. Abdul Kalam Technical University. He has guided 14 Ph.D. students and published over 50 papers in peer-reviewed journals. His research interests are the Synthesis and application of molecular NHC-based main group, organometallic compounds, and multi-functional coordination polymers/metal-organic frameworks towards catalysis, sensing, and water harvesting. He has been recognized with different laurels, to name a few, "Excellence-in-Teaching Award 2022", "Commendation letters" from Director, IIT Kanpur for teaching courses in Advanced Main Group Chemistry and Inorganic Chemistry Laboratory, "Indian Chemical Society Research Excellence Award" for Oral presentation at International Seminar on "Recent Advances in Chemistry & Material Sciences (2020), and "IIT Bombay Research Paper Awards" for the years 2007 and 2011.

Multifunctional Cuboctahedral MOFs of Imidazole-Based Benzoic Acids for Water Adsorption, Sensing, and Catalysis

ABSTRACT

Coordination polymers (CPs) or Metal-organic frameworks (MOFs) have gained enormous attention due to their simplicity in preparation, structural diversity, and applications in gas adsorption, separation of small molecules, catalysis, sensing of small molecules to hazardous materials, drug delivery, nonlinear optics, proton conductivity, and other biomedical related processes. Thus, the studies on MOFs/PCPs have now been extended to address the incorporation of frameworks having multifunctional properties. The robustness of the MOFs against hydro- and thermal stability under different pH solutions without losing their crystallinity and porosity is an essential criterion for the above potential applications. In this talk, the CPs/MOFs derived from imidazole-carboxylic acids, their robust nature in aqueous solution, and their applications towards sensing/remediation of hazardous materials and catalysis will be presented.

Prof. Amit Pratap Singh

Department of Applied Sciences, National Institute of Technology, Delhi

Dr. Singh is an Associate Professor and head, Department of Applied Sciences National Institute of Technology Delhi, India. Before joining NIT Delhi, he worked as an INSPIRE Faculty at the Department of Chemistry, IIT Roorkee. He was associated with the Department of Chemistry, Georg August University, Goettingen, Germany, during the year 2011-13 as a postdoctoral fellow. He was a recipient of the KSKRA ward in the year 2014, along with other national and international awards. His current research areas are the Design and synthesis of new porous materials with metal skeleton and their application in catalysis, chemical technology, host-guest chemistry (molecular adsorption and molecular recognition), and electrical, optical, and magnetic properties. He has published over fifty publications in top national and international journals/conferences with high citations. He has significantly contributed to the institutional development by serving as Dean Academic and Dean R & C at NIT Delhi.

POST-FUNCTIONALIZED ORDERED MESOPOROUS MATERIALS: APPLICATION IN CATALYSIS AND SENSING

ABSTRACT

Among many mesoporous materials, the Mobile Composition of Matter No.41 (MCM-41) is the most widely studied due to its well-defined, uniform shape and size of the pores over the micrometer length scale, which enable large organic molecules to be diffused much more quickly. Also, MCM-41 offers a high thermal and chemical robust solid matrix for the development of functionalized mesoporous materials. The post-functionalization of MCM-41 is one of the prominent ways to develop the functionalized solid mesoporous material for various applications. The present research showcases the development of MCM-41 functionalized solid mesoporous materials for catalysis and sensing applications. The catalytically important metal ions such as copper(Cu^{2+}) and palladium(Pd^{2+}) have been immobilized on MCM-41 through the functionalization method to produce solid Lewis acid catalyst Cu(II)-L-propylsilyl@MCM-41 (**MS1**) and Pd(II)-L-propylsilyl@MCM-41 (**MS2**), respectively. The solid catalyst **MS1** has been demonstrated to catalyze the aminolysis reaction, and **MS2** was used in the C-C coupling reactions. Both catalysts were used for more than ten consecutive catalytic cycles without significant loss of catalytic activity. However, functionalized MCM-41 based materials suitable for sensing applications were prepared by immobilizing boron-dipyrromethene (BODIPY) derivatives. Chemosensor BODIPY-propylsilyl@MCM-41 (**MS3**) and BODIPY-(COOH)-propylsilyl@MCM-41 (MS4) were synthesized and used for the efficient detection and removal of heavy metal ions from aqueous medium. Chemosensor **MS3** shows a turn-off emission response selectively for Hg^{2+}. In contrast, the emission intensity of **MS4** was enhanced multifold in the presence of trivalent (Cr^{3+}, Al^{3+}) metal ions and was utterly quenched in the presence of divalent (Cu^{2+}, Hg^{2+}) metal ions. The limit of detection was calculated to be in the nanomolar range for all detected metal ions in a pure aqueous medium for both the chemosensors. The synthesized mesoporous materials **MS1-4** were well characterized using N_2 adsorption-desorption, powder X-ray diffraction, TEM, FT-IR, and thermal analysis.

Dr. Saral Kumar Gupta

Department of Physical Sciences, Banasthali Vidyapith

Dr. Saral Kumar Gupta is an accomplished physicist and academic professional with a Ph.D. in Applied Physics and extensive expertise in Condensed Matter Physics, Semiconductor Nanotechnology, and Photonics. Currently serving as an Associate Professor at Banasthali University, he has a rich background in both theoretical and applied research. In addition to his current role, Dr. Gupta has enriched his academic journey with a valuable postdoctoral research experience at the University of Surrey (UK), where he served as a Research Fellow. This stint has further augmented his expertise, providing him with insights into cutting-edge developments in his field. Dr. Gupta has presented his work at numerous National and International Conferences, receiving accolades such as the Top Cited Paper award from IOP Publishing (UK). His research spans organic photonic devices, Semiconductor NanoPhotonics, Nonlinear optics, and Condensed matter theory. With a passion for teaching and mentoring, he has successfully supervised and awarded 12 Ph.D. students, contributing significantly to renewable energy, carbon nanotubes, graphene-based polymer heterostructures, and organic photovoltaic applications. Proficient in a range of computer tools and languages, Dr. Gupta brings a wealth of knowledge and experience to the field, making impactful contributions to academia and research.

MICRO-ANALYSIS IN SCIENCE AND ENGINEERING: FIELD EMISSION SCANNING ELECTRON MICROSCOPY (FESEM)

ABSTRACT

Micro-analysis in Science and Engineering often relies on advanced techniques like Field Emission Scanning Electron Microscopy (FESEM) to delve into the intricate details of materials and structures. FESEM is a powerful imaging tool that utilizes a finely focused electron beam to examine surfaces at extremely high resolutions, providing invaluable insights into the microstructure and composition of various specimens. This technique plays a pivotal role in diverse fields, from materials science to biological research, allowing scientists and engineers to observe and analyze fine details with exceptional clarity. By capturing high-resolution images and enabling elemental analysis, FESEM facilitates a comprehensive understanding of materials at the micro- and nanoscale, contributing significantly to advancements in science and engineering.

Prof. Praveen Bhatt

Professor and Head, Department of Physics, Baba Mastnath University,, Rohtak, Haryana-124021

Dr. Praveen Bhatt is working as a professor and head of the department of Physics at Baba Mastnath University, Asthal Bohar, Rohtak. He has guided 23 Ph.D. students, 18 M.Phil students and more than eight students are doing research under his supervision. He has published more than 70 research papers in SCI, Scopus, UGC-CARE and peer-reviewed journals and also attended more than 87 national and international (abroad and within India)conferences. His areas of interest are Atomic, Molecular and Laser Physics & Spectroscopy. He has also been a visiting Professor and Research Scientist at Banasthali Vidyapith, Banasthali Rajasthan and various leading Universities. He has a large volume of impactful publications in top International Journals with high citations and a unique expertise in technology development for the under-served.

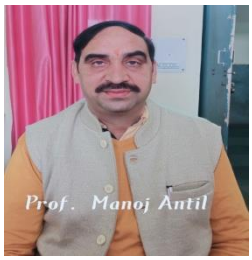
INTRODUCTION OF VEDIC ATOMIC PHYSICS

ABSTRACT

This study delves into the ancient wisdom of Maharishi Kanad and his remarkably advanced Atomic Theory, a profound yet often overlooked aspect of India's rich cultural and scientific heritage. Grounded in ancient texts like the Vedas and Upanishads, Maharishi Kanad's Atomic Theory provides a unique perspective on the fundamental nature of matter and the universe. The research aims to unearth and comprehend the intricacies of this atomic model, exploring its alignment with contemporary scientific understanding and its potential contributions to modern scientific discourse. By meticulously examining the philosophical and cosmological aspects embedded in Maharishi Kanad's teachings, this study seeks to bridge the gap between ancient knowledge and contemporary science. Additionally, the investigation evaluates the impact of the Atomic Theory on the spiritual and societal fabric of ancient India, shedding light on how this profound understanding of the cosmos influenced various aspects of daily life. Through a multidisciplinary approach that combines textual analysis, historical inquiry, and scientific comparison, this study strives to revive interest in Maharishi Kanad's contributions to atomic science and foster a deeper appreciation for the symbiosis of ancient wisdom and modern knowledge.

Prof. Manoj Antil

Department of Mathematics, Baba Mastnath University, Rohtak



Dr. Manoj Antil is working as a Professor and Head in the department of Mathematics at Baba Mastnath University, Asthal Bohar, Rohtak. He has qualified the CSIR(NET) examination in 2003. He did his Ph.D. in the area of fixed point theory from Guru Jambheshwar University of Science and technology, Hisar. He has published more than 80 papers in UGC-Care listed, Scopus indexed and SCI journals. In addition to this, he has a lot of publications with various International authors in the area of fixed point theory. He has taught the subjects like Real Analysis, Functional Analysis, Complex Analysis, Engineering Mathematics, Measure Theory and Integration. 15 students have completed their research work under the guidance of Dr. Manoj Antil. He got the research appreciation award at Lovely Professional University in 2017. He is also a potential reviewer in many indexed journals.

GOLDEN RATIO AND APPLICATIONS OF MATHEMATICS IN REAL LIFE

ABSTRACT

The Fibonacci numbers, a sequence of integers where each entry is the sum of the two entries before it, are the source of the golden ratio. Though Leonardo of Pisa is linked to this sequence, the Fibonacci numbers were originally initially developed 600 years before they were introduced to the West by the Indian mathematician Virahanka.

If the ratio of two quantities in mathematics equals the ratio of their total to the bigger of the two quantities, then the two quantities are in the golden ratio. The golden ratio is an irrational number that is equal to $(1+\sqrt{5})/2$, or approximately 1.618.

The golden ratio has a lot of real life and interesting applications in Art, Architecture, Music, Nature and Human being etc.. The golden ratio has been used in the geometric shape and design of many buildings, such as the Great Pyramids of Egypt.

In addition to this, mathematical techniques in various fields like engineering, physics, medicine, business, biology, industry, and computer science are used. Engineers use math to design structures, machines, and systems. Math enables engineers to create computer models and simulations. This helps them predict behavior, optimize designs, and test scenarios without building physical prototypes.

Dr. Jay Singh

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi- 221005, UP, India

Dr. Singh is an accomplished scientist and educator currently serving as an Assistant Professor at the Department of Chemistry, Institute of Sciences, Banaras Hindu University in Varanasi, Uttar Pradesh, India, since 2017. He obtained his Ph.D. degree in Polymer Science from Motilal Nehru National Institute of Technology in 2010, following which he completed his MSc and BSc degrees at Allahabad University, Uttar Pradesh. Throughout his career, Dr. Jay has gained extensive research experience through prestigious postdoctoral fellowships at institutions including the National Physical Laboratory in New Delhi, Chonbuk National University in South Korea, and Delhi Technological University in Delhi. His exceptional research capabilities have been recognized through notable fellowships such as the CSIR (RA), DST-Young Scientist Fellowship, and DST-INSPIRE Faculty Award. Dr. Jay's research primarily focuses on the development of nanomaterials synthesized chemically and biologically, as well as their nanobiocomposites, conducting polymers, and self-assembled monolayers. He has dedicated his efforts to the creation of clinically significant biosensors and sensors for the detection and estimation of various bioanalytes, including enzymes, antibodies, DNA, toxic chemicals, and gases. With over 125 research papers published in esteemed international journals and a remarkable citation count exceeding 4550, Dr. Jay's contributions have been widely recognized. He possesses an impressive h-index of 36, which indicates the impact and influence of his research. He has successfully undertaken numerous research projects funded by different agencies, further showcasing his ability to secure research grants. In addition to his research accomplishments, Dr. Jay has authored and edited more than 17 books and contributed over 50 book chapters for internationally renowned publishers such as Elsevier, Springer Nature, IOP, Wiley, and CRC. He has also taken on the responsibility of handling special issues for esteemed journals including Elsevier, Wiley, Springer, MDPI, and Frontiers. Currently, Dr. Jay's active research revolves around the fabrication of sustainable metal oxide-based biosensors for applications in clinical diagnosis, food packaging, drug delivery, and tissue engineering. His work has significantly contributed to the understanding of interfacial charge transfer processes and the sensing capabilities of metal nanoparticles. Dr. Jay Singh's extensive research contributions, publication record, and academic pursuits have established him as a highly respected scientist in the field of chemistry and nanomaterials. His dedication to advancing the field and his commitment to creating innovative biosensors and sensors for various applications continue to make a significant impact on the scientific community and society.

POTENTIAL OF NANOMATERIALS REVOLUTIONIZING BIOSENSORS IN CLINICAL APPLICATIONS

ABSTRACT

The most common application of nanotechnology for sensors in biomedical research is the use of nanomaterials to assist the standard enzymatic electrochemical detection of bioanalyte. The incorporation of nanomaterials into these sensors offers a variety of advantages including increased surface area, more efficient electron transfer from enzyme to electrode and the ability to include additional catalytic steps. The performance of a nanostructured metal oxide-based biosensor can be enhanced by tailoring the properties of the metal oxide–biomolecule interface through engineering of morphology, particle size, effective surface area, functionality, and adsorption capability and electron-transfer properties. Among the various types of nanomaterials that have been developed, nanostructured metal oxides have recently aroused much interest as immobilizing matrices for biosensor development. The nano structed metal oxides based on $NiFe_2O_4$, Cu_2O, Tm_2O_3 and CeO_2 have recently attracted much attention for the fabrication of miniaturized total cholesterol-based biosensor. I will focus on some of the recent results obtained at our laboratories relating to development of nano-structured metal oxides-based cholesterol biosensor for clinical applications.

Dr. Bhaskaran

Department of Chemistry, HNB Garhwal University (A Central University), Srinagar (Garhwal)-246174

Dr. Bhaskaran is currently working as Assistant Professor at the Department of Chemistry in H.N.B. Garhwal University, Srinagar Garhwal. Dr. Bhaskaran received his Ph.D degree from University of Delhi. He qualified for national level exams such as CSIR JRF and GATE for research fellowship and visited a world-class research institution British-Columbia, Vancouver for reserch programme. Dr. Bhaskaran has been working as assistant professor in Ramjas college since last 5 years. His research work has been recognized at national and international levels and published in several international journal.

EXPERIMENTAL AND QUANTUM CHEMICAL STUDIES OF IONIC LIQUIDS AS GREEN CORROSION INHIBITORS

ABSTRACT

The present study described the effect of synthesized imidazolium ionic liquids on mild steel corrosion in 0.5 M H_2SO_4 solution using electrochemical, surface morphological (SEM, AFM,) techniques, and quantum chemical calculations. The results show that the imidazolium ionic liquids (IILs) with heteroatom exhibit higher inhibition efficiency. The inhibition efficiency increase with increase in inhibitor concentration suggesting the occurrence of chemical adsorption. The surface analysis techniques further confirm that the corrosion inhibition occurs due to the adsorption of the inhibitor molecules at the metal/solution interface. The use of computational chemistry as a tool in the design and development of imidazolium ionic liquids has been greatly enhanced by the development of density functional theory (DFT). The various quantum parameters like EHOMO, ELUMO, energy gap (ΔE), electronegativity (χ) and fraction of electron transferred from inhibitor molecule to metallic atom (ΔN) have been calculated to understand the interaction between the ionic liquid and the mild steel.

TECHNICAL PRESENTATIONS

NCRAPS:CHEM-01

CATALYTIC PERFORMANCE OF RGO/$BiVO_4$ COMPOSITE MATERIAL ON MB DYE DEGRADATION

Manish Kumar , Rahul Vaish *
Department of Chemistry, Indian Institute of Technology, Mandi, India.
Email: rahul@iitmandi.ac.in

ABSTRACT

Water in today's world is one of the major essentiality of survival for the living beings. Fresh water reserve in the world being limited prohibits the humans from the reckless utilization of the resource. Among different pollutant sources that contaminate water, colored organic dyes from the textile industries occurs to be the major contributor. In view to remove the contamination from water, photocatalysis, piezocatalysis and combined piezo-photocatalysis processes would be promising technology. Photocatalysis takes use of photon energy present in light to generate electron-hole pairs in semiconductor materials which would be utilized for water remediation. Piezocatalysis use vibrational energy in the form of stress on the piezoelectric material which produces positive and negative charges on the materials surface which is harnessed to clean the dye contaminated water. There had been a quest to investigate new materials which would be cheap, easily available, recyclable and eco-friendly. In this regard we investigated the catalytic dye degradation on rGO/$BiVO_4$ composite material. Combining two different materials serves our ultimate purpose of enhanced cleansing of the contaminated water. $BiVO_4$ is good photocatalytic material while rGO enhances carrier mobility and charge separation. rGO/$BiVO_4$ composite material was prepared through ultrasonication and hydrothermal methods. Reduced graphene oxide (rGO)/bismuth vanadate ($BiVO_4$) composites with varying content of rGO (0, 1, 2, 3 and 5 wt %) were prepared and their catalytic dye degradation performance was investigated. Presence of both rGO and $BiVO_4$ phases was analyzed through Raman spectroscopy and X-ray diffraction techniques. Coupling interaction between both the phases was affirmed using transmission electron microscopy (TEM). We ought investigate the catalytic methylene blue (MB) dye degradation capability of the proposed sample and discover the best composite among the varying rGO content in terms of dye degradation. We ought to find initial increase in catalytic performance as we increase rGO content up to 2 wt% and hereafter decrease in performance was found. This would be probably since higher wt% of rGO covers most surface of $BiVO_4$.

NCRAPS:CHEM-02

APPLICATIONS OF NANO TECHNOLOGY IN AYURVEDA

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ABSTRACT

Ayurveda is thousands of years old medical system in India. Various herbs, metals and non-metals preparations are used as medicine in Ayurveda. In the Ayurvedic description, several metallic preparations called Bhasma are in clinical use since 8th century AD. The Bhasma (incinerated metals) is obtained by repeating these methods several times. In this process the toxic effects of the metals are not only nullified but are transformed into biologically active nanoparticles. Nanotechnology is the study of extremely small structures which covers the diverse area of matters at dimensions which are approximately between 1 to 100 nanometers. The nanoparticles are a miracle invention of the century that has opened novel avenues of applications in various fields. Nanomedicine is the relevance of nanotechnology in the area of healthcare, diagnosis, cure and prevention of disease which is relatively a new field of science and technology. Nanotechnology is the newly emerging field in the medical sciences. Ayurvedic medications and therapies are getting in trend because of their safety and efficacy. Integration of Ayurveda and nanotechnology may provide the best medicines to treat various lifethreatening diseases. Nanotechnology has enormous applications in drug delivery field. Nano drug delivery systems can reduce the drug consumption and side-

effects by lowering the deposition of the active agent in the non-targeted sites. This review will give insights on nanotechnology, its applications in health sector and contributions in the field of Ayurveda.

NCRAPS:CHEM-03

DEVELOPMENT OF SUPERHYDROPHOBIC/OLEOPHILIC FABRIC USING MODIFIED NANOTITANIA FOR OIL-WATER SEPARATION

Adeeba[1] , Abhilasha Mishra[*1] , Akanksha Rajput[1] , Pushpa Bhakuni Negi[2]
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ABSTRACT

In recent years, the increasing environmental issues arising from oil spills and industrial wastewater discharge have emphasized the need for finding efficient and sustainable solution for oil water separation. This research paper investigates the fabrication of an advanced superhydrophobic coating on cotton fabric surfaces to improve the process of oil-water separation. The coating is developed through the synergistic utilization of stearic acid and titania sol via the dip coating method. By varying the molar ratio of various constituents, threesol solution of titanium dioxide (TiO_2) were prepared using sol-gel technique. The Titania sol exhibited an average particle size of 39.35 nm and zeta potential value of 25.96 mV which shows good stability of sol solution. The Scanning Electron Microscopy (SEM) analysis was employed to examine the surface roughness and morphology of the superhydrophobic coating. The composition of the modified sol was characterized by Fourier Transform Infra-Red (FTIR), revealing peaks corresponding to Ti-O-Ti and Ti-O-Si bonds at wave numbers of 665.3 cm^{-1} and 894.5 cm^{-1} respectively. The coated fabrics displayed hydrophobic characteristics with low surface free energy values and demonstrated significant superhydrophobicity, with the maximum water contact angle (WCA) recorded at 158.5° and the minimum contact angle hysteresis at 5°. Mixtures such as Toluene-water, Cooking Oil-water and Chloroform-water were successfully separated by coated fabrics, with separation efficiencies of up to 97.5%. This study provides a promising solution for ecofriendly and effective oil water separation systems and as well as contribution to the advancement in materials for environmental applications.

NCRAPS:CHEM-04

MODELLING DNA-LIGAND INTERACTIONS THROUGH VARIABLE FORCE FIELD BASED MD SIMULATIONS

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ABSTRACT

In the field of MD simulations, force field refers to as the combination of a set of mathematical formulae and incorporated parameters that are used to evaluate the protein energy as a function of its atomic coordinates over the passage of time. And therefore, the choice of suitable force field to carry out MD simulation is of utmost importance. Apart from literature survey and previously reported results, there is no direct evidence regarding the choice of appropriate force field for a particular system. This entirely depends upon the type of system that is to be simulated and the parameters to be analysed. In the current research article, analysis of molecular dynamics trajectories for ligand-DNA interactions over two such force fields, AMBER03 & CHARMM27 have been done. The functional forms including the parameterization protocols of both the force fields are also studied and well discussed in this research article. It was found that energetics related to CHARMM27 force field were in better agreement with the RMSD of the complex than that of the AMBER03 force field and hence CHARMM27 force field can be a suitable choice to model DNA-ligand complexes for shorter simulations as the convergence criterions are met earlier with minimum or no deviations in the RMS plots.

NCRAPS:CHEM-05

STRUCTURAL INVESTIGATION OF SCHIFF BASE TRANSITION METAL COMPLEXES: MOLECULAR DOCKING AND ANTIMICROBIAL INVESTIGATION

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ABSTRACT

Schiff base transition metal complexes are a type of coordination molecule produced when a Schiff base ligand is coordinated to a transition metal ion. Because of these complexes varied structures and broad range of applications in bioinorganic chemistry, catalysis, and antibacterial, antifungal, anticancer, antiviral, antituberculosis, antidiabetic, antiproliferative, herbicidal, and anti-inflammatory properties, among other fields, these compounds have been studied in great detail. This article describes the synthesis of a new Schiff base ligand and its complexes with several transition metal ions. FTIR, NMR, UV-visible, ESR, PXRD and mass investigations were the spectroscopic techniques used to clarify the structure. The acquired results point a hexadentate structure of the synthesized metal complexes and a tetradentate binding mechanism of the ligand. Antimicrobial tests were conducted using the serial dilution method against two fungus strains and four different bacterial strains in order to determine the biological efficacy of the synthesized ligand and their metal complexes. Additionally, investigations on molecular docking were conducted, and the results show encouraging outcomes when compared to synthetic drugs.

NCRAPS:CHEM-06

MOLECULAR DOCKING AND ADMET STUDIES OF 1,3-BENZODIOXOLE-BASED CARBAMOYL-IMIDAZOLE DERIVATIVES TO REVEAL ANTICANCER PROPERTIES

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ABSTRACT

The treatment of cancer – a major health issue, needs fitter pharmaceutically active ingredients with additional positive results and fewer side effects. We have studied the derivatives of 1,3-bezodioxole to determine their interactions with tubulin protein involved in microtubule formation during cell proliferation. The molecular docking and ADMET - absorption, distribution, metabolism, excretion and toxicity predictions; were carried out with open-source software such as HEX server, AutoDock Vina, pkCSM and SwissADME. The derivative that has shown effective binding with protein and lies in the applicability domain according to pharmacokinetic and pharmacological studies were considered potential anticancer candidates.

NCRAPS:CHEM-07

NANOSTRUCTURED $ZNFE_2O_4$/RGO-MODIFIED ELECTRODE-BASED INTERFACES FOR ELECTROCHEMICAL IMPEDANCE MONITORING OF ADRENALINE

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ABSTRACT

This study introduces a promising biosensor designed for the detection of adrenaline (AD) in bovine serum albumin (BSA) real samples, with implications for the diagnosis and treatment of neurodegenerative disorders. The biosensor is constructed using a La/ZF/rGO/ITO bioelectrode, created through the electrophoretic deposition of zinc ferrite/reduced graphene oxide (ZF/rGO) nanohybrid, followed by the drop casting of laccase (La) enzymes. Material characterization and electrochemical studies indicate that the ZF/rGO nanohybrid enhances the electroactive surface, facilitating direct electron transfer between the electrode and electrolyte interface. Cyclic voltammetry and electrochemical impedance spectroscopy confirm that the ZF/rGO nanohybrid reduces the charge-transfer resistance (Rct) and increases surface adsorption, leading to a high diffusion coefficient (D) of 0.192 cm 2 /s. The biosensor demonstrates a high sensitivity of 0.71 Ω/μM cm 2 , a favorable linear range (0.1 to 140 μM with R 2 = 0.98), and a low limit of detection (LOD) of 12.5 μM. This showcases the synergistic effect of ZF and rGO in the La/ZF/rGO/ITO bioelectrode with AD. Additionally, the biosensor exhibits high selectivity and stability (55 days) in the presence of interfering substances and in BSA samples, highlighting its potential for biosensing applications in disease diagnostics, monitoring, and treatment in real-world scenarios.

NCRAPS:CHEM-08

CU(I)−CATALYZED CSP^3 -CSP^3 HOMO-COUPLING OF BENZYL THIOCYANATES TO ACCESS FUNCTIONALIZED BIBENZYLS VIA C(SP^3)-H BOND ACTIVATION

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ABSTRACT

Carbon-carbon bond formation reaction[1] is one of the most powerful tools in organic synthesis to construct the core skeletons of different building blocks in polymers, pharmaceuticals, dyes, supramolecular chemistry. [2] The wide pharmacological applications of bibenzyl compounds as immune enhancement, antitumor, antidiabetes, anti-aging, antiinflammatory agents have sparked extensive investigations of such molecules in the last few decades.[3] Homocoupling of benzyl halides is a classical approach to access bibenzyl skeletons where stoichiometric amount of strong reducing agents such as Fe, Ni, Li, Mn, In, Ti, Sm, Rh, Co, and Zn are utilized. Recently, heterogeneous photocatalysis has been developed to facilitate the formation of such compounds.[4] However, harsh reaction conditions, requirement of strongly reducing metals, complicated and costly metal complexes or photocatalysts restricted their synthetic utility.
Herein, a facile and cost-effective approach for the synthesis of bibenzyls via Csp^3 -Csp^3 homo-coupling of benzyl thiocyanates has been disclosed under Cu(I)-catalyzed conditions using Cs_2CO_3. The reaction proceeds via activation of unreactive C(sp^3)-H bond to under base promoted conditions to afford the homo-coupling product. Diverse substituents on the aryl ring are well-tolerated to afford the homo-coupled products in moderate to good yields under mild conditions.

NCRAPS:CHEM-09

DEVELOPMENT OF TRANSPARENT SUPERHYDROPHOBIC COATING FOR GLASS AND PLASTIC AND STUDY OF ANTIMICROBIAL CHARACTERISTICS

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ABSTRACT

Superhydrophobic coatings have gained substantial attention in recent years due to their potential applications in various industries. Biomedical and many more devices are made from a variety of materials, including plastics, polymers, metals and glasses. Adherence of microorganisms on equipment can cause infections in the human or animal body. To resists the growth of bacteria, mould, fungus, and other germs on these devices, antimicrobial coating were prepared. This research paper explores the development and characterization of antimicrobial superhydrophobic coatings on glass and plastic surfaces. Silica nanoparticles were prepared using sol gel process and further hydrophobically modified which is forming transparent antimicrobial coatings on glass and plastic. Confirmation of the dispersion of nano Silica in the solution was confirmed through Particle Size Analyser which is 45 nm and formation of silica nanoparticle in the sol was confirmed by IR spectra. The Zeta potential of sol was found -1-33mv, which is showing that the sol is quite stable. The surface morphological studies were done by Scanning Electron Microscopy (SEM) analysis which confirmed the uniformly distribution of nanostructures on coated surface, while in contact angle study a maximum water contact angle of coated glass was found 163.3° and coated piece of plastic having angle of 150º confirmed the coating's superhydrophobic nature. The effect of antibacterial activity for E. coli was observed at 1 hour and 24 hours. The results obtained from coated glass pieces showed less bacterial adhesion as compare to uncoated glass pieces. This indicates the durability and versatility of prepared coating.

NCRAPS:CHEM-10

DEVELOPMENT OF MESOPOROUS SILICA-BASED HETEROGENEOUS CATALYST FOR AMINOLYSIS REACTION UNDER SOLVENT-FREE CONDITION

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ABSTRACT

Aminolysis reaction produces β-amino alcohols, the intermediate of various biologically active natural products and chiral auxiliaries. In particular, heterogeneous catalysts play an important role in organic transformation reactions due to their easier recovery/separation from the reaction mixture. Functionalized mesoporous silicas have been employed in recent decades to develop heterogeneous catalysts.[1] Among various mesoporous materials, MCM-41 is extensively investigated in heterogenous catalysis reactions because of their large surface area, adjustable pore size (2-50 nm), and uniform arrangement of pores on the surface. The present work demonstrates the development of mesoporous silica-based heterogeneous catalysts and explores their catalytic application in aminolysis reactions. Briefly, the solid Lewis acid catalyst Cu(II)L-propylsilyl@MCM-41 was prepared by immobilizing the catalytically active Cu(II) metal ion on MCM-41 with the support of organosilica precursor. Then, this heterogeneous catalyst has been used to synthesize regioselective β-amino alcohol with high yield under solvent-free conditions. More importantly, this heterogeneous catalyst can be used for multiple cycles without losing its catalytic activity.

NCRAPS:CHEM-11

BODIPY- FUNCTIONLIZED MESOPOROUS MATERIAL: APPLICATION IN HEAVY METAL ION DETECTION

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ABSTRACT

Heavy metal contamination in driking water has severely threatened the environment and human health. Heavy metal ions such as Mercury(Hg^{2+}), Aluminium(Al^{3+}), Lead(Pb), and Chromium(Cr), show an adverse effects on the ecological system and human health. Mercury and aluminum are the most toxic non-biodegradable pollutants that exhibit acute toxicity to the human body, even in low concentration. Therefore, developement of efficient sesor for selective detection and separation of metal ions in an aqueous media is an emerging field in reserch community. In the present work, BODIPY-(COOH)-propylsilyl@MCM-41 (MS4) were synthesized and used for the efficient detection and removal of heavy metal ions (Hg^{2+} , Cu^{2+} , Al^{3+} and Cr^{3+}) in aqueous mediaum. The synthesized chemosensors MS2 were well characterized using N_2 adsorption-desorption, powder X-ray diffraction, TEM, FT-IR, and thermal analysis. The emission intensity of chemosensor MS4 is enhanced multifold in the presence of trivalent (Cr^{3+}, Al^{3+}) metal ions and is completely quenched in the presence of divalent (Cu^{2+} , Hg^{2+}) metal ions. The limit of detection(LOD) was calculated to be a nanomolar range for Cr^{3+} , Al^{3+} , Cu^{2+} and Hg^{2+} in aqueous media. Also, MS4 were demonstrated the removal of respected metal ions from the pure water samples up to 98%.

NCRAPS:CHEM-12

CARBAZOLE-ISONICOTINOYL HYDRAZONE AND ITS STRUCTURALLY DISTINCT ZINC(II)-COMPLEXES EXHIBITING REVERSIBLE MECHANOCHROMISM AND ACIDOCHROMISM: COMPARATIVE MULTI-STIMULI DRIVEN STUDIES VIA FLUORESCENCE READOUT

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ABSTRACT

Based on a donor-acceptor type hydrazone HL, namely (E)-N'-((9-ethyl-9H-carbazol-3- yl)methylene)isonicotinohydrazide comprising carbazole as donor and isonicotinoyl group as acceptor unit, two new Zn(II) complexes 1 and 2, have been investigated in detail for their photophysical properties in solid as well as solution state. Both 1 and 2 have been synthesized from the same ligand HL using zinc chloride and zinc nitrate hexahydrate respectively. Further, ligand HL, 1 and 2 have been systematically characterized by elemental analysis, HRMS, FTIR, ^{1}H &^{13}C-NMR spectroscopic studies. The structure of HL has been confirmed by single crystal X-ray diffraction. Interestingly, both HL and complex 1 displayed remarkable reversible mechanochromic luminescent behavior on grinding while complex 2 was not responsive to the mechanical force stimuli. The emission of pristine HL changed from blue to yellowish green after grinding in a mortar with a pestle while the emission of 1 in solid state changed from yellow to orange under irradiation of 365 nm UV light. In addition, HL and complex 1/2 exhibit anticipated acidochromic behavior on exposure to HCl/NH3 vapors. Notably, the mechanochromic luminescence behavior and the acidochromism of HL and 1 have been studied in-depth by PXRD, SEM morphological studies, TGA-DSC analysis. The PXRD pattern of HL and complex 1 vividly illustrates the noteworthy phase transformation from crystalline state to amorphous state. This study emphasizes on fact that a small structural variation can alter a system's distinctive behavior.

NCRAPS:CHEM-13

MICROWAVE ASSISTED OXIDATION OF WATER SOLUBLE CARBOHYDRATES LIKE MANNOSE BY CHROMIUM (VI) BASED COMPLEXES WITH TERTIARY AMYL CHROMATE.

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ABSTRACT

This study investigates the microwave-assisted oxidation of water-soluble carbohydrates, focusing on mannose, using chromium (VI) based complexes with tertiary amyl chromate. The utilization of microwave irradiation as an energy source enhances the efficiency of the oxidation process, aligning with sustainable practices and the principles of green chemistry. The chromium (VI) based complexes, particularly with tertiary amyl chromate, serve as effective oxidizing agents, facilitating the conversion of mannose into valuable products. The synthesized materials are thoroughly characterized using advanced analytical techniques, including spectroscopy (e.g., FTIR) Thermal analysis (TGA,DTA), Elemental analysis. The study elucidates the reaction pathways and mechanisms involved in the oxidation process, providing insights into the structural evolution of the resulting compounds. The materials obtained exhibit potential for energy-related applications, such as catalysis for fuel cells or energy storage devices, and societal applications, such as drug delivery systems or biomaterials.
The interdisciplinary nature of this research integrates principles from chemistry and materials science, contributing to the development of innovative Thermal analysis (TGA,DTA), Elemental analysis materials with dual significance for both energy and societal applications. The sustainable aspects of microwave-assisted synthesis and the utilization of water-soluble carbohydrates highlight the eco-friendly approach of this study. The findings not only advance our understanding of chromium (VI) based oxidation of carbohydrates but also pave the way for the design of materials that can address contemporary challenges in energy and healthcare, thus fostering sustainable development.

NCRAPS:CHEM-14

APPLICATION OF PRINCIPLES OF GREEN CHEMISTRY IN THE OXIDATION OF 1,4 CYCLOHEXANEDIOL USING TERTIARY BUTYL CHROMATE (TBC) AND TERTIARY AMYL CHROMATE (TAC)

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ABSTRACT

The application of the principles of Green Chemistry in the oxidation of1,4 Cyclohexanediol using Tertiary Butyl Chromate (TBC) and Tertiary Amyl Chromate (TAC) represents a significant advancement in environmentally friendly synthetic processes. The abstract outlines the key aspects of this approach, emphasizing the sustainable and efficient aspects of this chemical transformation. The oxidation of 1,4 cyclohexanediol with Tertiary Butyl Chromate and Tertiary Amyl Chromate demonstrates a commitment to green chemistry principles. These reagents, as highly efficient and selective oxidants enable the conversion1,4 Cyclohexanediol to valuable ketone or aldehyde products with minimal waste generation. The principles of green chemistry including the reduction of hazardous by-products and the use of catalytic or stoichiometric reagents are addressed in this methodology. The oxidation process minimizes the formation of undesired by-products resulting in higher atom economy and reduced environmental impact. These reagents enable the conversion of the starting materials into valuable ketones or aldehydes with minimal waste generation minimizing the use of resources of green chemistry is the reduction of hazardous by-products. Furthermore, the use of Tertiary Butyl Chromate and Tertiary Amyl Chromate is advantageous in terms of safety and toxicity. These reagents offer a safer alternative to traditional oxidants, such as chromium(VI) compounds by reducing the risks associated with hazardous materials, and thus aligning with green

chemistry's principle of hazard reduction. In conclusion, the application of green chemistry principles in the oxidation of 1,4 Cyclohexanediol with Tertiary Butyl Chromate and Tertiary Amyl Chromate exemplifies a sustainable and environmentally responsible approach to chemical synthesis. This abstract highlights the potential of this methodology to contribute to greener and more sustainable chemical processes in the future.

NCRAPS:CHEM-15

A NOVEL SMART ANALYTICAL TOOL FOR THE SUSTAINABLE DETECTION OF COBALT IN BIOSYSTEMS: MPP

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ABSTRACT

N1,N3-bis(3-(((E)-2,3,4-trihydroxybenzylidene)amino)propyl)malonamide (MPP), a symmetrical dipodal chelator, was effectively synthesised and characterized. It contains pyrogallol binding units which is attached to the malonate central moiety by propylene spacers. The fluorescent sensor MPP, which performs "OFF-ON" fluorescence sensing for Co(II) ions with remarkable selectivity and sensitivity, is based on the excited state intramolecular proton transfer (ESIPT) process. Studies show that the suggested sensor can detect Co(II) over a variety of physiologically and environmentally significant metal ions, including Na(I), K(I), Al(III), Cr(III), Fe(III), Fe(II), Co(II), Ni(II), Cu(II), and Zn(II). The sensor's fluorescence intensity has shown a linear response to Co(II) concentration in the range of 5 - 100 μM, with a detection limit of 8.75 x 10^{-5}. When cobalt ions are added, the ligand's emission intensity increases as a result of the complex's 1:2 (L:M) binding stoichiometry being formed. The pre-organized structure favoured the ligand for an efficient Co (II) encapsulation by imine nitrogen and pyrogallol oxygen donors with a high formation constant (log β = 34.13).

NCRAPS:CHEM-16

MICROWAVE ASSISTED SYNTHESIS: AN APPROACH EMBRACING SUSTAINABLE DEVELOPMENT

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ABSTRACT

Green technology, an environmentally friendly technology is developed and used in a way that protects the environment and conserves natural resources. Green technology is going the extra mile these days zipping well past the empire of solar power, into the illimitable world of innovative ideas that are hell bent on renovating the world to a more sustainable place. A part of the renewable energy branch of the environmental technology movement, the green technology importance cannot be ignored. Moving a step forward we have carried out microwave assisted synthesis of heterobimetallic complexes. Microwave-assisted synthesis is considered to be a promising green chemical approach because it reduces reaction time from days or hours to minutes or even seconds, and has many other advantages. It helps reduce side reactions and increase yields, uses fewer solvents or is almost solvent-free, has solid supported reactions, and improves purity. Further these complexes have been evaluated for a number of biological activities such as antifungal, antibacterial and anti-inflammatory activity. These complexes are then characterized by physicochemical and spectroscopic techniques such as IR, ^{1}H NMR, ^{13}C NMR, ESR.

NCRAPS:CHEM-17

THIAZOLE-BASED METALLOLIGANDS AND THEIR MOFS FOR MOLECULAR DETECTION

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ABSTRACT

This part of the work focuses on the thiazole-containing metalloligands and their extended Metal-organic frameworks (MOFs) that further exploited in the applicative field of luminescent sensing. MOFs are hybrid organic/inorganic 3D coordination polymers with open structures deriving from the self-assembly of poly(topic) ligands and metal ions or metal-based clusters. The typical ligands belong to this class are polycarboxylic and polydentate N-heterocyclic bases. The rational design and construction of MOFs have made rapid progress due to their intriguing structural variety and potential applications such as gas adsorption and separation, luminescence, catalysis, and sensing. A comprehensive literature review has been done on thiazole-containing MOFs. In this work, we have synthesized the metallo-ligands based on the Cu(II) and Zn(II) comprising 2-(2-Pyridyl)-4-methylthiazole-5-carboxylic acid organic moiety having –COO functional groups that have been structurally determined by X-ray analysis. The 1D-chained structure obtained by intermolecular hydrogen bond interactions is presented below. Further, we have also synthesized MOFs and discussed their diverse structures and associated properties especially in the field of molecular detection studies.

NCRAPS:CHEM-18

COMPARATIVE INSIGHTS ON PHOTOCHROMISM AND FLUORESCENT DETECTION OF SO_4^{2-} /CO_3^{2-} USING SALICYLALDEHYDE-PYRIDINE HYDRAZINE CONJUGATE AND ITS ZN(II)-COMPLEX

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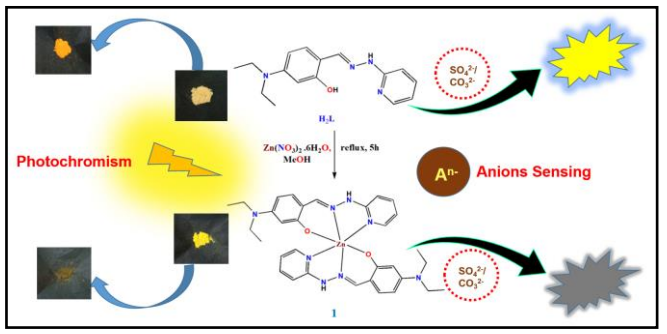
ABSTRACT

A new salicylaldehyde-pyridine hydrazine Schiff base (H_2L) and its Zn(II)-complex (1) have been synthesized and developed as novel fluorescent probes for the detection of SO_4^{2-} and CO_3^{2-} . The ligand and Zn(II)-complex have been characterized by different spectroscopic and analytical techniques like, FT-IR, ^1H & ^{13}C-NMR, mass, SC-XRD, UV/vis and fluorescence. Notably, ligand and Zn(II)-complex both serve as highly selective and ultrasensitive fluorescent probes towards SO_4^{2-} and CO_3^{2-}. H_2L gives fluorescence “turn-on” response in presence of SO4 2- (66%) and CO_3^{2-} (46%) whereas 1 gives fluorescence “turn-off” response towards SO_4^{2-} (85%) and CO_3^{2-} (71%) among various competing anions. Both H_2L and 1 also exhibit photochromic behaviour whereas thermochromic properties are shown by only H_2L.



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NCRAPS:CHEM-19

STUDY OF WATER QUALITY AND TOXICITY IN GROUNDWATER SOURCES OF ROHTAK DISTRICT, HARYANA .

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ABSTRACT

Water is the main constituent of Earth's hydrosphere and the fluids of all known living organisms. It is an excellent solvent that can dissolve most minerals that come in contact with it. Therefore, in nature water always contains chemicals and biological impurities i.e. suspended and dissolved inorganic and organic compounds and microorganisms. These compounds may come from natural sources and leaching of waste deposits. Our water resources are being polluted at a very fast rate. Due to increased industrialization, human population, use of fertilizers in the agriculture and manmade activities, it is highly contaminated which results in undesired changes in physical, chemical and biological characteristics of water.
Physical: Colour, Odour, Temperature
Chemical: pH, metals, alkalinity, sulphate, carbonates, bicarbonates, sodium, potassium, calcium, chloride, bromide, magnesium and fluoride. Heavy metals like lead, mercury in water cause serious health effects like damage to brain and kidney, bloody diarrhoea, abdominal pain even in trace amount.
Biological Parameters: Bacteria, algae, protozoan.
In terms of direct effect on human health biological parameters are more important than physical and chemical parameters. Human beings and another animals discharge large number of intestinal bacteria into stool and urine, the bacteria therefore appears in drinking water when the water sources contaminated with stool. In India most of the population is dependent on ground water for drinking purposes, so continuous monitoring of large number of quality parameters is essential for effective maintenance of water quality as quality of water is a vital concern for mankind.

NCRAPS:CHEM-20

ANALYSIS OF SOIL SAMPLE TO DETERMINE ITS PHYSICAL AND CHEMICAL PARAMETER FROM ROHTAK DISTRICT, HARYANA

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ABSTRACT

Soil is a intricate and dynamic natural resource that plays a important role in agriculture and environmental sustainability. The physicochemical properties of soil is essential for crop production and environmental conservation. A number of factors, including soil pH, electrical conductivity (EC), phosphorus (P), potassium (K), sulfur and organic carbon, determine the physichochemical qualities of soil. After Fifteen sample soil samples were taken at a depth of 0.02 meters, their pH values ranged from 7.20 to 8.30, indicating that soils were neutral to slightly alkaline. The conductivity was ranging from 0.15-1.18 ds/m , phosphorous was ranging from 2.79-9.89 kg/ha, organic carbon was found to be 0.24-0.72 and potassium 44.07-450.74 kg/ha, sulphur 40.07- 410.30ppm.This analysis provides valuable information for farmers that promotes agricultural productivity.

TETRASUBSTITUTED IMIDAZOLE: SOLVATOFLUOROCHROMISM, AIE, TRACE WATER DETECTION AND PH SENSING PROPERTIES

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ABSTRACT

Tetrasubstituted Imidazole derivatives **R-1** and **R-2** have been designed with flexible and rigid backbone respectively. The design strategy enabled entirely different behaviour of **R-1** and **R-2** in different media. Taking advantage of their flexible and rigid structure, the solvatofluorochromism, Aggregation Induced Emission (AIE), trace water detection and pH sensing properties have been explored. The probe **R-1** shows excellent solvatofluorochromism compared to **R-2**. For **R-1** the emission in Hexane is observed at 418 nm while in Acetone it is at 636 nm with 259 nm redshift. On the contrary, for **R-2**, only 95 nm redshift was noticed. Interestingly, the **R-1** and **R-2** also exhibited excellent multi AIE in more than one solvent like DMSO, THF, and ACN. Furthermore, the response of **R-1** and **R-2** toward the HCl was very efficient in aqueous media. For **R-2**, in the solution (80 % H_2O-DMSO, v/v), the peak 420 nm was enhanced, and redshift to 522 nm in pH range of 1.0 to 13.0, while for **R-1** only enhancement of emission is observed. The **R-2** also showed very exotic properties of trace water detection in THF.

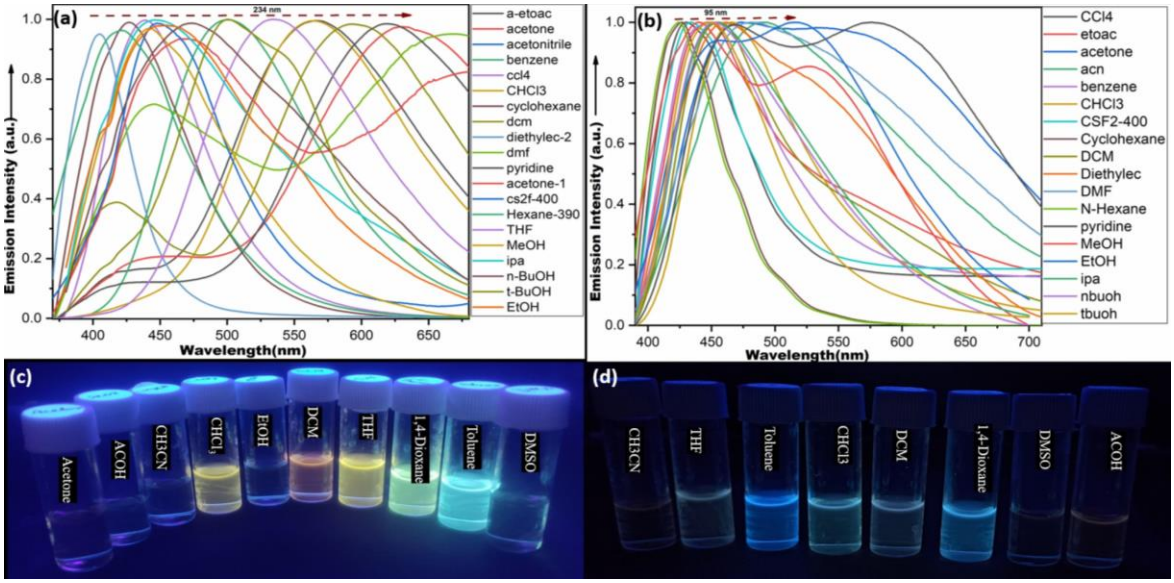

Figure: Normalized emission spectra and pictures of **R-1** (a & c) and **R-2** (b & d) in different solvents (λ_{ex} = 360 nm).

NCRAPS:CHEM-22

SINGLE BENZENE-BASED FLUOROPHORES (SBBF)

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ABSTRACT

Fluorescence-based materials and associated techniques (analytical, imaging, and sensing techniques) have been highlighted over the last century throughout various basic research fields and industries. To date, hundreds of organic fluorophores have been developed, and many studies have introduced new rationales for the fluorophore design and the analysis of the relationship between its structure and photophysical properties both in the solution- and solid-state. Often, within industry, the multiple aromatic rings and/or π-conjugated skeleton have been preferred which generally cause problems in terms of solubility, purification and processing of organic materials. In order to overcome these issues, many researchers have focused on the development of compact (small size, no π-extension) and unique fluorophores that can be used in optics and biology, and single-benzene-based fluorophores have been considered as an ideal candidate among them. Single benzene is a six-membered aromatic ring in which pie-conjugation within the benzene backbone. When EDG and EWG-type push-pull systems are connected appropriately, excellent fluorescence properties can be harnessed with even single benzene core.

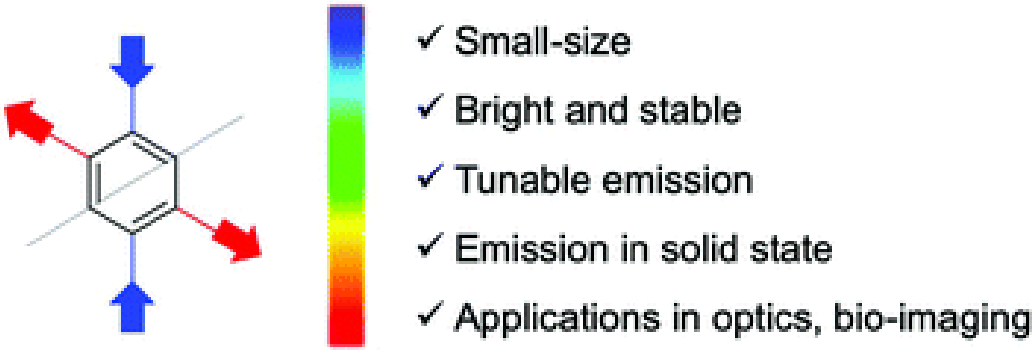

Figure 1. Single-benzene-based fluorophore (SBBFs)

NCRAPS: ENG-01

THREE-LEVEL SEVENTH-ORDER WEIGHTED ESSENTIALLY NON-OSCILLATORY SCHEMES

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ABSTRACT

Accurately determining shock structures is crucial for assessing the loads on supersonic flights. Achieving precision in aero-thermal load estimation for high Mach number flows demands the use of higher-order highresolution schemes. This study introduces a specific higher-order high-resolution scheme renowned for its exceptional shock-resolving capabilities. While many seventh-order schemes typically achieve only fourth or seventh-order accuracy, the presented scheme can attain accuracy levels of fourth, sixth, or seventh order. Notably, it precisely satisfies the Taylor series with zero residues, unlike many existing schemes that yield small non-zero residues. This accomplishment is attributed to a novel weighting function that breaks the direct connection between the smoothness indicator and the weighting function. The scheme's effectiveness is validated using gas dynamics Euler equations, particularly in scenarios involving step-like discontinuities such as shock

tube problems and double Mach reflection test cases. Across various test cases, the proposed scheme consistently demonstrates minimal errors and exhibits outstanding shock-resolving properties.

NCRAPS: ENG-02

AN INVESTIGATION ON THE COMPONENT EFFICIENCIES OF SUPERSONIC EJECTOR

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ABSTRACT

This report aims to investigate different component efficiencies present in CRKEC based ejector model. This study calculates the efficiencies of component on-design and off-design condition. This study shows the effect of the inlet, secondary, and exit pressure on the efficiencies of the nozzle, mixing, diffuser and entrainment efficiency of supersonic ejector. The definitions of ejector component efficiencies in literature are given. There is a discussion of how ejector shapes, operating circumstances, and working fluid properties affect ejector efficiency. This review will be useful for future research on ejector efficiency, optimal design, and control of ejectors and ejector systems.

NCRAPS: ENG-03

ELECTROSPUN NANOFIBROUS MEMBRANE FOR EFFICIENT BACTERIAL REMOVAL AND ELECTROCHEMICAL SENSING OF BIOLOGICAL DRUGS.

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ABSTRACT

Due to their essential significance in healthcare and environmental applications, innovative materials have attracted a lot of attention for their development of effective filtration systems and biosensors. The electrospun nanofibrous membrane used in this research is a major step forward since it serves two important purposes: efficient bacterial eradication and sensitive electrochemical sensing of biological medicines. The electrospun nanofibrous membrane, made with a straightforward and inexpensive method, displays a complex nanostructure that improves its performance1 . After extensive testing, we were able to prove that it effectively eliminates bacterial pollutants, making it a suitable contender for use in hospitals and other medical facilities. Additionally, a highly sensitive electrochemical biosensor for the detection of biological substances has been developed by capitalizing on the membrane's special surface features. The electrochemical system is highly sensitive and selective, allowing for continuous monitoring in real time2 . This study not only demonstrates the adaptability of electrospun nanofibrous membranes but also emphasizes its potential in resolving pressing issues in healthcare and environmental safeguarding. Our membrane is a promising option for a wide range of applications, from biosensors to pharmaceutical diagnostics, thanks to its synergistic combination of efficient bacterial eradication and biological drug detection.

NCRAPS: ENG-04

CONSTRUCTION STAGE ANALYSIS OF A TUNNEL OBLIQUE TO A SEWER LINE

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ABSTRACT

The construction of metro tunnels addresses urban transportation challenges, offers numerous benefits, and contributes to more sustainable and efficient cities. Metro systems play a vital role in enhancing mobility, reducing traffic congestion, improving environmental quality, and fostering economic development. Analyzing metro tunnels using FEA software is essential to ensure the safety, structural integrity, and efficiency of these critical transportation infrastructure projects. At the crown of tunnel is very critical as the bending moment is 177.8 kNm, shear force is minimum where bending moment is maximum and vice-versa and the factor of safety was 1.13 increasing to 2.27 when we were moving toward lateral position of tunnel, for making informed decisions during the design, construction, and operation phases, ultimately ensuring the tunnel's functionality and safety. Geotechnical and structural modelling and analysis are conducted using GTS NX. This paper focuses on addressing the analysis of an underground metro tunnel.

NCRAPS: ENG-05

EXPERIMENTAL INVESTIGATION ON EFFECTS OF THERMAL AND PHYSICAL PROPERTIES OF BIODEGRADABLE HYBRID NANO FLUID USING TWO STEP METHOD

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ABSTRACT

In the presence of the green technology or biodegradable Vegetable oils are emerging as replacement for mineral oil as base oils because of their properties of high viscosity index, high flash point, low toxicity, low volatility and high biodegradability. Nano fluids are a relatively new class of fluids which consist of a base fluid with nano-sized particles (1–100nm) suspended within them. The hybrid nano material and its characterization is vital role in the machining operation .In this paper carried out the synthesis and characterization of biodegradable hybrid Nano fluids and its combination of base material. The SiC and TiO_2 as a Nano particle with base fluid as a palm oil, surfactant used as Sodium Dodecyl Sulfate (SDS) to maintain the stability of fluids. All samples are prepared with Individual and Hybrid mode, 1) Palm oil (Base fluid Standard base without any emulsifier/ surfactant), 2) Palm oil + Sic, Nano particle (0.1% Vol, 0.2% Vol, and 0.3% Vol), 3) Palm oil + TiO_2 , Nano particle (0.1% Vol, 0.2% Vol, 0.3% Vol) ,4) Palm oil + SiC+TiO_2 , Nano particle (0.1% Vol, 0.2% Vol, 0.3% Vol).the result shows that FTIR methods and results shows that the sample no. 8, 9 and 10 biodegradable Hybrid nano fluids is better than the biodegradable nano fluids of sample no. 1 to 7. The zeta potential values was found to increases when volume concertation is 1%, 2% and 3%. At biodegradable hybrid nano fluids samples (Palm Oil+1 % Vol. SiC +TiO_2), (Palm Oil+2 % Vol. SiC +TiO_2), (Palm Oil+3 % Vol. SiC +TiO_2) and results shows that the increase the stability, physical, thermal and rheological properties of biodegradable hybrid nano fluids using the application machining application.

NCRAPS: ENG-06

THE INFLUENCE OF INJECTION PRESSURE AND EXHAUST GAS RECIRCULATION ON A VCR ENGINE FUELED BY MICROALGAE BIODIESEL

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ABSTRACT

Biodiesel has been chosen as a decent alternative to diesel in the context of establishing environmentally pleasant conditions and saving petroleum-based resources for the next generations. It is well established that biodiesel-powered diesel engines may achieve equivalent outcomes to diesel engines. The current investigation was done to study the effect of injection pressure (190, 210 and 230bar) and Exhaust gas recirculation (5%, 10% and 15%) using a single-cylinder Variable compression ratio diesel engine running on a B20 (20% MB +80% PD) blend of Microalgae biodiesel. This experimentation was carried out in two stages. During the first stage of experimentation, efficiency and emission characteristics studied of a diesel engine with a B20 blend of Microalgae biodiesel at various fuel injection pressures along with the fresh air and during the second phase, the fresh air is mixed with 5%, 10% and 15% exhaust emission and experimentation was carried out. It was discovered that increasing the injection pressure boosted the brake thermal efficiency by 2.35%. BSFC was decreased by 3.57% and reduced CO, HC and smoke emissions by 52.94, 45.31 and 51.32% as compared to diesel at standard IOP and by 30.43%, 27.08% and 22.91% compared to B20 blend at 210bar IOP but the NOx emission has increased by 3.14% as compared toIOP210bar for B20 blend. Also EGT at IOP 230 bar was increased by 1.72% as compared to IOP210bar During the second phase, experiments were carried out with EGR at 5%, 10% and 15% at different IOP; the result revealed that with 10% EGR, the NOx emission at 230bar IOP reduced by 41.42% and by 53.79 % in comparison to the standard B20 blend condition without much affecting the other performance and emission parameter. In addition, the performance and emission characteristics of a B20 blend of Microalgae biodiesel at IOP 230 bar outperformed other injection pressures.

NCRAPS: ENG-07

APPLICATION OF HASHING VECTORIZER FOR CLASSIFYING MEDICAL TEXT WHILE HANDLING IMBALANCE OF CLASSES

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ABSTRACT

As a result of the widespread implementation of Electronic Health Record (EHR) systems, learning of medical text has lately been highlighted as a promising area to improve healthcare. It is extremely difficult to create efficient deep learning models given how complicated medical texts are, with their varied lengths, heterogeneous text kinds, and plenty of medical words. Deep learning models have recently been used to categorize unstructured text in the healthcare industry, with encouraging results. However, unbalanced data sets where a select few classes predominate, have made it difficult for these models to be reliable in real-world applications. Rare classes require additional model restrictions for robust performance in the absence of sufficient training data. For solving the challenges faced during development, Deep Learning (DL) models, Hashing Vectorizer algorithm is applied on medical texts which is a suitable framework for text-based data, providing better data efficiency and comparable performance to few-shot language models and can be successfully applied to medical note data. In this paper the complicated medical data of Tuberculosis has been classified using Hashing Vectorizer Algorithm using Pandas for preprocessing. This classified data will help in analyzing the statistics of any particular disease by the

related professionals. This DL Algorithm can be extended for all other medical texts also. Methodology using the categorization of TB pathology reports, which demonstrates a significant improvement in model performance for uncommon classes is assessed. Additionally, the influence of terms is also assessed.

NCRAPS: ENG-08

DESIGN AND ANALYSIS OF HYBRID SOLAR OTFT

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ABSTRACT

Solar energy is the most abundant renewable source of energy available to humankind. At present the solar cells used for harnessing solar energy are generally based on inorganic semiconductors like silicon. But due to their structurally rigidity, high input and maintenance cost and non-biodegradable nature, room has been created for emerging alternatives like organic solar cells. While organic transistors have successfully entered commercial applications space, the performance of contemporary organic solar cells is still lower compared to silicon technology. Therefore, there is a need to develop a multipurpose hybrid device capable of working as an organic thin film transistor (OTFT) and organic photovoltaic cell (OPV) capable of generating electricity from the sun as well as consuming it in its absence. This would dramatically reduce the number OTFTs as wells OPVs required in portable solar powered systems like organic smart wears, solar lighting devices, communication devices etc. The hybrid device would be functionally equivalent to an OTFT as well as OPV, whereas structurally it would be equivalent to a single OTFT device in terms of material composition and size. Consequently, a compact and robust energy harnessing system could be developed by utilizing hybrid solar OTFT. Also, it would be cost effective due to the ease of fabrication and low cost of organic materials. In this research article a single layer hybrid solar OTFT has been designed and analyzed, which is improvised to work as a bottom gate bottom contact (BGBC) OTFT as well as an OPV. The analysis shows that it is possible to use an OTFT as an organic solar cell provided improvisation in structural architecture and material composition of the OTFT is effectively done.

NCRAPS: ENG-09

PREDICTIVE MODEL FOR SMART AGRICULTURE USING MACHINE LEARNING

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ABSTRACT

Agriculture holds a significant position in India's economic and employment landscape. A common challenge faced by Indian farmers is the lack of adherence to appropriate crop selection based on soil requirements, resulting in the cultivation of crops without a well-structured Crop Recommendation System. This adversely affects productivity of crop yields. Precision agriculture emerges as a solution to this issue, characterized by the utilization of a soil database derived from the farm, expert-provided crop recommendations, and the incorporation of parameters such as soil quality from soil testing lab datasets. The proposed system takes input data on soil quality, including Nitrogen, Phosphorous, Potassium, and pH values, as well as weather-related information such as Rainfall, Temperature, and Humidity. This information is utilized to predict the optimal crop for cultivation and enhancing crop productivity. The research employs datasets obtained from the Kaggle website, utilizing machine learning algorithms to analyse the data. The study focuses on key parameters to determine the

most suitable crops for cultivation in specific regions, aiming for heightened productivity. Among the various machine learning algorithms applied, the Random Forest and Naïve Bayes Algorithm demonstrated superior results, achieving a remarkable accuracy score of 99.09%.

NCRAPS: PHY-01

TEMPERATURE DEPENDENT DIELECTRIC, IMPEDANCE AND CONDUCTION BEHAVIOUR OF NIO MODIFIED CUO COMPOSITES.

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ABSTRACT

In the recent years, exploration of the characteristics of the metal oxide based composites has wide range of applicability and has gained the interest of the scientific community. In view of this in the current work, CuO modified with NiO nanocomposites containing the varying amount of NiO (0.05, 0.10, 0.15 & 0.20) has been synthesized using the energy efficient mechanical mixing method. The composites of above mentioned stoichiometric proportions are synthesized by altering the amount of NiO. The characteristics of the synthesized composites were uncovered by the advanced characterization techniques. The temperature dependent electrical properties such as dielectric permittivity, electrical impedance & conductivity have been explored. The effect of substitution of NiO on electrical conductivity and conduction behavior of prepared ceramic composites has also been studied.

NCRAPS: PHY-02

FIBER ORIENTATION IN FLOWING FIBER SUSPENSIONS

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ABSTRACT

The alignment of fibers in a flowing suspension plays an important role in the production process of fiber composites. In a mold flow process the local distribution of fiber orientations depends on the shear rate and the flow geometry. After hardening this orientation distribution is frozen, and the resulting fiber composite shows anisotropic material properties.A widespread model equation for this process is the Folgar-Tucker equation. It introduces the orientation tensor as a coarsened measure of the fiber orientation distribution. Analytical solutions of this nonlinear differential equation are hardly investigated in the literature. A reduction of the equation to a linear problem will be presented, thus leading to analytical solutions of the Folgar-Tucker equation. These analytical solutions serve as benchmarking solutions for numerical schemes and are compared to numerical results.The Folgar-Tucker equation is based on Jeffery equation for the rotation of a single fiber, an additional orientation diffusion term and a closure relation for the fourth order orientation tensor. As an outlook some generalisations of this classical model are discussed.

NCRAPS: PHY-03

FIRST PRINCIPLES CALCULATIONS ON THE OPTICAL PROPERTIES OF ABA STACKED TRILAYER SILICENE

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ABSTRACT

In this work, we have carried out the study of the optical properties of ABA stacked trilayer Silicene. The unit cell structure of 2D Silicene has been constructed using the surface builder tools of materials studio. **CASTEP** code based on Density Functional Theory (DFT) prescription is used for the present calculation [1]. ABA stacked trilayer Silicene is constructed with 6 atoms in the unit cell. The optical properties are analyzed and interpreted with the help of electronic band structures. Silicene as a single layer exhibits unique features. These features are found to be reduced in ABA stacked trilayer Silicene [2]. The imaginary part of dielectric function is calculated from electronic band structure. The real part of dielectric function is calculated using Kramers Kronig relation. With these values, n and k are calculated. From the calculated values of ε1, ε2, n, and k, optical properties like absorption, reflection, and electron loss function are analyzed. The optical properties are studied and analyzed along both parallel (||) and perpendicular ($\perp$) polarization directions of the electromagnetic field. The results are compared with the properties of single and bilayer materials [3], the analysis of which and the in-depth investigations of the present work would enable the prediction of their potential applications in the optical and optoelectronic industries.

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NCRAPS: PHY-04

COMPARATIVE STUDY OF LEAD IODIDE-POLYMETHYL METHACRYLATE POLYMER COMPOSITES AND POLYVINYL ALCOHOL AS A X-RAY SHIELDING MATERIAL

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ABSTRACT

Nowadays, there is continuously increasing the importance of X-rays in fields like medical diagnosis, cancer treatment, nuclear fission energy, X-ray scanning machines for airport and railway station entry and in treatment of food for preservation. But the exposure to X-rays will be harmful for the users of such facilities. Doctors, operators and researchers are required to be protected from the high energy ionizing radiations like X-rays and gamma rays. So to protect them, proper shielding is necessary. Radiation Shield is one of the methods for protection. It creates a barrier between a person and source of radiation and block the radiation through photo emission and scattering by a barrier material. People working near X-rays are required to wear protective clothing to avoid radiations.Most commonly used, shielding material is lead glasses or rubberized lead sheets. Recently light polymer sheets are replacing heavy glass sheets. To prepare lead polymer sheets lead compounds are mixed with polymer. In the present work, we have selected to mix lead iodide in different polymer

composites to analyze their X-ray shielding capabilities and compared their different parameters. Different Polymer composites sheets of lead iodide were prepared by solution method. These sheets of Polymer composites were subjected to soft X – rays (30KeV- 60KeV) switching studies at room temperature. These sheets found to provide the X- ray absorption with different percentage than conventional shielding material of lead.

NCRAPS: PHY-05

PARTIAL AND TOTAL CROSS SECTION DETERMINATION OF CHF_3 BY ELECTRON IMPACT

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ABSTRACT

For measuring ionization cross section of inner shells of a molecule ,electron impact method is one of most effective and useful tool. It has a vast range of applications in various fields as radiation analysis, plasma and atmospherics physics, low temperature study and many more. Using this method different fragmented ions from the molecule CHF3 , CF^+_3,CHF^+_2,CF^+_2,CHF^+,CF^+,F^+,CH^+,C^+ are being formed. In this highly energized e^- are incident on targeted molecule Further scattered, ejected as well as recoil ions are examined in terms of energy, momentum and angular distribution is studied and their cross section is measured. A semi empirical approach is used and applying modified Jain and khare formula partial and total cross section is caculated and result is compared with already existing data achieved by different method and both found to be in good agreement.

NCRAPS: PHY-06

ELECTRON IMPACT IONIZATION CROSS SECTION FOR BF3

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ABSTRACT

Calculation of electron impact total and partial ionization cross sections for halide molecules like , BF3,BCl3 molecules etc. We are performing this by using semi-empirical formula based on Jain Khare formalism. As previous data seem to exist for differential cross sections, we have derived the partial and total ion ionization cross section from these differential cross sections from ionization threshold up to different energies and compared with available experimental and theoretical data.

NCRAPS: PHY-07

RAMIFICATION OF ND $^{3+}$ SUBSTITUTION ON STRUCTURAL, OPTICAL AND DIELECTRIC PROPERTIES OF $LAPO_4$ CERAMICS

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ABSTRACT

Phosphor-procured emitting diodes are most significant and technologically source especially for solid state illumination applications due to its enormous potential. The 4f electrons in lanthanide based orthophosphate materials have been attracted a lot of attention in current research for light emitting applications in semiconductor industry. For remarkable

resolution in solid state illumination applications such as Light Emitting Diodes, rare earth modified phosphate materials become important candidates and materials of choice. While some other rare earths modified phosphates which belongs to this category have been very in red, blue, &green light emitting diodes with exceptional light-emitting properties. Fuel cells, refractory materials, heat-resistant materials, monazite or xenotime structural phases of rare earth phosphate are particularly important for their usage in high temperature photonic conductors. The requirement for light-emitting diodes in solid-state lighting applications is the focus of current research, and phosphates are emerging as viable materials for such vital applications. In present paper, we report structural, optical, luminescence and dielectric properties of Nd 3+ modified LaPO 4 at La 3+ site. The Nd 3+ modified ceramics have been synthesized using Auto Combustion method. The structural phase analysis has been confirmed from X-ray diffractograms whereas micro-structural analysis studied using SEM micrographs. The SEM micrographs also gives us information about grains growth and densification. The effect of Nd 3+ substitution on band gap studied from Taue's plot whereas PL data gives information about excitation wavelength. The dielectric measurements have been recorded using impedance analyzer.

NCRAPS: PHY-08

PARTIAL DIFFERENTIAL CROSS-SECTION ANALYSIS FOR $CCLF_3$ MOLECULE DISSOCIATIVE IONIZATION: A SEMI-EMPIRICAL STUDY AND COMPARATIVE VALIDATION

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ABSTRACT

In this research paper, we conducted an evaluation of the partial differential cross-section for the dissociative ionization of the CClF3 molecule, spanning from the ionization threshold up to 5000 electron volts (eV). This study underscores the practicality of employing Mass Spectroscopy, utilizing a semi-empirical approach. To determine the electron impact ionization cross-section for $CClF_3$ molecules, we adopted a semi-empirical formula that combines elements from Bethe theory and Binaryencounter theory. The results we computed were subjected to comparisons with both experimental and theoretical data. Notably, the various cross-sections we calculated exhibited a remarkable level of agreement with previously established data.

NCRAPS: PHY-09

A REVIEW ON METHYLENE BLUE DEGRADATION ACTIVITIES OF VARIOUS TRANSITION METAL OXIDES NANOCOMPOSITES

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ABSTRACT

In recent time, the major issue faced by the society is to get clean water for the drinking purpose. One of the most common chemical that renders water unsafe for drinking is industrial dyes. Out of so many dyes, Methylene Blue (MB) dye is the one that is used in textiles causing dye effluent contamination. It is non-biodegradable, poisonous and carcinogenic which is hazardous for environment and human health. Therefore, it is necessary to create an effective, environmentally acceptable method of removing MB from wastewater. Nowadays, metal oxides based semiconductor is used as a photo catalyst for removing organic dye in wastewater. But their photocatalytic efficiency is constrained due to large forbidden gap and large recombination time of electron hole pairs. Thus, researchers continuously worked to improve the degradation efficiency using a dopant or by forming nanocomposites. Therefore, in the current review article, the synthesis method of metal oxide (MO) nanoparticles and their photocatalytic efficiency toward MB dye have been discussed.

NCRAPS: PHY-10

EFFECT OF ZINC OXIDE DOPANT ON THE STRUCTURAL, OPTICAL, AND MAGNETIC PROPERTIES OF A-FE_2O_3 NANOCRYSTALLINE STRUCTURE

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ABSTRACT

Recent research demonstrates that unique progressive properties of nanomaterials have contributed to significant advancements in several fields. Therefore, in the current study zinc oxide (5%, 10%, and 20%) – doped Fe_2O_3 nanoparticles were synthesized by co-precipitation method and then treated with microwave radiation. Further, the prepared samples were calcined for two hours at a temperature of 600°C and the samples were characterized using various techniques to check their suitability in various applications. For that purpose, initially the formation of nanoparticles was confirmed using X-Ray diffraction analysis (XRD) data and found a hexagonal crystalline structure. The grain size was also calculated using Debye Scherrer formula which increased from 23nm to 30 nm with increase in doping. Through transmission studies, it was observed that the band gap decreases with increase in doping concentration. In all the calcined samples, the alpha and gamma mixed-phase graphs were constrained by the Infrared (IR) peak positions at 540 cm^{-1} and 625 cm^{-1} in the range of the Ultraviolet–visible (UV-Vis) spectrometer. The magnetic properties of the prepared sample were analyzed by Vibrating sample magnetometer (VSM), and it was observed that the saturation magnetisation decreases as doping concentration of zinc oxide increases.

NCRAPS: PHY-11

FIRST PRINCIPLE INVESTIGATIONS OF K DOPED $CUINSE_2$ FOR OPTOELECTRONIC APPLICATIONS

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ABSTRACT

$CuInSe_2$ is a ternary compound and a fine viable substitute of polycrystalline silicon for photovoltaic applications. In this work we computationally investigated the consequence of K atom doping in $CuInSe_2$. The structural, electronic, and optical features of the K doped $CuInSe_2$ compound was calculated using the full potential linearized augmented plane wave approach. Furthermore, the Wien2k algorithm performs the most accurate Tran-Blaha modified BeckeJohnson (TB-mBJ) exchange approximation. To ascertain the optical efficacy of compound under study, optical parameters including the real and imaginary dielectric tensor, absorption coefficient, reflectivity, and refractivity are computed. For $Cu_{0.8125}$ $K_{0.1875}$ $InSe_2$, the energy band gap value revealed via TB-mBJ is 1.07eV. According to states adding K doping to the Cu site in $CuInSe_2$ improves the band gap value, indicating its potential use in solar devices. The compound acquired optical and electronic properties significantly implied that it would be useful in optoelectronic applications.

NCRAPS: PHY-12

SYNTHESIS AND CHARACTERIZATION OF MIXED PHASE MANGANESE OXIDE NANOPARTICLES PREPARED BY SIMPLE CO-PRECIPITATION METHOD

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ABSTRACT

With their exceptional qualities such as high specific surface area, a high fraction of surface atoms, non-toxicity, and excellent redox properties, manganese oxide nanoparticles—a transition metal oxide with a variety of crystal phases, morphologies, and structural diversity— are attracting attention for use in several storage science applications, particularly in batteries, supercapacitors, energy conversion, environmental catalysis, and wastewater treatment [1-2]. To fully explore their application potential, it is important to have precise control over several factors such as particle size, morphology, surface area, and Mnx $^{+}$ oxidation state. [3] The present study describes the synthesis of manganese oxide nanoparticles through a facile coprecipitation method that employs double precursor salts of manganese, namely manganese sulphate and potassium permanganate, along with three surfactants: KCl (cationic), Polyethylene glycol (PEG-Non-ionic), and sodium dodecyl sulphate (SDS-anionic), respectively. At 500 °C, the samples are subsequently annealed. Samples are examined using XRD, both as prepared and annealed. In the absence of any calcination treatment, the MnO_2 - precursor was primarily an amorphous phase with indistinct amorphous α-MnO_2 crystal patterns for all the samples. Well-defined crystalline prominent peaks of α-Mn_2O_3 with some traces of α-MnO_2 visible for samples prepared with different surfactants and without surfactants after calcination at 500°C. Crystallite sizes and macrostrains etc are estimated. By using this one-spot calcination method, mixed phases of α-MnO_2 and α-Mn_2O_3 were produced. The thermogravimetric analysis also supports the results

NCRAPS: PHY-13

ELECTRON IMPACT IONIZATION CROSS SECTION OF CARBON COMPOUNDS

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ABSTRACT

Cross sections of many different types of carbon compounds can be determined by various techniques during the last decades. Electron impact ionization of rare gas ions is an important process in high energy chemical processes, such as in planetary atmospheres and in plasma physics. Inelastic collision between electrons and molecules are dominated by channels yielding both electrons and positive ions. We have study of ionization rate coefficients as a function of electron temperature in the units of energy for the individual cations produced in electron collision with the organic molecule.

NCRAPS: PHY-14

INVESTIGATION OF STRUCTURAL AND OPTO-ELECTRONIC FEATURES OF RB_2TLSBX_6 (X = CL, BR) MATERIALS FOR PHOTOVOLTAIC AND SOLAR CELL APPLICATIONS.

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ABSTRACT

In this article, we have investigated theoretically the structural, electronic, and optical properties of the Rb_2TlSbX_6 (X = Cl, Br) double Perovskite compounds. All the calculations are done by using Perdew-Burke-Ernzerh generalized gradient approximation (PBE-GGA) as embodies in Wien2k [1]. And NANODCAL code [2,3]. From both the methodologies, it is found that the energy gap of studied halide Perovskite compounds lies in the energy range 1.10 –1.70 eV which is appropriate range for optoelectronics and solar cell applications. The formation of individual energy bands of Rb_2TlSbX_6 (X = Cl, Br) compounds are explain with help of density of state (DOS) spectra. The narrow band gap, exceptional optoelectronic properties, good light absorption capacity, excellent environmentally favourable characteristics, and are devoid of toxicity, makes Rb_2TlSbX_6 (X = Cl, Br) compounds promising for photovoltaic and optoelectronic applications.

NCRAPS: PHY-15

SYNTHESIS PROCESSES, AND APPLICATION OF ZNO NANOSTRUCTURES AS PHOTOCATALYSTS: A REVIEW

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ABSTRACT

POPs are chemical compounds with a carbon basis that are resistant to environmental deterioration and may not be totally eliminated despite treatment procedures. Their persistence may have detrimental health effects on both people and wildlife. Thus, due to its enormous potential as a green and eco-friendly technique for the elimination of POPs to strengthen the security of pure water, the solar photo catalysis process has drawn increasing attention. Given that they are inexpensive, non-toxic, and more effective at absorbing a significant portion of the solar spectrum than TiO_2, ZnO nanostructures have been demonstrated to be major photocatalyst candidates to be employed in photo degradation. However, there are a number of factors that must be taken into account for continued development. Reviewing POP photo-degradation mechanisms and recent advancements in ZnO nanostructured production methods, including doping, heterojunction, and modification techniques, as well as advancements in ZnO as a photocatalyst, are the goals of this research. The review's second goal is to assess the immobilization of photocatalyst and suspension systems while considering their potential and upcoming difficulties.

NCRAPS: PHY-16

RECENT ADVANCEMENT IN PEROVSKITES MATERIALS FOR OPTOELECTRONIC AND PHOTOVOLTAIC APPLICATION.

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ABSTRACT

This article suggests development of perovskites materials for the Solar cell applications. Although the traditional perovskites materials exhibit significant promise in photovoltaic applications, they face notable challenges. These challenges encompass issues with long-term stability, toxicity, material considerations, and scalability. However, recent advancement in Double perovskites, on the other hand, offers several advantages that potentially mitigate these drawbacks like enhanced stability, tunable bandgaps, reduced toxicity concerns, better charge carrier mobility etc. Because of their tunable bandgaps, double perovskites have prospective applications in photovoltaics, where they could improve solar cell performance and efficiency by absorbing a wider range of light , showing better optoelectronic properties and thermal conductivity. Additionally, This paper deals with Lead-free halide double perovskites which have shown immense improvement with passage of time with power conversion efficiency beyond 25%. Moreover, A comprehensive analysis of literature indicates that lead free double perovskites exhibit favourable optoelectronic properties and enhanced stability, positioning them as promising candidates for various applications. Further, the review concludes with the challenges and latest application in optoelectronic solar cell devices.

NCRAPS: PHY-17

DETERMINATION OF CROSS-SECTION OF INORGANIC MOLECULE THROUGH ELECTRON IMPACT IONIZATION

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ABSTRACT

In our research, we will expand the semi-empirical Jain and Khare formula to determine the partial and total ionisation cross-section of an inorganic molecule and its fragmentation ions due to electron impact at incident electron energy. The calculated cross-sections will then be compared to other theoretical cross-sections and the most current experimental data.

NCRAPS: PHY-18

IONIZATION CROSS SECTION PROCESS FOR MOLECULES BY ELECTRON IMPACT

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ABSTRACT

In this paper, we report modified calculation for total ionization and total cross sections for molecules. We describe the recent progress in the development of the semi-empirical approach developed by Jain-Khare for the calculation of ionization cross section for molecules by electron impact. We calculate this for different molecules upon electron impact at different energies. These energies lie from around threshold to 3000 eV. The present results are compared with available experimental data and other theoretical data wherever available.

NCRAPS: PHY-19

PARTIAL AND TOTAL CROSS SECTION DETERMINATION OF ORGANICCOMPOUND BY ELECTRON IMPACT

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ABSTRACT

For measuring ionization cross section of inner shells of a molecule, electron impact method is one of most effective and useful tool. It has a vast range of applications in various fields as radiation analysis, plasma and atmospherics physics, low temperature study and many more. Using Jain Khare method for different fragmented ions from the organic compound, Further scattered, ejected as well as recoil ions are examined in terms of energy, momentum and angular distribution is studied and their cross section is measured. A semi empirical approach is used and applying modified Jain and khare formula partial and total cross section is calculated and result is compared with already existing data achieved by different method and both found to be in good agreement.

NCRAPS: PHY-20

PARTIAL AND IONIZATION CROSS SECTION PROCESS FOR MOLECULES BY ELECTRON IMPACT

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ABSTRACT

In this paper, for measuring ionization cross section of inner shells of a molecule, electron impact method is one of most effective and useful tool. It has a vast range of applications in various fields as radiation analysis, plasma and atmospherics physics, low temperature study and many more. We describe the recent progress in the development of the semi-empirical approach developed by Jain-Khare for the calculation of ionization cross section for molecules by electron impact. We

calculate this for different molecules upon electron impact at different energies. These energies lie from around threshold to 4000 eV. The present results are compared with available experimental data and other theoretical data wherever available.

NCRAPS: PHY-21

FERMI ARC SURFACE STATES AND ELECTRONIC BAND STRUCTURE OF THE WEYL SEMIMETAL IN TAP

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ABSTRACT

Weyl semimetals open a new scope in physics and materials science and they provide the first realization of Weyl fermions and shows Fermi arc surface states. But they found rare in nature. Family of transition metal pnictide was first predicted as a Weyl semimetal candidates. Using photoemission spectroscopy Weyl fermion cones and nodes in the bulk and the fermi arc on the surface directly observed. Weyl fermions have distinct chiralities either left-handed or right-handed. ARPES data is used to study the bulk and surface electronic structure of the Weyl semimetal TaP. TaP crystal is a body-centered tetragonal Bravais lattice.The basis constists of two Ta atoms and two P atoms. X-ray diffraction measurement showed the lattice constants of TaP samples. In this crystal structure, each layer is shifted relative to the layer below by half a lattice constant i either the x or the y direction.

NCRAPS: PHY-22

EVALUATION OF ELECTRON IMPACT IONIZATION CROSS SECTION FOR RADIOACTIVE MOLECULE

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ABSTRACT

We report here the total and partial ionization cross section for radio molecules by Electron Impact. To calculate this we use the semi-empirical formulation based on the well-known Jain-Khare formulation. In this article we are presenting data for energies ranging from threshold to different value. Our results are compared with available experiment and theoretical data wherever available. The present study also establishes the validity of the semi empirical approaches.

NCRAPS: PHY-23

UNRAVELLING IONIZATION DYNAMICS: A SEMI-EMPIRICAL EXPLORATION OF PARTIAL IONIZATION CROSS SECTION IN ORGANIC COMPOUNDS

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ABSTRACT

This paper endeavours to unravel the intricacies of ionization processes in organic Compounds. Employing a semi-empirical approach, we calculate the total ionization cross sections across the energy spectrum, ranging from threshold to 5000 eV. Through a systematic comparison with existing results, we enhance the semi-empirical formula, specifically tailoring it for the calculation of partial differential cross sections in Organic Compounds. The foundation of our semiempirical model rests upon the Jain & Khare formalism, promising a comprehensive understanding of ionization phenomena.

NCRAPS: PHY-24

PHYSICAL-CHEMICAL EXAMINATION OF SECUNDERABAD, TELANGANA'S GROUNDWATER

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ABSTRACT

Physico chemical analysis of groundwater comprehends about present status of water for household and industrial purposes. Due to coercion of human activities, industrialization and urbanisation, the groundwater genesis is disrupted gradually. Thus, safe , healthy, odorless and pure water has become a matter of deep concern. This study sets one's sight on the chloride levels of various drinking sources, especially in state of Telangana. Here we have examined various water quality parameters such as pH, TDS, electrical conductance, total hardness, magnesium, calcium, total alkalinity, bicarbonate, carbonate,etc.

NCRAPS: PHY-25

DETERMINATION OF ELECTRON IMPACT IONIZATION CROSS SECTIONS OF CS MOLECULE

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ABSTRACT

The electron impact ionization of CS has been investigated across a range of electron energies, spanning from the threshold to 2500 eV. A double-focusing sector field mass spectrometer with reversed geometry, featuring enhanced ion transmission characteristics, was utilized for this study. This configuration enables the comprehensive and controlled collection of mass-selected parent and fragment ions, facilitating the precise measurement of quantitative electron impact ionization cross-sections. Absolute partial ionization crosssection functions were determined for CS by semi empirical Jain and Khare formulism. Additionally, the total ionization cross-section determined and compared with previous experimental and theoretical findings.

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NCRAPS: PHY-26

PARTIAL AND TOTAL CROSS SECTION DETERMINATION OF CHF_3 BY ELECTRON IMPACT

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ABSTRACT

For measuring ionization cross section of inner shells of a molecule, electron impact method is one of most effective and useful tool. It has a vast range of applications in various fields as radiation analysis, plasma and atmospherics physics, low temperature study and many more. Using this method different fragmented ions from the molecule CHF_3, CF_3^+ , CHF_2^+ ,CF_2^+ ,CHF+ ,CF^+ ,F^+ ,CH^+ ,C + are being formed by highly energized e^- are incident on targeted molecule Further scattered, ejected as well as recoil ions are examined in terms of energy, momentum and angular distribution is studied and their cross section is measured. A semi empirical approach is being used and applying modified Jain and Khare formula partial and total cross section is calculated and result is compared with already existing data achieved by different method and both found to be in good agreement. The Threshold energy being discussed in this paper is 0-5000ev.

NCRAPS: PHY-27

ELECTRON IMPACT IONIZATION: A COMPREHENSIVE ANALYSIS USING AN ENHANCED SEMI-EMPIRICAL MODEL

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ABSTRACT

In this study, we have refined S.P. Khare's theoretical semi-empirical model to compute total cross sections for electron impact ionization of organic molecules, spanning the energy range from the ionization threshold to 5000 eV. Our focus is on comprehending partial and total ionization cross sections for organic molecules and their fragmentation ions at diverse energy levels. The calculated cross sections exhibit remarkable agreement with experimental data, particularly for fragment ions. However, notable discrepancies emerge, underscoring the necessity for further exploration. This research significantly contributes to the broader comprehension of electron impact ionization, with implications extending to plasma studies, fusion modeling, astrophysics, and planetary atmosphere modeling.

NCRAPS: PHY-28

COMPOSITE OF VANADIUM OXIDE AND ACTIVATED CHARCOAL: ELECTROCHEMICAL AND ANTI-MICROBIAL STUDIES

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ABSTRACT

Activated carbon based composite of V_2O_5 nanoparticles was prepared via one pot hydrothermal synthesis showing enhanced capacitive performance in comparison with pure V_2O_5 nanoparticles. AC absorbs more electrolyte as compared to V_2O_5 nanorods due to its high porosity leading to its enhanced charge storage and higher performance. SEM and TEM images indicate that the growth of V_2O_5 nanorods has taken place around AC microsized particles and fully interact with each

other. The electrochemical study of the material revealed a modified charge storage behaviour of the composite and specific capacitance of 545.56 F g^{-1} at 0.6 A g^{-1} current density. The low value of series resistance (12 Ω) and negligible charge transfer resistance show that the interaction between carbon and V_2O_5 has led to enhancement in the electrolyte-electrode interaction which results in better performance. The composite was also tested for anti-microbial properties which revealed that the material demonstrated bactericidal activity by inhibiting the respiration activity and thus damaging the cellular components.

NCRAPS: PHY-29

VANADIUM AND ACTIVATED-CARBON BASED ACTIVE MATERIALS FOR SUPERCAPACITORS

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ABSTRACT

Supercapacitors are advanced designs of capacitors that have a higher energy density than conventional capacitors. Supercapacitors are promising for energy storage. The performance of a supercapacitor is mainly influenced by the active materials. In nano derivatives of carbon such as graphene, reduced-graphene-oxide (RGO), carbonnanotubes (CNTs), which have been studied as active materials, activated carbons are low-cost and have large surface area but low electrical conductivity. Similarly, among various metal oxide materials, the low cost, low toxicity, layered structure and multiple oxidation valences of nano structured V_2O_5 makes it outstanding among other oxide materials. This review mainly discusses the active electrode materials based on Vanadium and activated carbon.

NCRAPS: PHY-30

CROSS-SECTION OF INORGANIC ATOM THROUGH ELECTRON IMPACT IONIZATION AT DIFFERENT ENERGY RANGE

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ABSTRACT

In our research work, we will expand the semi-empirical Jain and Khare formula to determine the partial and total ionization cross-section of Inorganic atom and its fragmentation ions due to electron impact at different incident electron energy above from ionization threshold. Comparing the calculated cross-sections with other theoretical cross-sections and the experimental evidence that is currently available.

NCRAPS: PHY-31

STRUCTURAL INNOVATION IN AZOLE COMPOUNDS: ENHANCING EFFICACY AND STABILITY

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ABSTRACT

The present study emphasizes the structural modification of azole-based heterocyclic compounds to improve their therapeutic efficacy and stability. Azole compounds, notably used for their antimicrobial properties, often face limitations in clinical settings due to reduced efficacy against resistant strains and stability issues. In addressing these challenges, our research focuses on chemical modifications to the azole nucleus and its adjacent functional groups. This approach aimed to enhance the compound's interaction with biological targets, increase resistance to enzymatic degradation, and improve overall pharmacological properties. The study involved the synthesis of various azole derivatives, followed by their characterization using techniques like NMR, IR spectroscopy, and mass spectrometry. The antimicrobial efficacy of these compounds was assessed through Minimum Inhibitory Concentration (MIC) assays, demonstrating a significant increase in activity against resistant pathogens. Furthermore, stability tests revealed enhanced resilience to physiological conditions. These findings suggest that structural innovation in azole compounds can lead to more effective and stable therapeutic agents, providing a new direction in the development of antimicrobial drugs. The study's implications extend beyond antimicrobial therapy, opening possibilities for their use in treating other diseases.

NCRAPS: PHY-32

TOTAL AND ABSOLUTE IONIZATION CROSS SECTION FOR RADIOACTIVE ATOMS

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ABSTRACT

We report here the total and partial ionization cross section for radioactive atoms by Electron Impact. To calculate total and absolute ionization cross section, we use the semi-empirical formulation based on the well-known Jain-Khare formulation. In this article we are presenting data for energies ranging from threshold to different value. Our results are compared with available experiment and theoretical data wherever available.

NCRAPS: PHY-33

RADIATION CHARACTERIZATION OF RECTANGULAR MICROSTRIP ANTENNA IN COMPLEX PLASMA MEDIA

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ABSTRACT

This paper presents the radiation charaterstics of rectangular microstrip antenna in complex plasma media. In present world microstrip antenna play a key role for wireless services. Rectangular microstrip antenna have many advantages like low cost, easy to fabricate, small in size, simple structure , feedline flexibility etc. Rectangular Microstrip antenna have also many of applications like radar, mobile communications, space , healthcare etc. We study how the Impedance , gain, Resonant

frequency, E-H field effect the radiation pattern for the rectangular microstrip antenna in complex plasma media. The microstrip antenna designed at the frequency of 5GHz.

NCRAPS: PHY-34

EVALUATION OF ELECTRON IMPACT IONIZATION CROSS SECTION FOR RADIOACTIVE ATOM

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ABSTRACT

We report here the total and partial ionization cross section for radioactive atom by Electron interaction. To calculate this, we use the semi-empirical formulation based on the well-known Jain-Khare formulation. In this article we are presenting data for energies ranging from threshold to different value. Our results are compared with available experiment and theoretical data wherever available. The present study also establishes the validity of the semi empirical approaches.

NCRAPS: PHY-35

REFLECTING RESPONSE OF $HgGa_2S_4$ IN SOFT X-RAY REGIME: DFT COMPUTATIONS

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ABSTRACT

$HgGa_2S_4$ is adamantine ordered vacancy compound of $A^{II}B_2^{III}X_4^{VI}$ family which crystalizes in tetragonal defect chalcopyrite structure with space group I-4. In this work, we present its frequency dependent reflectivity using full potential linearized augmented plane wave method with the latest modified Becke-Johnson potential. The optical reflectivity is shown in Fig 1. At the zero energy level the calculated amplitude of reflectivity is found to be 0.155 and 0.150 for perpendicular and parallel directions. Present reflectivity curve shows almost 70% reflectivity near 14 eV. Moreover, real part of the dielectric function $\varepsilon_1(\omega)$ shows negative values between 8 eV and high side of the shown spectra. On the basis of real part $\varepsilon_1(\omega)$ and reflectivity curves, it is concluded that $HgGa_2S_4$ can be employed as soft X-rays reflector, besides its use in optoelectronic devices.

NCRAPS: PHY-36

QUANTUM CHAOS IN THE SACHDEV-YE-KITAEV MODEL: EXPLORING LYAPUNOV EXPONENTS AND CONFORMAL SYMMETRY

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ABSTRACT

Our work focuses on the quantum aspects of chaos in quantum field theory. We start with classical dynamical systems, then chaotic systems and their Lyapunov exponents. Next, we explore the relationship between quantum and classical chaos. We examine the SYK model, which has similar properties, and derive the Schwinger-Dyson equation for the two-point function. We also obtain the leading order correction for the four-point function and investigate the chaotic behavior in SYK to compute the Lyapunov exponent.

NCRAPS: PHY-37

SOLVATOCHROMIC ESTIMATION OF GROUND AND EXCITED STATE DIPOLE MOMENTS IN THE LASER DYE NILE BLUE 690

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ABSTRACT

In this comprehensive study, we experimentally investigate the solvatochromic influence on the photophysical characteristics of the fluorescent dye Nile Blue 690. Our primary objective is to examine the dipole moments of Nile Blue 690 using the solvatochromism method by analyzing absorption and fluorescence spectra in various solvents with varying polarities. We utilized diverse models to assess the dipole moments of the chosen molecule. This involves considering microscopic solvent polarity parameters, including Bakhshiev, Bilot-Kawski, Kawski-ChammaViallet, Lippert-Mataga, and Reichardt, in both the ground and excited states and conducted a meticulous comparative analysis of the calculated dipole moments. The findings reveal a consistent pattern: the molecule examined exhibit a lower dipole moment in their ground state compared to their singlet excited state. This finding provides valuable insights into the molecular behavior under diverse solvatochromic conditions, contributing to a deeper understanding of the dynamic interplay between molecular structures and their environment.

NCRAPS:MATH-01

EFECT OF ROTATION ON THE ONSET OF CONVECTION IN MAGNETIC NANOFLUIDS CONTAINING GYROTACTIC MICROORGANISMS

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ABSTRACT

The focus of this work is on employing linear stability analysis to investigate the initiation of the bioconvection (B_{convec}) phenomenon in the presence of rotational influences. In this study, we examine a water based magnetic nanofluids $W_b - M_g N_f$ that contains gyrotactic microorganisms, taking into account the influence of gravity. The motion of the microorganisms is considered to be motile and of small size, rendering the inertial effects negligible. The employed model incorporates the combined impact of two slip mechanisms, namely Brownian motion and thermophoresis, as suggested by J. Buongiorno (J. Buongiorno, "Convective transport in nanofluids", Journal of Heat Transfer, 128(3), 240–250, 2006), in addition to magnetophoresis. To solve the resulting eigenvalue problem, a numerical method utilizing MATLAB's EIG function is utilized. The critical Rayleigh number Ra_c is determined through neutral stability curves $(N_s C_{urves})$ to analyze the system, considering the governing parameters. The Taylor number T_a is employed to investigate the influence of rotation, revealing that it stabilizes the system.

Keywords: Rotation, Bioconvection, Magnetic nanofluids, Microorganisms

NCRAPS:MATH-02

NUMERICAL SOLUTION OF DELAY DIFFERENTIAL EQUATIONS USING HAAR WAVELET COLLOCATION METHOD

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ABSTRACT

The Haar wavelet collocation approach is introduced in this paper to find numerical solutions to delay differential equations. Some proportional delay problems are solved to demonstrate the efficiency and dependability of the method. The solutions obtained are compared to the exact solution and existing solution to measure the accuracy of the output obtained. To further strengthen the reliability of the method, error analysis is also performed. Finally, it is concluded that with the increase in resolution level, the accuracy of the solution improves.

Keywords: Delay differential equation, HAAR wavelet, collocation points, numerical solution error

NCRAPS:MATH-03

NUMERICAL ANALYSIS OF SORET AND DOFOUR IMPACTS ON MHD HYBRID NANOFLUID FLOW PAST A NONLINEAR STRETCHABLE SHEET

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ABSTRACT

This study evaluates the unsteady laminar flow, heat transfer, and mass transfer of conventional nanofluids against those of newly emerging hybrid nanofluids. Boundary layer heat transfer has been improved with the help of hybrid nanofluid, a new kind of conventional fluid. Using the Darcy-Forchheimer flow inside the vicinity of a nonlinearly passable stretched surface in the context of nonlinear heat radiation, we deal with water to be the base fluid and copper and aluminium oxide to be nanoparticles. Similarity conversion is familiar with reduced governing models into dimensionless variables, and the bvp4c approach is adpoted to acquire the solution numerically. The numerical parametric study, supervised to check out the impact of different physical parameters on the problem, also provides useful comparisons. Variations in fluid parameters are used to sketch out the resulting graphs. Coefficient of surface drag, heat flux, and mass flux are all numerically interpreted. The high resistance offered by local inertia coefficient causes an increase in the skin's friction. Numerical tests with change of Dufour (which rates the holdings of gradient of concentration's essence on heat exchange) have put on display that gradient of concentration is high profitable in the context of hybrid nanofluid, and this is true both in the fluid regime and in the case of hybrid nanofluids. Also it is noted that Soret number is a measure of the degree to which a solute's diffusivity in a fluid is altered by changes in temperature.

Keywords: Hybrid nanofluid, Non-linear stretching sheet, Darcy-Forchheimer flow, Soret-Dufour effects.

NCRAPS:MATH-04

MULTI SLIP EXPLORATION OF WILLIAMSON MATHEMATICAL MODEL IN TRIHYBRID NANOFLUID FLOW OVER WEDGE, CONE AND PLATE

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ABSTRACT

Primary motive of this research work is to conduct a study for the tri-hybrid nanofluid flow with different particles shape. CuO, Ag, Cu are dispersed in H_2O. Suction/injection along with porous medium is introduced for the non-Newtonian Williamson mathematical model fluid flowing over the wedge, cone and plate. The impacts of electromagnetic field with heat source were incorporating for the radiative flow. Mass transfer is also embraced with multi slip boundary layer flow. All the effects were displayed in mathematical formulation of the flow which then transfigure into ODE's by utilising the similarity transformations. Graphical forms of the parameters are portrayed with the aid of bvp4c solver in MATLAB software.

Keywords: Suction/injection, tri-hybrid, Williamson mathematical model, multi slip, Suction/injection.

NCRAPS:MATH-05

CONVERGENCE OF PERIODIC FUNCTIONS IN HÖLDER'S CLASS BY TRIPLE PRODUCT MEANS

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ABSTRACT

Signals, which are periodic functions, belonging to various classes have been processed using various summability transforms. Also, abundant researchhave been carried out to estimate the error between the input and output signals. Singh [2] defined the Hölder's i.e. H_ω space and also approximated the functions belonging to this space using the product summability $(C,1)(E,1)$ [2]. In this article, we first introduce the triple product transform i.e. $(N,p_n)(C,1)(E,1)$ on the H_ω space via conjugate of Fourier series.

Keywords: Degree of Approximation, Fourier series, (C, 1)(E, 1) means.

NCRAPS:MATH-06

SOLUTION OF AN INTEGRAL EQUATION VIA FISHER TYPE HYBRID CONTRACTION IN CONTROLLED METRIC SPACE

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ABSTRACT

In the present manuscript, we shall introduce a new notion of Fisher type hybrid contraction in controlled metric spaces and prove some fixed point results for such type of contraction. Some non-trivial examples will be discussed to prove the validity of our results. Some results from the literature are also deduced from the main results. As an application, an integral equation is also solved by making use of our results.

Keywords: Fisher type hybrid contraction, fixed point, controlled metric space.

NCRAPS:MATH-07

A NEW TOOL TO SOLVE DATA RELATED PROBLEM WITH SOURCE CODING THEOREM

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ABSTRACT

The most significant aspect of the new generalization of entropy $._k h(\Re)$ that we provide in this study is its ability to derive the most significant entropies that are well recognized and have an impact on applied mathematics and information theory. In

this article, some important characteristics of $_{.k}\ h(\Re)$ have been investigated. Also presented a new generalized mean code word length $_{.kl}\ I = \frac{1}{k-1}\log_D\left\{\frac{\sum(\Re_t)^{l_D - m_t(k-1)}}{\Re_t}\right\}$ and obtained the source coding theorem relationship between $(\ )_k\ h(\Re)$ and $_{.kl}\ \mathrm{I}$.

Keywords: The Huffman and Shannon Fano coding techniques, average codeword length, Kraft's inequality, the source coding theorem, and code alphabets.

NCRAPS:MATH-08

VISCOPLASTIC FLUIDS FLOW ANALYSIS IN MULTIMEMBRANE FITTED POROUS CHANNEL

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ABSTRACT

Bingham plastic fluid flow driven by multi-membrane pumping mechanism in porous media is presented mathematically. The motivation behind this mathematical analysis is to examine the rheological effects of Bingham Plastic fluid on flow analysis, wall shear, pressure distribution, pumping characteristics, stream line patterns and discuss the importance for the physiological transport phenomena. Considering creeping flow nature of physiological transport, lubrication approach is utilized. Analytical approaches are adopted to derive the closed form solutions and graphical results are simulated using MATLAB code. The examination revealed that the movement of substances in the channel is greatly influenced by the difference in timing between the phases of the two walls channel. The analytical results indicate that the flow characteristics and pumping characteristics are significantly affected by the plasticity of the fluids as well as permeability parameter. Such types of results are highly recommended for the designing of the micro-valveless pumping actuator to control the microscale transport phenomena of physiological systems.

NCRAPS:MATH-09

JENSEN'S FUZZY INEQUALITIES, CSISZAR Φ- FUZZY MEASURE, BOUNDS AND APPLICATION IN PATTERN RECOGNITION

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ABSTRACT

In mathematics, inequalities are utilized to analyse the overall size of quantities. They can be utilized to compare integers, factors, and different other mathematical expressions and Inequalities are especially helpful for tackling issues including least or greatest possible qualities. The goal of our paper to present new Jensen's fuzzy inequality through convex function in term of (r, s) parameters and by this result we will propose some relations for Csiszars's fuzzy measure and their bounds. Next we will present pattern recognition problem under Hellinger fuzzy measure.

Keywords: Fuzzy Set, Jensen type Fuzzy Inequality, Csiszar Fuzzy Measure, KL Fuzzy Measure, Hellinger Fuzzy Measure, Pattern Recognition

NCRAPS:MATH-10

PARAMETRIC PROPERTIES OF NEW F-DIVERGENCE MEASURE

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ABSTRACT

Here we discussed the parametric properties of new f-divergence functional. There are many papers published on these measures. This measure is also known as Jain and Saraswat measure which is established in 2012. The applications of this measure in the form of series using the properties of convexity have been established in this article.

Keywords. Fisher information, New f-divergence measure, parametric measure of information etc.

NCRAPS:MATH-11

THERMAL ANALYSIS OF CHEMICALLY REACTIVE MAGNETIZED FLUID FLOW THROUGH ROTATING HORIZONTAL CHANNEL IN THE OCCURRENCE OF HALL CURRENT AND RADIATION

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ABSTRACT

The aim of the current study is to analyze the chemical reactive MHD natural convective flow through the porous medium occupied horizontal channel rotating in its plane in the presence of hall current and thermal radiation. The governing equations of the velocity field, temperature and mass transfer are modelled, and their closed-form solutions are also obtained. In addition, shear stress, rate of heat transfer and rate of mass transfer are also calculated for pertained flow constraints. It is perceived that fluid velocity detracts in the x and y direction with the rise in the rotational parameter and growth in the heat source and radiation decrease the temperature field.

Keywords : Chemical reaction, Coriolis force, Radiation effects, MHD, Horizontal channel, Hall current, Heat source.

NCRAPS:MATH-12

MULTI-MEMBRANES BASED PUMPING FLOW OF NANOFLUIDS: MICROSCALE HEAT AND MASS TRANSFER ANALYSIS

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ABSTRACT

The microscale heat transfer is now very much essential to analyse and applicable in various smart thermal devices like microchannel heat sinks, micro heat pipes, thermosyphon, and micro heat exchangers, etc. In bio microfluidics point of view, the microscale heat transfer is very much significant to examine when the biological fluids are being transported by the natural pumping mechanism at micro scale. Inspired from the significant role of microscale heat transfer, nanofluids and natural pumping mechanism (i.e., membrane-based pumping), a biothermal based pumping flow model is developed mathematically and analysed computationally with help of MATLAB coding. A Ghost-Valve model for the membrane pumping formulated by the Yasser [17] is considered. For the microscale heat and mass transfer through microchannel, suitable approximation based on the lubrication theory has been adopted for analytical solution. For the mathematical formulation, conservation principles for mass, momentum, energy and nanoparticle fraction are considered. The results for pressure gradient, velocity distribution, volumetric flow rate, shear stress, streamlines, isotherms, nanoparticle fraction, Nusselt numbers, and Sherwood numbers, are computed using MATLAB software. Additionally, entropy generation is analysed for the microscale heat transfer in the multimembranes fitted microchannel to examine dissipated useful energy and degradation of the performance of thermal based pumping systems. Results reveal that the entropy generation increases with higher values of the thermal Grashof number, concentration Grashof number, Brinkmann number, and lower values of relative temperature. It is further reported that the membrane-based pump can effectively control micro level fluid flow and heat transfer in microchannel.

Keywords: Heat Transfer; Nanofluids; Ghost-valve model; Time phase lag; Nusselt Number; Entropy Generation.

NCRAPS:MATH-13

KAEHLERIAN PROJECTIVE RECURRENT MANIFOLDS OF UMBILICAN HYPERSURFACE

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ABSTRACT

Murgescu (1970) studied generalized weyl spaces, and Negi (2017) deliberated on Kaehlerian conharmonic bi-recurrent spaces. After that, Negi (2018) studied hyper asymptotic curves on Kaehlerian hypersurfaces. In the present paper, the author calculates Kaehlerian projective recurrent manifolds of umbilical hypersurface with a comprehensive weyl conharmonic recurrent curvature tensor and a projective recurrent curvature tensor.

Keywords: Kaehlerian weyl space, Weyl recurrent space, Conharmonic curvature tensor, Projective curvature tensor.

NCRAPS:MATH-14

S-CONVEX FUNCTIONS AND JAIN-SARASWAT'S FUNCTIONAL DIVERGENCE

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ABSTRACT

This article presents a new inequality for s-convex functions based on Jain-Saraswat's functional divergence measure. Functions that are convex are particular cases of s-convex functions. In addition, some special cases at different values of s have also been discussed in terms of divergences. A discussion has also been held on the verification of the obtained results.

NCRAPS:MATH-15

CONVOLUTION THEOREM ON SUM TRANSFORM AND APPLICATIONS OF SUM TRANSFORM

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ABSTRACT

Let (x) be a piecewise continuous real valued function. A transform called SUM transform is defined as $S_{\propto}[f(x)]_{(s)} = \frac{1}{s_n}\int_0^{\infty} f(x) \propto^{-sx} dx$ where, $x \geq 0$, $\alpha \in (0,\infty) - \{1\}, m_1 \leq s \leq m_2$, $m_1, m_2 > 0$. In this paper, we study the convolution theorem on the SUM transform and solve some of the problems in the engineering field using the new transform.

Key words: : Transform, SUM Transform, Convolution.

NCRAPS:MATH-16

RELATION-THEORETIC FIXED POINT THEOREMS FOR GENERALIZED Θ − Φ-CONTRACTION IN G-METRIC SPACES

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ABSTRACT

The work is intended as an attempt to motivate idea of f generalized θ − ϕcontraction in G- metric space. We wish to investigate few fixed-point theorems in G- metric space for generalized θ −ϕ- contraction with the help of ternary relation. Also, we have stated a fixed-point result for the right monotone function. We have given an illustration to assist our result.

Keywords: Ternary relation, G-metric space, t - complete metric space, t - continuous, T-closed, Generalized $\theta - \phi$ Contraction

NCRAPS:MATH-17

STUDY THE EFFECTS OF HEAT AND MASS TRANSFER OVER A NON-LINEAR STRETCHING SHEET WITH CROSS-FLUID FLOW

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ABSTRACT

To investigate the effects of heat and mass transfer with cross-fluid flow over a nonlinear stretching sheet. The given system of governing partial differential equations is altered into a system of highly non-linear ordinary differential equations with the help of appropriate similarity variables. The system of ordinary differential equations is reduced to the initial value problem by the shooting technique. The solution to the initial value problem is attained by the MATLAB bvp4c solver in the form of graphs and tables. Graphs represent the effect of parameters like Weissenberg number (We), Prandtl number (Pr), Schmidt number (Sc),and power law index on the velocity temperature and concentration profiles. The study accomplishes that for increasing values of the We velocity profile decreases and the growing values of the Prandtl number (Pr) lessened the temperature profile. The concentration profile increases for the increasing values of the Weissenberg number and the Schmidt number.

Keywords: Heat transfer, Mass transfer, Cross Fluid, Nonlinear stretching sheet, Weissenberg Number

NCRAPS:MATH-18

APPLICATION OF NEW FUZZY MEASURE IN MULTI-ATTRIBUTE DECISION-MAKING

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ABSTRACT

In this paper,we examined the multi-attribute decision-making application and the procedures that support it. Additionally, with the aid of an example utilising a new Fuzzy divergence measure that was previously researched, this application in the MADM case study has been discussed in terms of how to choose the optimal market for investment. we looked at application in multi-attribute decision-making and the processes that make it legitimate. Additionally, this application in the MADM case study has been described in terms of how to pick the best market for investment with the aid of an example using a new Fuzzy divergence measure that was previously investigated.

Keywords: New fuzzy divergence measure, Properties, Multi Attribute Decision making, Applications, Numerical presentation.

NCRAPS:MATH-19

HOPF LIGHTLIKE HYPERSURFACES OF INDEFINITE KENMOTSU SPACE FORM

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ABSTRACT

The object of present paper is to study the properties of Hopf lightlike hypersurfaces of indefinite Kenmotsu space form with an (ℓ, m)-type connection .

Keywords: : Hopf lightlike hypersurfaces, Kenmotsu manifold.

NCRAPS:MATH-20

ON ALMOST YAMABE SOLITON OF SASAKIAN MANIFOLD

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ABSTRACT

The object of present paper is to study the properties of almost Yamabe soliton on Sasakian manifold with Da-homothetic deformation and Schouten-van Kampen connection

Keywords: Schouten van Kampen connection, Sasakian manifold, Yamabe soliton.

NCRAPS:MATH-21

RAMAN SIGNATURE OF THE INTERACTION BETWEEN FUNCTIONALIZED MWCNT AND THE LIQUID CRYSTALLINE SYSTEM (4DBA)

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ABSTRACT

Liquid crystalline systems provide the best molecular matrix as a host for carbon nanotubes (CNTs) due to their fluidity character that controls the molecular ordering. The anisotropic shape of the CNTs makes them highly suitable nanoparticles that can be embedded in liquid crystalline systems to achieve uniform tunable dispersion. The uniform and stable dispersion of CNTs in the liquid crystalline host is challenging due to strong Vander Waal forces between CNTs. The functionalization of CNTs is one of the most popular techniques to achieve the dispersion system in an LC host due to the covalent bonding between CNT and LC systems. The COOH functionalized multi-wall carbon nanotubes (F-MWCNT) provide effective sites to interact with LC systems with the carboxylic group at the terminal. Raman spectroscopy is used as a probe to investigate the interaction between 4DBA and F-MWCNT through COOH---COOH dimer formation. Comparative Raman analysis of 4DBA, 4DBA + bare MWCNT, and 4DBA + F-MWCNT spectra show bands associated with the COOH group giving strong evidence of interaction between 4DBA and F-MWCNT. Raman study reveals the mechanism of dimer formation between F-MWCNT and 4DBA.

Keywords: 4DBA, MWCNT dispersion, F-MWCNT, Liquid crystal.

NCRAPS:MATH-22

APPROXIMATING FIXED POINT VIA F ITERATIVE ALGORITHM WITH SOLUTION OF A DELAY DIFFERENTIAL EQUATION

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ABSTRACT

The paper reports convergence, stability and data dependence results for the operators satisfying contractive conditions and contractive condition of rational expression using F iteration scheme in Banach space. With the help of suitable numerical examples, it is claimed that iteration process is more efficient than many other iterative schemes available in literature. As an

application, we have proposed solution to a delay differential equation. Our results are new and extend and improve many corresponding results available in the literature.

Key Words: delay differential equation, data dependence result, F-iteration.

NCRAPS:MATH-23

FIXED POINT THEOREMS FOR GENERALIZED (Ψ − Φ)-WEAK CONTRACTIONS IN S − METRIC SPACE

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ABSTRACT

In the present paper, we introduce a new notion of generalized (ψ − φ)-weak contraction in the setting of S − metric space. Further,some fixed point results are also proved by using this new notion. An example is also provided to support our result.

Key Words: fixed point, generalized (ψ − φ)-weak contraction, S − metric space.

NCRAPS:MATH-24

HYERS-ULAM STABILITY OF GENERALIZED QUADRATIC FUNCTIONAL EQUATION IN NONARCHIMEDEAN $(n,)$ NORMED SPACES

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ABSTRACT

In this research paper, we introduce a generalized quadratic functional equation and prove its Hyers-Ulam stability. Some results of literature are also proved, which are directly consequence of our main results.

Keywords: Hyers-Ulam stability; Non-Archimedean $(n,)$ Normed Spaces; Quadratic functional equation.

NCRAPS:MATH-25

Best proximity points for cyclic Meir – Keeler – Khan Contractions

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ABSTRACT

In the present manuscript, we introduce a new notion of cyclic Meir – Keeler – Khan contractions. In addition to this, we shall prove a theorem to ensure the existence and uniqueness of a best proximity point for cyclic Meir – Keeler – Khan contractions. An example is also provided to prove the validity of our result.

Keywords: Cyclic contraction, Best proximity point, Cyclic Meir- Keeler – Khan contraction.

NCRAPS:MATH-26

Fixed point theorems for generalized contraction in G –metric spaces

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ABSTRACT

In this paper, a new notion of generalized contraction is introduced in G – metric spaces. With the add of this new notion some fixed point results are also proved in the mentioned spaces. Some suitable examples are also provided to prove the validity of our results. An application is also provided by making use of our results.

Keywords: Fixed point, G – metric space, Generalized contraction.

NCRAPS:MATH-27

ON CESÀRO SUMMABLE VECTOR VALUED DIFFERENCE SEQUENCE SPACES

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ABSTRACT

In the present study, we explore the notion of difference sequence spaces to introduce and study a new kind of Cesàro summable difference sequence spaces of vector valued sequences with the aid of paranorm and modulus function. In addition to this we extend the concept of statistical convergence which lead to a new sequence space that coincides with one of the above defined Cesàro summable difference sequence spaces, under the restriction of bounded modulus function.

Keywords : Difference sequence spaces, Paranorm, Statistical convergence, Modulus function.

NCRAPS:MATH-28

A LTNE APPROACH ON THE EFFECT OF TRANSVERSE HYDROMAGNECTIC ON MIXED CONVECTION IN A CHANNEL FILLED BY POROUS MEDIUM

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ABSTRACT

In this paper mixed convection in a vertical porous channel along with transverse hydromagnetic effect is reported. The fluid in channel is assumed electrically conducting and flow is due to external pressure gradient and the buoyancy force. In order to describe the flow in porous medium non-Darcy-Brinkman-Forchheimer extended model is considered here. The local thermal non-equilibrium (LTNE) model is used and the governing equations are solved numerically using the Chebyshev spectral collocation method and a significant agreement is found with the analytical solution in the special case. An extensive focus is given to the influence of physical parameters, inter-phase heat transfer coefficient (H), Hartman number (M), and

Darcy number (Da) on the fluid flow mechanism at fixed values of other parameters. The numerical results show that The fluid flow as well as heat transfer are reduced on decreasing media permeability via reducing the values of Da. Both Nuf & Nus reduce on reducing Da. The velocity is reduced in the middle region of the channel on increasing M, while it is increasing near the walls. The influence of H and M on temperature is meagerly.

NCRAPS:MATH-29

NUMERICAL INVESTIGATION OF HEAT TRANSFER CHARACTERISTICS FOR VARIOUS CPU DESIGNS

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ABSTRACT

Due to the rise in demand of computers with high computing power, there is significant advancement in electronic omponents inside the CPU cabinet every 6 months. The life of these electronic components is greatly affected by their working temperatures. Therefore, it is necessary to maintain the temperature of these devices within acceptable limits. Forced air cooling inside the CPU cabinet is a widely used technique for this purpose. Heat sinks are another way of increasing the heat transfer rate. The present study analyses the effect of different probable improvement cases implemented in the basic CPU cabinet. These improvement cases include changing the position and number of fans, changing the type of heat sink, and changing the inlet cross section. By making use of commercially available CFD softwares like Ansys Fluent and Icepak, the cooling effect in the CPU cabinet is analysed.

NCRAPS:MATH-30

THE OPTIMIZATION OF THE REGIONAL DISTRIBUTION OF COVID- 19 VACCINATIONS, TAKING INTO ACCOUNT LOGISTICAL AND QUALITY CONCERNS

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ABSTRACT

The effective and fair allocation of COVID-19 vaccinations within a certain geographical area presents a complex issue, requiring a thorough optimization approach that considers logistical and quality considerations. This abstract offers a succinct summary of the primary factors and goals involved in tackling the intricacies of vaccine distribution. The global COVID-19 immunization campaign, characterized by its unparalleled magnitude and time sensitivity, highlights the necessity of developing strategic plans that are specifically designed to address the distinctive conditions of each location. The successful management of logistical obstacles, such as supply chain operations, final-stage delivery, and live monitoring, is essential in conjunction with the crucial task of preserving vaccine quality by strictly adhering to cold chain regulations. The objective of this study is to devise tailored optimization approaches that effectively manage the trade-off between efficiency and quality assurance during the distribution of COVID-19 vaccinations within a defined geographical area. This study aims to investigate the influence of geographical characteristics, population density, and pre-existing healthcare infrastructure on the logistical aspects of distribution. Additionally, it seeks to provide novel strategies to effectively tackle these issues. Achieving equitable distribution necessitates the implementation of specific strategies aimed at reaching populations that are vulnerable and excluded. The primary aim of this research is to provide valuable insights that can aid in the development of distribution hubs, the incorporation of modern technology for real-time monitoring, the fostering of collaboration with local healthcare providers, and the implementation of community engagement activities. These efforts are intended to improve

vaccine acceptance rates. This project aims to provide adaptive distribution frameworks by integrating data-driven insights and a nuanced awareness of the local situation. The primary objective is to support policymakers, healthcare professionals, and stakeholders in maximizing the allocation of COVID-19 vaccinations, so making a valuable contribution to the worldwide endeavor to alleviate the consequences of the pandemic. The mathematical model described in this study offers a comprehensive framework for optimizing the allocation of COVID-19 vaccinations within a certain geographical region, taking into account various logistical and quality considerations. The achievement of its successful execution necessitates the engagement of pertinent stakeholders and the ongoing improvement of the approach through the utilization of empirical data nd adaptation to changing circumstances. Engage in collaborative efforts with healthcare authorities and decision-makers to incorporate the model within the decision-making framework for the distribution of COVID-19 vaccines. The optimization challenge aims to determine the most efficient allocation of vaccine doses to various locations, with the objective of decreasing overall costs while ensuring compliance with logistical and quality requirements.

NCRAPS:MATH-31

A LINEAR PROGRAMMING APPROACH TO ENSURING EQUITABLE DISTRIBUTION OF COVID-19 VACCINES IN DEVELOPING COUNTRIES

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ABSTRACT

The equitable dissemination of COVID-19 vaccinations in underdeveloped nations presents a crucial worldwide dilemma, necessitating smart allocation techniques to guarantee impartial and effective coverage. This paper introduces a mathematical approach that utilizes Linear Programming (LP) to efficiently distribute vaccination doses among underdeveloped countries. The model incorporates crucial variables such population magnitude, healthcare infrastructure capability, susceptibility to the virus, financial limitations, and worldwide vaccine availability. The linear programming (LP) model is constructed using decision variables that indicate the quantity of vaccination doses assigned to each country. The goal function seeks to optimise the fair allocation of resources by giving weights to countries according to certain criteria. Constraints are imposed to ensure compliance with global vaccine supply, population coverage targets, healthcare capacity, vulnerability concerns, and budget limits. The non-negativity constraints guarantee that the vaccination allocations will always be greater than or equal to zero. The model is designed to be flexible, taking into account dynamic factors such as emerging viral strains and fluctuating vaccination availability. It highlights the significance of timely data updates to facilitate ecision-making. The LP solver, such as the simplex method or interior-point approaches, is used to determine the best solution that achieves a fair distribution while considering logistical limitations. The results obtained from the linear programming (LP) model offer practical and effective guidance for policymakers and health organizations. These insights help in distributing COVID-19 vaccinations in a way that maximizes their impact and reduces inequalities among developing countries.

The approach recognizes the interdependence of global health and emphasizes the need for coordinated endeavors in addressing the pandemic. This mathematical model is a useful tool in the ongoing efforts to distribute COVID-19 vaccinations fairly and efficiently. It contributes to the worldwide aim of obtaining universal immunity and overcoming the problems posed by the epidemic in underdeveloped countries.

Keywords: Linear Programming,Equitable Vaccine Distribution,Optimization ,Vulnerability Index, Budget Constraints ,Global Vaccine Supply.

NCRAPS:MATH-32

EFFECT OF THERMAL RADIATION ON THE EVOLUTION OF TWO-DIMENSIONAL WEAK SHOCK WAVES IN A PERFECT GAS CONTAINING DUST PARTICLES

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ABSTRACT

The current paper presents an analysis of the evolution of weak shocks in a two-dimensional flow of a perfect gas with small solid dust particles, considering the effects of thermal radiation. The analysis covers both planar and axisymmetric scenarios. The shock-evolution equation has been constructed using the wavefront expansion method. This equation confirms the presence of discontinuities in the normal derivatives of physical variables and describes the process of wave generation and evolution. The shock-evolution equation was used to analyse the influence of shock-Mach number and thermal radiation on the evolutionary behaviour of shock waves in planar and axisymmetric flow geometries. The results were presented through figures and tables using the computational software package MATHEMATICA 11.0. Throughout the study, a consistent delay in the creation distance of shocks is found for higher values of specific heat ratios. Additionally, it is important to mention that in axisymmetric geometry, the generation of weak discontinuity happens earlier compared to the planar case. This highlights the significant influence of flow configuration on the process of shock evolution.

NCRAPS:MATH-33

SUSTAINABLE ECONOMIC ORDER QUANTITY MODEL WITH DETERIORATION, CARBON EMISSION AND CARBON TAX

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ABSTRACT

In current scenario, consideration of carbon emissions and deterioration in an inventory model has become essential. This research paper investigates a sustainable economic order quantity inventory model for deteriorating products considering carbon emissions and carbon tax. So, this proposed model incorporates the carbon emissions emitted from two activities: storage and deterioration. Due to consideration of carbon emissions, this sustainable economic order quantity problem involves carbon emission tax. In this sustainable model, total cost function and total carbon emissions function are derived. Further, order quantity and cycle time are determined by optimizing total cost and total carbon emission. A solution procedure is presented to obtain the optimal solution. The convexness of total cost function is exhibited by analytical approach as well as graphical approach. Finally, a numerical analysis is set to verify this model and moreover an analysis of sensitivity is performed to investigate the effects of key model parameters on optimal policy.

Keywords: Sustainable economic order quantity model; Deterioration; Carbon emissions; Carbon tax.

NCRAPS:MATH-34

VELOCITY AND THERMAL WALL SLIPS IMPACT ON THE BOUNDARY LAYER FLOW OF NANOFLUID OVER A NON-LINEAR STRETCHING SHEET IN POROUS MEDIA ALONG WITH MAGNECTIC FIELD

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ABSTRACT

The objective of this research is to analyse the behaviour of magnetohydrodynamic nanofluid flow over a non-linear stretched sheet embedded in a porous medium along with thermal and velocity slips. The partial differential equations are transformed into non-dimensional ordinary differential equations by employing the similarity transformation. The finite difference Keller box implicit (FDKBI) method yields the numerical solutions. The achieved results are depicted graphically. Notably, our findings reveal the intricate influence of several factors, such as velocity slip factor $\boldsymbol{\lambda}$, thermal slip factor $\boldsymbol{\beta}$, stretching factor n, magnetic parameter $\boldsymbol{M}$, Brownian parameter $\boldsymbol{N_b}$, thermophoresis parameter $\boldsymbol{N_t}$ permeability parameter $\boldsymbol{K}$ on temperature $\boldsymbol{\theta(\eta)}$, concentration $\boldsymbol{\xi(\eta)}$ and velocity $\boldsymbol{f'(\eta)}$, also unveiling $\boldsymbol{n}$.

Keywords Nanofluids, Magnetohydrodynamics, Porous media, Keller-box method.

NCRAPS:MATH-35

NUMERICAL INVESTIGATIONON VORTICITY OF HYDROMAGNETIC TWO-PHASE FLOW THROUGH TWO PARALLEL PLATES IN AROTATING SYSTEM

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ABSTRACT

In this paper, an attempt has been made to find the vorticity of incompressible fluid in the hydromagnetic two-phase flow through two parallel plates in a rotating system. variations in the vorticity are studied through vorticity profiles, and some very important conclusions are drawn. it is also observed that the flow in both the regions is self-superposable. the conditions for the flow in both the regions is self-superposable. the conditions for the flow in both regions to become irrotational are found.

Key words: MHD, Vorticity, Parallel plates.

NCRAPS:MATH-36

A COMPARATIVE STUDY OF STOCK MODEL APPROACHES FOR MANAGING FLEXIBILITY IN THE EXECUTIVE 3-ECHELON MULTI-LEVEL SUPPLY CHAIN

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ABSTRACT

Supply chain resilience has become increasingly critical in the dynamic world of global commerce, where disruptions are a constant threat. This paper explores the intricate relationship between stock model flexibility and supply chain resilience, using the Executive 3-Echelon Multi-Levels as a case study. Mathematical equations are employed to quantify flexibility and its impact on resilience. The study demonstrates the significance of a balanced approach to supplier, manufacturer, and retailer flexibility. It provides valuable insights and practical strategies to enhance supply chain resilience, ensuring organizations can thrive in today's unpredictable business environment.

Key Words: Supply chain resilience, stock model flexibility, sensitivity analysis, information visibility, , collaboration, strategic planning, adaptability, sustainability

NCRAPS:MATH-37

AN ANALYSIS OF THERMOELASTC DAMPING IN MICROPLATE RESONATORS WITH MODIFIED COUPLE STRESS THEORY AND QUINTANILLA MODEL

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ABSTRACT

The micro-electro-mechanical system (MEMS) resonators are designed to have low energy dissipation, which is associated with high quality factors. In couple stress theory, considering the size effect is necessary to explain such problem when plates have micro/nanoscale thicknesses. The main objective of proposed work is to obtain an analytical expression for TED quality factor (Q) of size-dependency micro-plate resonators by employing the modified couple stress theory (MCST) with the condition of plane stress and heat conduction for Quintanilla model. We consider thin silicon micro-plate resonators to explore how the parameter of length-scale affects TED's quality factor. The variation of TED has been examined in terms of the parameter of length-scale, micro-plate thickness, and normalized frequency and also looked into the impact of phase lag parameter on TED. A comparative study of the proposed model and conventional continuum theory (CCT) has been explained. The present work states that the quality factor of resonators with an infinitesimal thickness may increase by considering small values of parameter of phase lags under the modified couple stress theory.

Keywords: Thermoelastic damping; Thin micro-plate resonators; Size-effects; Quality factor; Modified couple stress theory; Quintanilla model.

NCRAPS:MATH-38

DYNAMICAL SYSTEMS ANALYSIS OF $f(R,G)$ COSMOLOGICAL MODEL WITH DARK SECTOR COUPLING

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ABSTRACT

In this study, we thoroughly investigate the stability of linear coupling within the dark sector of the Universe. Our focus is on the cosmological feasibility of $f(R,G)$ gravity theories, and we employ a dynamical system approach to achieve this analysis. The central technique involves transforming the evolution equations into an autonomous system of ordinary differential equations by utilizing appropriate variables. We apply this framework to a specific category of models characterized by $(R,G) = \alpha R^m + \beta G^n$. Subsequently, we analyze a comprehensive examination of the solutions produced by these models and the associated stability properties.The model has an attractor that leads to late-time accelerated expansion, which aligns with our observations. This work contributes to a deeper understanding of the interplay between various components within the dark sector and the overall dynamics of the Universe, shedding light on the potential implications of $f(R,G)$ gravity theories.

Keywords: Modified gravity, Cosmological model, Dynamical system, Gauss–Bonnet term.

NCRAPS:MATH-39

LINEAR PROGRAMMING PROBLEM ON WOMEN'S HEALTH MANAGEMENT

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ABSTRACT

The purpose of this study article is to investigate how a linear programming issue might be defined with an emphasis on women's health management. Next, we'll create a mathematical model that minimizes the effective cost of a healthy meal throughout the day by optimizing a diet program based on the number of calories required for daily intake, diet budget, and the healthiest meal distribution in a day.

Keywords: Women's health, Diet Plan, Optimization

NCRAPS:MATH-40

SHIFTING OF DOCTORS BY USING LINEAR PROGRAMMING PROBLEM

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ABSTRACT

Linear programming problems are one of the strategies used in Operations Research. In this study, we use Linear Programming to optimize doctor shifts in hospitals. In this task, we will maximize the hospital's profit by scheduling and changing doctors to give continuous tutorship service.
Keywords: Shifting, Doctors, Profit, Linear Programming Problem, Optimization

NCRAPS:MATH-41

IMPLICATIONS OF UNIFORM CONVERGENCE - AN OVERVIEW

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ABSTRACT

In this article notion of uniform convergence with its implications is discussed. As a necessary tools, first of all, we briefly introduce the concept of pointwise convergence. Then we discuss uniform convergence with few illustrated examples. Finally, we investigate three important aspects namely uniform convergence and continuity, uniform convergence and integrability, and uniform convergence and differentiability with some illustrated examples.

Keywords: Pointwise Convergence, Uniform Convergence, Continuity, Differentiability.

NCRAPS:MATH-42

SOME THEOREMS ON DEFINITE ALMOST PRODUCT METRIC MANIFOLDS

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ABSTRACT

Negi (2017) has derived some theorems on almost product and decomposable spaces, and Negi et al. (2019) have premeditated an analytic HP-transformation in almost Kaehlerian spaces. In this paper, we have find out some theorems on definite almost product metric manifolds.

Keywords: Almost product manifolds, Kaehlerian manifolds, Riemannian spaces and Contact manifolds.

NCRAPS:MATH 43

EFFICACY OF THIRD DIFFUSING COMPONENT AND MODULATED ROTATION ON HEAT AND MASS TRANSPORTS IN NEWTONIAN FLUID SATURATED POROUS MEDIUM: A COMPARATIVE STUDY

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ABSTRACT

A weakly non-linear theory is employed to examine the effect of rotational modulation and the third diffusive component on transports in the Rayleigh B`enard convection in an extended Brinkman-Darcy porous layer. The porous layer is extended infinitely in x- direction, and z- axis is taken in upward direction. Temperature and concentration of both the solutes at lower plate are higher than the upper plate. The time dependent rotational speed of fluid is assumed to be modulated by small parameter ϵ^2 with amplitude (δ). A linear differential matrix method is adopted to analyze the behavior of the system. A non-autonomous differential equation known as Ginzburg Landau's equation has been derived by employing Fredholm-solvability condition. The expression of critical Rayleigh number is obtained for the three different cases; clear fluid Layer, Darcy porous

Layer and Sparsely packed porous layer (Brinkamn model), and the impact of dimensionless parameters on stationary convection are also discussed. The convective transports are measured in terms of Nusselt number (Nu) and Sherwood numbers (Sh1, Sh2) for both the solutes and the effect of modulation and other dimensionless parameters on these convective transports are deliberated through the graphs plotted by the software MATHEMATICA12. Moreover, it is found that the heat and mass transports in fluid layer is greatest, and lowest in sparsely packed porous layer among the considered three different models.

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