



**A COMPENDIUM OF RESEARCH PAPERS PRESENTED IN
THE INTERNATIONAL CONFERENCE ON
FRONTIER AREAS IN CHEMICAL TECHNOLOGIES-2019 (FACTs-2019)**

July 25-26, 2019

**Conference Organized By
Department of Industrial Chemistry
(DST FIST, DST PURSE and UGC SAP Assisted Department)
School of Chemical Sciences
Alagappa University**

**(Accredited with A+ Grade by NAAC (CGPA 3.64) in the Third Cycle)
Karaikudi-630 003, Tamil Nadu, India**

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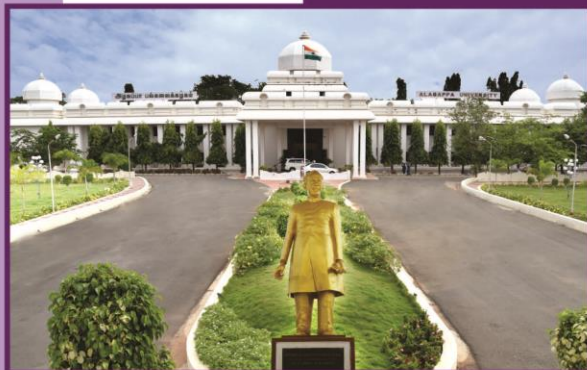
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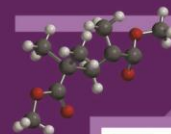
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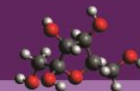


INTERNATIONAL CONFERENCE ON
**FRONTIER AREAS IN
CHEMICAL TECHNOLOGIES – 2019**

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ALAGAPPA UNIVERSITY

(A State University Established in 1985)
Karaikudi - 630003, Tamil Nadu, India



SCHOOL OF CHEMICAL SCIENCES
DEPARTMENT OF INDUSTRIAL CHEMISTRY

(DST- FIST, PURSE & UGC-SAP Assisted Department)



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Frontier Areas in Chemical Technologies

**A Compendium of Research Papers presented in the International Conference FACTs
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Preface

Chemical technologies involving Green Chemistry, Materials Chemistry, Electrochemistry, Textile Chemistry, Nanoscience, Computational Chemistry, etc., are the challenging as well as fascinating branches of advanced technologies and they find applications in almost all areas of Science and Technology. It is important for the researchers, educators and developers from academic institution and industries to know the research and recent developments that have been made on various aspects of Chemical and Electrochemical Sciences and Technologies. The present conference on **Frontier Areas in Chemical Technologies (FACTs-2019)** is the Third International Conference organized by the Departments of Industrial Chemistry to focus on the update of recent advancements in different areas of chemical science and technologies. The aim of this international conference is to provide a forum to all the chemists, physicists, biologists and material scientists and technologists and researchers to discuss their recent findings and information and to promote cooperation both nationally and internationally. The invited talks and papers focus mainly on various advanced aspects of Chemical Technologies such as Electrochemical Technologies, Nanoscience and Technology, Sensor Technologies, Supramolecular and Photochemical Technologies, Green Chemical Technologies and other allied technologies.

It is indeed a matter of great pleasure and satisfaction to the Editors to present this volume containing collection of abstracts of the presented in the International Conference on FACTs- 2019 held at Alagappa University, Karaikudi during 25th and 26th July-2019. There are about 08 Invited Talks, 67 Oral Presentations and 132 Poster Presentations. In addition, the programme includes open forum discussions. About 250 delegates from various Research Institutes, Universities, Colleges and Industries in India including four Invited Speakers from overseas participate in the conference.

The editors are thankful to **Prof. N. RAJENDRAN**, Vice-Chancellor, Alagappa University, Karaikudi for supporting all the activities of this International Conference and advising in promoting the research culture among the young researchers. Our sincere thanks are to **Prof. H. Gurumallesh Prabu**, Registrar, all the **Syndicate Members** and Authorities of Alagappa University, Karaikudi for their constant support and encouragement. Sincere thanks are due to the Organizing Committee Members of the conference, Faculty Members, Research Scholars and Students of the Departments of Industrial Chemistry. We also thank all the authors for submitting their abstracts in time.

We hope all the delegates had a pleasant stay in Karaikudi and stimulating discussions during the International Conference on FACTs-2019.

Editors



Professor **N. Rajendran**
Vice - Chancellor

ALAGAPPA UNIVERSITY

Vallal Alagappan Valagam, Karaikudi - 630 003, Tamil Nadu, India.

(A State University Established by the Government of Tamil Nadu, Recognised by UGC.

Accredited with 'A+' Grade by NAAC (CGPA : 3.64) in the Third Cycle,

Graded as Category - I University and Granted Autonomy by MHRD - UGC)



MESSAGE

I am happy to note that the Department of Industrial Chemistry, School of Chemical Science is organizing an International Conference on "Frontier Areas in Chemical Technologies - 2019 (FACTs - 2019)" on 25th - 26th July 2019.

The Department of Industrial Chemistry has a pride of place at Alagappa University. The Department has richly contributed to the academic ambience and quality enhancement of Alagappa University. The Department's contribution to 'h' index of the university is noteworthy. Currently, the application of Chemical Technology has become more widespread because it offers diverse benefits in almost all spheres of science. With the advent of a new technology-driven global economy, revolutionary advances have been made in almost all sectors. There is an urgent need to apply Chemical Technology to solve environmental problems and to encourage the replacement of existing products with new products that are more environment friendly throughout their life cycles.

I am sure that the conference will encourage the participants to deliberate and exchange ideas on the diversified topic and to learn about recent developments in Chemical Technology. My compliments are due to the Faculty, Research Scholars and Students of the Department of Industrial Chemistry, for their enthusiasm in organizing this conference with an objective to undertake studies and research in the frontier areas of Chemical Technology.

I congratulate the organizers for bringing international experts to Alagappa University campus for interdisciplinary communication between scientists, teachers, and students so as to bring innovations in the applications of Chemical Technology.

I wish the International Conference all success.


(N. Rajendran)

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Prof. H. Gurumallesh Prabu
Registrar

Date: 17.07.2019



MESSAGE

It gives me great pleasure to learn that the Department of Industrial Chemistry, Alagappa University is organizing an International Conference on “Frontier Areas in Chemical Technologies” (FACTs - 2019) on 25th and 26th of July 2019.

The International Conference aims to deliver a platform for the young researchers to develop and bring forth the latest advances in all areas of chemical science including the interfaces with related disciplines such as biology, medicine, and material science. In this regard, it is appropriate that the Department of Industrial Chemistry, has taken efforts to arrange this International Conference with invited lectures from eminent personalities in India and abroad with paper presentation by academicians, scientists, scholars, and industrialists.

I am sure that all the delegates would be greatly benefited by the deliberations of this conference with many innovative ideas.

I wish the Conference a grand success.


(Prof. H. Gurumallesh Prabu)

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Karaikudi 630 003



Dr. G. Paruthimal Kalaingan M.Sc., Ph.D.,
Senior Professor and Head
Convener - FACTs - 2019



WELCOME TO THE DELEGATES

On behalf of the Staff and Students of the Department of Industrial Chemistry, Alagappa University, Karaikudi, I am pleased to extend a hearty welcome to all the delegates of the International Conference on Frontier Areas in Chemical Technologies (FACTs - 2019) during 25 - 26 July 2019.

Though the conference announcement was at short notice, there was an overwhelming response. About 199 technical papers and 8 Invited Lectures were received during this short notice of time. These cover a wide range of topics and are programmed to be deliberated in 6 sessions.

I am delighted to the response received from Academicians, Scientists from R & D Institutions and Chemists from Industries. The Conference would also provide a common platform to share their ideas / achievements of research into industrial applications to reach the common man and also help to establish a strong academic - research - industrial relationship. I hope that, the Conference will provide the unique opportunity for participants to interact and share the knowledge and experience.

I wish the delegates for enjoyable and memorable stay at karaikudi.

Dr. G. Paruthimal Kalaingan

CONTENTS

INVITED TALKS (IT)

		P. No
IT 1	Engineering Purely Organic Materials for Light Harvesting & Photon Upconversion <i>A. Jean-Luc Ayitou</i>	1
IT 2	Development of Some Diagnostic and Analytical Techniques Aided by and Using Fluorescence Spectroscopy <i>Ashok Kumar Mishra</i>	3
IT 3	Hybrid Nanocomposite-supported Metal Nanocatalysts for the Catalytic Reaction <i>Kang Hyun Park</i>	5
IT 4	Nanostructured NiPd/OMC: An Efficient Bifunctional Electrocatalyst for Hydrogen Production via Overall Urea Electrolysis <i>Muthuchamy Nallal</i>	7
IT 5	Hybrid Nanomaterials for Advanced Oxidation Processes <i>Sambandam Anandan</i>	8
IT 6	Recent Developments in Counter Electrode Materials for DSSCs <i>A. Subramania</i>	9
IT 7	The Preparation of Nanoparticles (NPs) by Top Down Approach and their Potential Industrial Application <i>Toemsak Srikhirin</i>	11
IT 8	High Energy Batteries for Defense Application <i>G. A. Pathanjali</i>	12

ORAL PRESENTATION (OP)

OP 01	MWCNT coated glassy carbon electrode used 2-hydroxy-1,4-naphthoquinone for oxygen reduction. <i>J. Antony rajam, A. Gomathi and C. Vedhi</i>	15
OP 02	Development of proton conducting polymer composite membranes for fuel cell application. <i>M. Aparna and P. Hemalatha</i>	16
OP 03	Ionic liquid functionalized hetero atom doped PNF-MWCNT and BNF-MWCNT and its Enhanced catalytic ability in clean energy and pollution control applications. <i>Murugesan Balaji, Pandiyan Nithya, Veerasingam Muthulakshmi, Arumugam Mayakrishnan, Sonamuthu Jegatheeswaran, SamayananSelvam, Ganesan Selvanathan and Mahalingam Sundrarajan</i>	17
OP 04	Synthesis and characterization of melamine core GI generation starburst dendrimers using 2,2 bis(hydroxymethyl) propionic acid and their potential application antioxidant. <i>P. Balu, S. Gajalakshmi and D. Thirumalai</i>	18

OP 05	Electrochemical performance of Cr based LiCoO ₂ nanofibres as electrode material for hybrid supercapacitors. <i>G. Bhuvanalogini</i>	18
OP 06	Enhancement in power conversion efficiency of angular luminescent solar concentrator employing RE ion based polymer composites. <i>V. G. Brindha, M. Kottaisamy, S. R. Srikumar and V. Vasu</i>	19
OP 07	Green Synthesis of Novel 1,3-Dithiazo Fused Heterocyclic Compounds and their Antituberculosis Studies. <i>S. Chitra, P. Manisankar and S. Muthusubramanian</i>	20
OP 08	Synthesis of Triphenylamine-based D-pi-A Molecules for OFET Applications. <i>P. Devibala, R. Dheepika and S. Nagarajan</i>	21
OP 09	Tetranuclear Palladacycles of 3-acetyl-7-methoxy-2 <i>H</i> -chromen-2-one derived Schiff bases: Efficient catalysts for Suzuki-Miyaura coupling in aqueous medium. <i>S. Dharani, G. Kalaiarasi, D. Sindhuja, V. M. Lynch, R. Shankar, R. Karvembu and R. Prabhakaran</i>	22
OP 10	Starburst Unsymmetrical Triarylaminines for <i>p</i> -channel OFETs: Improving Device Performance by Solvent Engineering. <i>R. Dheepika, Anisha Shaji and S. Nagarajan</i>	23
OP 11	Tailored sulfonated poly (vinylidene fluoride-co-hexafluoropropylene) nanocomposite membranes using poly (ethyleneimine) functionalized reduced graphene oxide for vanadium redox flow battery applications. <i>K. Divya, M. Sri Abirami Saraswathi and A. Nagendran</i>	24
OP 12	A Novel Duckling Toy Microbial Fuel Cell for Treating the Sewerage wastewater and generation of electricity for powering the danger zone alert lamp over the Sewerage Canals. <i>K. Gunaseelan and S. Gajalakshmi</i>	25
OP 13	<i>In vitro</i> antidiabetic and antioxidant activities of 2-(3,4-dihydroxyphenyl)-3,5,7 trihydroxy-4 <i>H</i> -chromen-4-one isolated from the methanolic leaf extract of <i>Andrographis echinoides</i> . <i>S. Gurupriya and L. Cathrine</i>	26
OP 14	Development of ruthenium doped graphitic carbon nitride for highly sensitive non-enzymatic glucose sensing. <i>Habibulla Imran and Venkataraman Dharuman</i>	27
OP 15	Room temperature hydrogen sensing property of polypyrrole/polyaniline conducting polymer blends synthesized by interfacial polymerization. <i>Heiner Albaris and Gurunathan Karuppasamy</i>	28
OP 16	Low-cost and eco-friendly synthesis of silver nanoparticles using <i>tridax procumbens</i> leaf extract and its larvicidal activity <i>A. LeemaRose, S. Vidhya, Pa. Harini Priya and F. Janeeta Priya</i>	28
OP 17	Synthesis of Anchored Nicotinic Acid Hydrazide Graphene Oxide for Efficient Electrochemical detection of Caffeine. <i>Jemini Jose, Subramanian Viswanathan and Sreeja P B</i>	29

OP 18	Cu ₂ NiSnS ₄ nanoparticles grown onto graphene as an efficient nanohybrid counter electrode for high-performance DSSC. <i>R. Jeniffa, M. Vignesh and A. Subramania</i>	30
OP 19	Asafetida-resin Stabilized MoO ₃ Nanoparticles Encrusted with Ruthenium Bipyridine an Effective Transducer for Electrochemistry of Butein. <i>Gaurav Pandey, Pandiyaraj Kanagavalli and Murugan Veerapandian</i>	31
OP 20	High capacity and enhanced cycling stability of K ⁺ -doped LiNi _{1/3} Mn _{1/3} Co _{1/3} O ₂ Cathode Materials for Lithium-ion batteries. <i>K. Kalaiselvi and G. Paruthimal Kalaignan</i>	32
OP 21	Synthesis of zinc complex using pyridoxal based Schiff base: functional mimics of histone deacetylase 6 isoform. <i>K. A. Karthick and A. Tamil Selvi</i>	33
OP 22	Photophysical and spectral properties of Boron Difluoride curcumin complex dye and their derivatives: a DFT study. <i>Selvam Karthick, Chinnalagu Dhilip Kumar and Gopalakrishnan Gopu</i>	34
OP 23	New understanding on sustainable fabrication enhanced photocatalytic performance of Pr ₆ MoO ₁₂ /g-C ₃ N ₄ nanocomposite for the degradation of organophosphate pesticide (Methyl Parathion). <i>S. Karuthapandian</i>	35
OP 24	Overview of modified carbon paste electrode with chitosan composite. <i>AL. Kavitha and H. Gurumallesh Prabu</i>	36
OP 25	Electrochemical and spectroscopic approach for iodide ion sensing by ferrocene based schiff base receptor (Fc-AEP). <i>N. Kavitha, R. Jenny, A. Rishwandhani and N. Sengottuvelan</i>	37
OP 26	Fluorogenic mercury ion sensor based on pyrene-amino mercapto thiadiazole unit. <i>B. Kirthika Rani and S. Abraham John</i>	38
OP 27	Mechanism proposed for the prepared Chitosan-ZnO nanocomposite. <i>R. Krishnaveni</i>	39
OP 28	A convenient electrochemical method for the preparation of bromohydrin using NaBr as electrolyte. <i>Y. Jenifer, K. Kulangiappar, T. Raju, V.M. Shanmugam and D. Velayutham</i>	40
OP 29	Preparation of Palladium Nanoparticles in a Microemulsion and their Application for the Heck Reaction. <i>R. Mangaiyarkarasi, M. Priyanga and S. Umadevi</i>	40
OP 30	Synthesis of nitrogen-doped RGO/BaWO ₄ nanocomposites with highly enhanced photocatalytic activity. <i>M. Mohamed Jaffer Sadiq and G. Paruthimal Kalaignan</i>	41
OP 31	Electrodeposition of Pd-Ni from a deep eutectic solvent system: effect of additives and hydrodynamic conditions. <i>S. Mohanapriya and A. Subbiah</i>	42

OP 32	Sulfur-doped carbon quantum dots incorporated iron oxide nanoparticles for a sensitive electrochemical determination of antipsychotic drug olanzapine <i>Ganesan Muthusankar, RamadhassKeerthika Devi and Gopalakrishnan Gopu</i>	43
OP 33	Highly photoactive Ag-ZnO/Fe ₂ V ₄ O ₁₃ (AZF) nanocomposite for effective environmental remediation. <i>K. Gowthami and I. Muthuvel</i>	44
OP 34	Synthesis and characterization of Mn doped CuCo ₂ S ₄ for supercapacitor applications. <i>P. Naveenkumar and G. Paruthimal Kalaigan</i>	44
OP 35	Constructing a g-C ₃ N ₄ /MnV ₂ O ₆ p-n heterojunction photocatalyst for organic pollutant degradation. <i>M. Nithya, U. Sathya and Keerthi</i>	45
OP 36	Comparison of corrosion inhibition performance of a symmetrical schiff base in acid media. <i>G. Pandimuthu and A. Sankar</i>	46
OP 37	Experimental and theoretical studies of the inclusion complex between biphenyl thiol derivatives and β-cyclodextrin <i>K. Paramasivaganesh and T. Stalin</i>	46
OP 38	Synthesis and characterization of cobalt based metal-organic framework for asymmetric supercapacitor performance <i>T. Ponmuthuselvi and S. Viswanathan</i>	47
OP 39	Hydrazine based schiff base ferrocene derivative as optical and electrochemical sensor for the detection of copper(II) and iodide ions. <i>S. Poornima, M. Sethupathi, N. Kavitha, R. Praveena and N. Sengottuvelan</i>	48
OP 40	Ceramic membranes for photo-catalytic dye degradation. <i>S. Prakash, G. Paruthimal Kalaigan and P. Manisankar</i>	49
OP 41	Preparation and characterization of TiO ₂ thin film by artist spray gun pyrolysis method for perovskite solar cell applications. <i>Pratheep Panneerselvam and Subramania Angaiah</i>	50
OP 42	Orientation and energy based stable supramolecular interaction of 3-Hydroxyflavone and quercetin with native and modified β-cyclodextrins. <i>A. Praveena, R. Rajamohan and MadiFatiha</i>	51
OP 43	Titanium Dioxide Nanocatalyst for Photocatalytic Degradation of Acid red dye under solar irradiation. <i>Preeja. P. Thattil and A. Leema Rose</i>	52
OP 44	Development and Performance Evaluation of PANI Pigmented hybrid Organic Coating as an Alternative to Chromate Primer. <i>K. Namsheer, Punniyakotti Parthipan and Subramania Angaiah</i>	53
OP 45	Nortriptyline and Nortriptyline:β-cyclodextrin loaded on electrospun PAN nanofibers as a carrier for antibacterial activity. <i>R. Rajamohan and A. Subramania</i>	54

OP 46	Sugarcane Juice Clarifying Capacity of Green Synthesized Nano CaO. <i>Ramesh Duraisamy, Majur Mading Makur and Tewodros Birhanu</i>	55
OP 47	Thermal stability and antibacterial properties of chitosan-magnesium oxide nanocomposite. <i>T. Revathi and S.Thambidurai</i>	56
OP 48	Efficiency Enhancement of Methylammonium Tin Iodide Perovskite Solar Cell using Benzyltrimethyl Ammonium Iodide as an Additive. <i>K. Sakthi Velu, B. Suganya Bharathi, G. Vigneshkumar, N. Vimalasruthi, S. Esakkimuthu and T. Stalin</i>	57
OP 49	Fluorometric and colorimetric “Off-On-Off” Relay sensor for $\text{CN}^-/\text{Cr}^{3+}$ in RAW264.7 cells. <i>Sanay Naha and Sivan Velmathi</i>	58
OP 50	Corrosion inhibition study of a new synthetic schiff base derived from drug compound on mild steel in acid medium. <i>A. Sankar and K. Paramasivaganesh</i>	59
OP 51	Synthesis and characterization of triazinecored imidazole polymers. <i>Chokalingam Saravanan and Paulpandian MuthuMareeswaran</i>	60
OP 52	Ruthenium catalyzed intermolecular hydroacylation of unactivated alkenes: ruthenium hydride-xantphos as a pre-catalyst for an intermolecular Markovnikov selective hydroacylation reactions. <i>Saravanakumar Shanmuganathan</i>	61
OP 53	Fabrication of 2D-MoWS ₄ MXene asymmetric supercapacitor and its supercapacitive performance studies. <i>K. Satheshkumar, M. Vignesh, B. Balakrishnan and A. Subramania</i>	63
OP 54	Synthesis and characterization of triazine based porous polymer. <i>M. Senthilkumaran, C. Saravanan, P.Puthiaraj and P. Muthu Mareeswaran</i>	64
OP 55	Redox-additive mediated electrochemical activity of invasive weed derived onion-like porous carbon for supercapacitor application. <i>Sathyanarayanan Shanmugapriya and Ramakrishnan Kalai Selvan</i>	65
OP 56	Synthesis and characterization of cadmium sulfide quantum dots and its analytical application in the photocatalytic degradation of rhodamine B under solar light. <i>K. Sivakumar and T. Poongodi</i>	66
OP 57	Electrochemistry and electrochemiluminescence of Luminol/DCHA. <i>M. Sornambigai C. V. Raju and S. Senthil Kumar</i>	66
OP 58	Poly (ether imide) ultrafiltration membranes tailored with poly (hexamethylene biguanide)woven copper oxide nanoparticles for water treatment applications. <i>M. Sri Abirami Saraswathi, K. Divya and A. Nagendran</i>	67

OP 59	One-pot multicomponent synthesis of Spiro bis phenyl pyrazolone piperidium salt derivatives. <i>Srinivasan Prabhakaran and Sivan Velmathi</i>	68
OP 60	Synthesis and characterization of n-chloropicolinamide: a new, mild, stable, effective and efficient oxidant for organic substrates. <i>M. Subalakshmi and V. Priya</i>	69
OP 61	Preparation and Characterization of Novel Electrospun Alumina/Poly (vinylpyrrolidone) Nanofibrous Mats with Antibacterial and Antioxidant Properties for Protecting Cells from Oxidative Stress <i>Suganya Bharathi Balakrishnan and Stalin Thambusamy</i>	69
OP 62	Highly efficient recyclable Cu-(I)-SBA clay catalyst for conversion of Nitroarenes to Aminoarenes. <i>Thennila Muthukumar, Muthumanickam Shenbagapushpam and Selvakumar Kodirajan</i>	71
PP 63	Fabrication and Characterization of Nanostructured Cd _{0.5} Zn _{0.5} S based Sensitizer for Photovoltaic Applications. <i>P. Vasantha Kumar and S. Rajashabala</i>	72
PP 64	Dimethyl Dioxirane and ZnO Nanocatalyst Assisted Photocatalytic Degradation of Methylene Blue Dye. <i>S. Vinotha and A. Leema Rose</i>	73
OP 65	Electrochemical Biosensor for Aflatoxin B1 in wheat flour <i>S. Viswanathan, S. Marimuthu and Cristina Delerue-Matos</i>	74
OP 66	Antioxidant potent diimines. <i>G. Thirunarayanan</i>	75
OP 67	Effect of moisture, temperature and humidity on the manufacture of firework composition <i>K. Srinivasan, T. Stalin, and L. C. Nehru</i>	190

POSTER PRESENTATION (PP)

PP 01	Plant-extract assisted green synthesis of silver nanoparticles using <i>nyctanthes arbor-tristis</i> flower at room temperature. <i>V. Abinaya and H. Gurumallesh Prabu</i>	77
PP 02	Synthesis and characterization of groundnut-ZnO composites. <i>R. Aiswarya and S.Thambidurai</i>	77
PP 03	Plant mediated green synthesis of TiO ₂ and MgO nanoparticles using <i>abutilon indicum</i> flowers extract and their antibacterial activity. <i>V. Aiswarya, M. Balaji, P. Nithya, S. Gowri, K. Kottaisamy and M. Sundrarajan</i>	78
PP 04	Cyclic Voltammetric Studies on New Nitro Chalcones. <i>A. Akilan and S. Senguttuvan</i>	79
PP 05	Structural, Photo-physical and Biomedcial applications of Curcumin-based Novel Conjugated Triazine Centred Metal Complexes. <i>Fr. L. Alphonse and P. Tharmaraj</i>	80
PP 06	Selective Sensing of Dopamine on Mn ₂ O ₃ -TiO ₂ -Graphene Nano structured electrodes. <i>Arockiajawahar Anancia Grace, Karutha Pandian Divya and Venkataraman Dharuman</i>	81
PP 07	Effect of pH on the Physical and NLO Behavior of Ammonium Dihydrogen Phosphate (ADP) crystals. <i>J. Anandakumaran and G. Ramasamy</i>	82
PP 08	Corrosion inhibition of carbon steel in 1m hno ₃ solution by <i>Aubutilon X Hybridum yellow</i> extract/powder as an eco-friendly inhibitor using weight loss method. <i>V. Anusiya, M. Muthu Kaviya, C. Ramya and M. Srimathi</i>	83
PP 09	Relation between biomarker enzyme and tissue damage of clam, <i>donax faba</i> exposure to lead. <i>C. Archana Devi, C. M. Ramakritinan and A. K. Kumaraguru</i>	83
PP 10	A novel schiff base ligand and its complexes for sensor application. <i>V. Aruldeepa, P. Tharmaraj and C. D. Sheela</i>	84
PP 11	Synthesis and electrochemical characterization of high voltage cathode material (LiCo _{0.5} Mn _{1.5} O ₄) for lithium ion batteries. <i>N. Azhagumeenal, N. Radha and S. T. Nishanthi</i>	85
PP 12	Photophysical studies on Donor-Acceptor blends of Picene-PTCDI. <i>B. Balambiga, R. Dheepika and S. Nagarajan</i>	86
PP 13	Hydrothermal approach of nano silver doping on the CuO nanomaterial and study of its photocatalytic activity under UV-light. <i>E. Bharathi, G. Sivakumari, B. Karthikeyan and S. Senthilvelan</i>	87

PP 14	Synthesis, characterization and antimicrobial activities of poly (N-tert-amylacrylamide-co-acrylamide-co-2-acrylamido-2-methylpropane sulphonic acid sodium salt) Zinc oxide nanocomposite hydrogels. <i>K. Bharathi and P. Pazhanisamy</i>	88
PP 15	Ionic liquid assisted synthesis of tri-doped N, P, F and N, B, F-MWCT and their prevention activities of bacterial biofilm-associated with orthopedic implantation. <i>G. Bhuvaneshwari, N. Uthayakumar, M. Balaji, P. Nithya, S. Jegatheeswaran, S. Selvam, K. Pandian and M. Sundrarajan</i>	88
PP 16	Effect of Different Chemical Treatment on Thermal, Morphological and Mechanical Properties of Short Pineapple Fiber Reinforced with Unsaturated Polyester/ Ceramics powder/Nanosilica filled Hybrid Nanocomposites for Automotive Application. <i>Chinnappa Arumugam, Senthilkumar Arumugam and Sarojadevi Muthusamy</i>	89
PP 17	Synthesis of zirconia doped Zinc oxide nanoparticles and Evaluation of interaction between NPs and calf thymus DNA. <i>K. Chinnasamy, S. Umamatheshwari and C. Sankar</i>	91
PP 18	Surfactant assisted synthesis of ZnS for supercapacitor applications. <i>Chinnalagu Dhilipkumar, Perumal Naveen Kumar, Selvam Karthick and Gopalakrishnan gopu</i>	92
PP 19	Formulation and characterization of water borne rust converter coating <i>S. Dhineshkumar, S. Palanisamy, S. Rajesh, S. Viswanathan</i>	93
PP 20	Carbazole encapped compartmental copper (II) complexes for antibacterial and theoretical optoelectronic studies. <i>Divakar Kumaravel, Baranipriya Sampathkumar, Mario Leo Joseph and Wilson Bosco Paul Michael</i>	94
PP 21	Synthesis, characterization and electrochemical studies of benzalazine supported polyaniline and copper(II) chloride nano sized composite. <i>B. Divya, D. Kanagavel and C. Vedhi</i>	95
PP 22	Isatin based ratiometric probe: Selective sensors for Cu ²⁺ and Hg ²⁺ ions in aqueous samples. <i>D. Divya, Ramanjaneyulu Mala and Sathiah Thennarasu</i>	96
PP 23	Synthesis, spectral, x-ray crystallography and biological properties of <i>n</i> -heterocyclic mixed ligand Co(III) complexes containing 1,10-phenanthroline and sodium azide <i>C. Elamathi, F. Dallemer, A. Madankumar and R Prabhakaran</i>	97
PP 24	Synthesis and Characterization of Poly (3,4-ethylenedioxythiophene)-Nickel oxide nanocomposites for Solar cell applications <i>A. Emi Princess Prasanna and C. Vedhi</i>	98
PP 25	Antibacterial and Antioxidant properties of Vitamin B ₃ -Poly(methyl methacrylate)/ α-Cyclodextrin Electrospun Nanofibers <i>S. Esakkimuthu, B. Suganya Bharathi and T. Stalin</i>	99

PP 26	<i>Solanum Procumben</i> leaves extract mediated green synthesis of Ag-Pd/Mn ₃ O ₄ nanoparticles and its antibacterial activity V. Gayathri, B. Pavithra, P. Nithya, M. Balaji, K. Bama, S. Jegatheeswaran, S. Selvam and K. Kottaisamy, M. Ramalakshmi and M. Sundrarajan	99
PP 27	Synthesis and characterization of metal oxide nanoparticles. S. Gomuraj and A. Mathavan	100
PP 28	Physico chemical characteristics and compositional studies of palm kernel oil. R. Govindaraju	101
PP 29	Synthesis, Characterization, Biological Studies and Fluoride Sensing of Salicylaldehyde Schiff Base Derivative. S. Gurusamy, S. Ramapandian and A. Mathavan	102
PP 30	Synthesis and evaluation of triazine based chemosensor for the detection of Co ²⁺ Ion. J. Jone Celestina, P. Tharmaraj, A. Jeevika and C. D. Sheela	103
PP 31	Precipitation synthesis and characterization of cadmium doped WO ₃ nanoparticles S. Kalaiarasi and R. R. Muthuchudarkodi	104
PP 32	Synthesis, spectral characterization and biological activities of metal(II) complex from Mannich base ligand. C. Kalaivanan, M. Sankarganesh, M. Yosuva Suvaiyin and G. Banukarthi	104
PP 33	A highly selective and sensitive colorimetric and fluorescent triazole sensor for Ni(II) ion. K. Kaleeswari and A. Tamil Selvi	105
PP 34	Electrochemical sensing of Atenolol by synthetic polymeric receptor. X. Robin Clara, P. Karthika, T. Kalpana and S. Viswanathan	106
PP 35	Facile Construction of a Supramolecular Organic Framework Using Naphthyl Viologen Guests and CB[8] Host via Charge-Transfer Complexation. Kanagaraj Madasamy, David Velayutham and Murugavel Kathiresan	106
PP 36	First principles calculations of the phase stability of rutile SnO ₂ . B. Kanimozhi, S. R. Srikumar and V. Vasu	108
PP 37	Thermal Studies of Cyclohexane, Sulfone and Maleimide containing Polybenzoxazine hybrid matrices. C. Karikal Chozhan, A. Chandramohan and M. Alagar	108
PP 38	Phosphorus and Silicon containing polybenzoxazine hybrid matrices: Thermal and Morphological properties. C. Karikal Chozhan, A. Chandramohan and M. Alagar	109
PP 39	Green synthesis of Iron oxide Nanoparticles using <i>Avicennia Marina</i> leaf extract. P. Karpagavinayagam, G. Kavitha and C. Vedhi	110
PP 40	Fabrication of silica particles connected onto the cellulose nanofibre/poly(lactic acid) nanocomposite for better thermal and mechanical properties. Karpuraranjith Marimuthu, Yuanfu Chen and Young-Soo Seo	111

PP 41	Fabrication of Cupric oxide decorated β -cyclodextrin nanocomposite immobilized Nafion as a high performance electrochemical sensor for L-tyrosine detection. <i>A. Karthika, A. Suganthi and M. Rajarajan</i>	112
PP 42	Jacobsen catalyst driven Friedel-Crafts intramolecular cyclization of inert terminal alkenes: Synthesis of 1 <i>H</i> -Indene derivatives from Baylis-Hillman adducts. <i>S. Karthikeyan, J. Helen Ratna Monica and Karthik Krishna Kumar</i>	113
PP 43	Molybdenum Disulfide nanosheets - chitosan hybrid composites high performance for and anticancer antibacterial activity <i>K. Kasirajan, M. Balaji P. Nithya and M. Karunakaran</i>	114
PP 44	Physical and Electrochemical characterization of pulse current electrodeposited Ni-TiN nanocomposite coatings <i>S. Kasturibai and G. Paruthimal Kalaigan</i>	115
PP 45	Synthesis and characterization of Titanium doped Zinc Sulphide nanoparticles for corrosive resistant application. <i>M. Kavitha and R. R. Muthuchudarkodi</i>	116
PP 46	Effect of soil copper on root of <i>Rhizophora annamalayana</i> under Wastewater Treatment. <i>K. Kayalvizhi and K. Kathiresan</i>	117
PP 47	“Clickable” block copolymer surfactants for the synthesis of color resilient latex. <i>N. Keerthika and S. G. Ramkumar</i>	117
PP 48	<i>Meso</i> -substituted Porphyrins for Bottom-gated OFETs by Solution Processing Technique. <i>Komal Kurlekar, R. Dheepika and S. Nagarajan</i>	118
PP 49	Synthesis, characterization and biological studies of Ov(iv) & Bi(iii) metal complexes. <i>K. Krishnaveni, A. Lajwen zuleka and A. Mathavan</i>	119
PP 50	Synthesis, Characterization, DNA-Binding and Biological Studies of Surfactant Cobalt(III)-IP-Dodecylamine Complexes <i>V. Krishnaveni and N. Kumaraguru</i>	120
PP 51	synthesis of 10-hydroxy-11 <i>h</i> -benzo[b]fluoren-11-ones and 6-hydroxy-7 <i>h</i> -benzo[de]anthracenes-7-ones via domino fries-scholl reaction. <i>M. Kumaresan, K. K. Balasubramanian and Sumathi Sowrirajan</i>	121
PP 52	Microwave assisted synthesis of fluorescent nitrogen doped carbon quantum dots for a selective sensing of Mercury(II) ions <i>AR. Maheswari, G. Muthusankar, G. Gopu</i>	122
PP 53	Ionic liquid mediated synthesis and characterization of ZnO nps by <i>leucas aspera</i> leaves extract with enhanced photocatalytic and biomedical applications <i>J. Maheswari, J. Saranya, M. Balaji, P. Nithya, V. Muthulakshmi, C. Subbu, M. Karunakaran and M. Sundrarajan</i>	123
PP 54	Adsorption and Electrochemical Studies of p-Tolylsulfoxide for oil pipeline in 1.0N HCl. <i>I. Malar vizhi, M. Pavithra, S. Selvaraj and K. Kalirajan</i>	124

PP 55	Design and synthesis of piperazine-piperidone H37 inhibitors with improved pharmacokinetic profiles <i>M. Mangalam, C. Sebastian Antony Selvan and C. Sankar</i>	125
PP 56	Synthesis, spectroscopic investigation and DFT study of 4-((4-fluorophenyl)diazenyl)-2-formylphenyl methyl carbonate. <i>G. Manikandan and A. Arokiasamy</i>	126
PP 57	Mn(II) complex containing 1,3 β -diketone and/or ancillary Pyrazolyl ligand. <i>A. Manikumar and Nagarajan Loganathan</i>	127
PP 58	Morphology directed synthesis of cadmium oxide nanomaterials based on modified kirkendall Effect. <i>A. Manimekalai</i>	128
PP 59	Effect of substituents on the ^1H - NMR chemical shifts of 6-(4'-substitutedphenyl)-4-methyl-2-oxo-1, 2, 3, 6-tetrahydropyrimidine-5-(n-phenyl)carboxamides <i>S. Manimekalai and K. Radhakrishnan</i>	128
PP 60	Electrochemical degradation of Mordant Blue 9 using flow reactor. <i>A. Manonmani, S. Dhineshkumar, S. Rajesh, S. Viswanathan</i>	129
PP 61	Synthesis, growth, structure, supramolecular architecture and Hirshfeld surface analysis of crown ether polyoxomolybdate complex: NLO applications <i>S. Sivaraman and R. Markkandan</i>	130
PP 62	Development of Abundant and Active Catalyst Host for Oxygen Evolution Reaction in Alkaline Medium. <i>V. Maruthapandian and V. Saraswathy</i>	130
PP 63	Tertiary composite material used for nanofibrous formation in biomedical application. <i>A. Mayakrishnan, M. Balaji, P. Nithya, V. Muthulakshmi, K. Ramanujam, V. Maheshkumar and M. Sundrarajan</i>	131
PP 64	Lyotropic liquid crystal directed synthesis of anisotropic copper microparticles and their application in catalysis. <i>P. R. Meyyathal and S. Umadevi</i>	132
PP 65	Electrochemical performances of surface modified CePO_4 -coated LiMn_2O_4 cathode materials for rechargeable lithium ion batteries. <i>P. Mohan, K. Srinivasan and G. Paruthimal Kalaigan</i>	133
PP 66	Synthesis of photo-responsive polysiloxane-based azobenzene liquid crystalline elastomers prepared by hydrosilation reaction. <i>K. Mohana, and S. Umadevi</i>	134
PP 67	Green approach for synthesis of Yb_2O_3 nanoparticles by <i>couroupita guianensis</i> abul leaves extract and biomedical applications. <i>V. Muthulakshmi, M. Balaji, P. Nithya, A. Mayakrishnan, H. Gurumalles prabu, A. Rukmani and M. Sundrarajan</i>	134

PP 68	Synthesis and applications of gold nanoparticles using fenugreek seed extract with their antibacterial, UV protection and anticancer. <i>P. Boomi, S. Muthumanickam, T. Indhumathi, RM. Ganesan and M. Karunakarn</i>	135
PP 69	Fabrication of Bromelain Decorated on Polyvinyl alcohol/Hydroxy ethyl cellulose Nanofibers and their Applications as Wound Dressings <i>P. Muthuselvi, B. Suganya Bharathi and T. Stalin</i>	136
PP 70	Chemical synthesis and characterization nano size poly (aniline-co-ethyl-4-aminobenzoate) copolymers and its spectroelectrochemical studies. <i>A. Nagarajan, Giftynol Elizabeth and R. Sasikumar</i>	137
PP 71	Electric field induced exciton binding energy in a Narrow Band gap Nanomaterials <i>M. Narayanan</i>	138
PP 72	A study on extraction, isolation and phytochemical evaluation of <i>tarenna asiatica</i> leaves. <i>G. Nithya, D. Lourdu Robert, Y. Muzakkira, A. Arokia Nepolean Raj and V. Collins Arun Prakash</i>	139
PP 73	Facile green synthesis of CeO ₂ and Ag doped CeO ₂ nanoparticles using ionic liquid medium and their antibacterial activity <i>P. Nithya, M. Balaji, V. Muthulakshmi, A. Mayakrishnan, S. Jegatheeswaran, S. Selvam, K. Bharathi and M. Sundrarajan</i>	139
PP 74	Development of functional antibacterial papers using Chitosan/Agar-Silver nanoparticles (Cht:Agar-AgNPs) <i>S. Nivethitha, K. Gopinath and C. Balalakshmi</i>	140
PP 75	Novel FeVO ₄ assisted Photocatalytic degradation of aqueous Methyl Violet solution under Sunlight irradiation. <i>S. Thillainatarajan, L. Firthawsha Yasmin, S. Parthiban, K. Gowthami and I. Muthuvel</i>	141
PP 76	Ni-CNT nanocomposites based electrochemical sensor for simultaneous determination of epinephrine and dopamine. <i>Perumal Manivel and V. Suryanarayanan</i>	142
PP 77	Cyclic Voltammetric Studies on New 2-Acetylnaphthone Chalcones. <i>R. Poongodi and S. Senguttuvan</i>	143
PP 78	Characterization of polymer electrolyte membrane based on blend polymer (PVP+PPA) with magnesium sulphate. <i>S. Prabu, M. Shanmugam, P. Manimegalai and R. S. Diana Sangeetha</i>	143
PP 79	Synthesis, characterization and biological studies on indole derivatives. <i>B. Prakash and O. Raina</i>	144
PP 80	Comparative Study on Nanoencapsulated Synthetic and Ayurvedic Matters; In vitro Evaluation of Neuroprotective and Antimicrobial Efficacies <i>Prakashkumar Nallasamy, Thenmozhi Ramalingam, Vijayalakshmi Ganesan and Suganthy Natarajan</i>	145

PP 81	Synthesis and thrombolytic activity of nitrogen containing hetero cyclic compounds. <i>V. Priyadarshini, K. Sundaresan and K.Tharini</i>	146
PP 82	Antimicrobial studies of schiff based novel ligand and its complexes. <i>M. Priyadharsani, P. Tharmaraj and C. D. Sheela</i>	147
PP 83	Novel & Smart sensing of Acetate & Hypochlorite ions with fluorescence Turn-on: Application in real sample analysis. <i>Ganesan Punithakumari and Sivan Velmathi</i>	147
PP 84	Synthesis, characterization of ferrite nanoparticles and its sunlight photocatalytic activity <i>O. Raina and B. Prakash</i>	149
PP 85	A novel electrochemical dopamine sensor based on hierarchical MoS ₂ wrapped CuMn ₂ O ₄ nanocomposite modified gold electrode. <i>Rajesh Madhuvilakku and Shakkthivel Piraman</i>	149
PP 86	Synthesis and characterization of a titanium based metal organic framework <i>S. Vishvatha, T. Ponmuthuselvi, S. Rajesh, S. Viswanathan</i>	150
PP 87	<i>Justicia</i> leaf assisted reduced Graphene Oxide /Zinc Oxide nanocomposite for antibacterial applications. <i>R. Rajeswari and H. GurumallesPrabu</i>	151
PP 88	Poly paraphenylene diamine/titanium dioxide/exfoliated graphite nanocomposites: synthesis, characterisation and application. <i>V. Rajeshwari and Jessica Fernando</i>	152
PP 89	Electrochemical, thermodynamic and adsorption studies for the corrosion inhibition of mild steel by henna extract in acid medium. <i>R. Rajkumar and C. Vedhi</i>	153
PP 90	Thin film formation of Phyla Nodiflora Linn leaves extract on mild steel in Acid Environment by Adsorption Studies <i>V. Rama, I. Malarvizhi, P. Deeparani and S. Selvaraj</i>	154
PP 91	Crystal Growth, Structure, Characterization and Theoretical studies of D-valinium picrate. <i>J. Anandakumaran and G. Ramasamy</i>	154
PP 92	Synthesis of Silver doped nano Zinc oxide and Evaluation of interaction between NPs and calf thymus DNA. <i>M. Ramesh, C. Sankar and S. Umamatheswari</i>	155
PP 93	Electrochemical degradation of malachite green dye using dsain a batch reactor. <i>C. Rani and K. Santhi</i>	156
PP 94	Physico chemical analysis of different soil samples in and around Thiruvavar District, Tamilnadu-India. <i>H. Rasith Ali and P. Sudha</i>	157
PP 95	Green Route Synthesis of Novel Nano composite material based on Nickel Oxide/ <i>Ocimum americanum</i> leaves extract derived Carbon for superior Supercapacitor applications. <i>M. Revathi and K. Thileep Kumar</i>	158

PP 96	Ionic liquid mediated synthesis and characterization of titanium di oxide nanoparticles by <i>tabernamentana divaricata</i> leaves extract with enhanced biomedical applications <i>S. Revathi, V. Bhuvaneshwari, R. Rajiv Gandhi, S. Ambika, M. Muthulakshmi M.Rajan and M. Sundrarajan</i>	159
PP 97	Synthesis and characterization of PVP-ZnO composite for enhanced antibacterial activity <i>A. Roshni and S. Thambidurai</i>	160
PP 98	All solid-state high-performance electric double layer capacitor fabricated using environment benign biomass-derived starch as the source for both degradable bio-electrode and bio-polymer electrolyte. <i>Palanisamy Rupa Kasturi and Ramakrishnan Kalai Selvan</i>	161
PP 99	Substantial investigation towards corrosive inhibition properties of <i>stachytarpheta jamaicensis</i> leaf extract on mild steel in 1.0 N HCl medium. <i>Mathu Sudhan, P. DeepaRani, S. Selvaraj, K. Kalirajan and C. Sangeetha</i>	162
PP 100	Biological synthesis and characterization of silver nanoparticles from seeds of lawsonia inermis and their antibacterial activity <i>R. Sangeetha, V. Komala, N. Dharsini Devia and N. Priya</i>	163
PP 101	Study of inhibition potential of synthesis green inhibitor on mild steel in acid medium <i>P. Sakunthala</i>	163
PP 102	Synthesis of carbon doped WO ₃ nanomaterials for photocatalytic applications. <i>K. Santhi, S. Karuppuchamy and C. Rani</i>	164
PP 103	Sensing Performance of B ₁₂ N ₁₂ Nanocage Towards Toxic Azides Detection: A Computational Study. <i>M. Saraswathi and S. Rajashabala</i>	165
PP 104	Antibacterial and photocatalytic application of Ag doped ZnO nanoparticles assisted by <i>Vitis Vinifera</i> . <i>K. Saravanadevi and A. Dinola</i>	166
PP 105	Soil microbial fuel cell assisted safe disposal of hexavalent chromium adsorbed <i>Chalcas Koenigii</i> leaves biochar. <i>C. Sathya and A. N. Senthilkumar</i>	167
PP 106	Synthesis and characterization of Chitosan-Gold nanoparticles with pdma hybrid composite <i>M. Senthilkumar and P. Manisankar</i>	168
PP 107	Maleonitrile schiff base derivative as a chemosensor for the detection of Cr ²⁺ and HSO ⁴⁻ ions and its bio-imaging application in living cells <i>M. Sethupathi, M. Thirumalaikumar, N. Sengottuvelan, P. Kumar</i>	169
PP 108	Adsorption of Nickel (II) from Aqueous Solution onto ZnCl ₂ Activated Carbon Prepared from Stems of <i>Leucas Aspera</i> . <i>A. Shanmugalingam and A. Murugesan</i>	170

PP 109	Studies on effect of aqueous solubility, <i>In-vitro</i> dissolution rate, Antimicrobial, Antibiofilm activity of Torsemide: β -Cyclodextrin inclusion complex. <i>Arumugam Shanmuga Priya, Jeyachandran Sivakamavalli, Baskaralingam Vaseeharan and Thambusamy Stalin</i>	171
PP 110	Green corrosion inhibitor for carbon steel by <i>Abutilon Indicum</i> powder/extract in 1 M HCl using weight loss method. <i>B. Shrigayathiri, U. Hajara Banu and M. Srimathi</i>	171
PP 111	Density functional study of the electronic and structural properties of several polymorphs of MgH_2 . <i>R. Shrivalli and V. Vasu</i>	172
PP 112	Cyclopentadienyl Ruthenium complexes of ferrocenyl ligands: synthesis, spectral Characterization and their biological evaluation. <i>M. Sindhu, R. Prabhakaran and P. Kalaivani</i>	173
PP 113	Evaluation of groundwater quality in the coastal stretch of Cuddalore District, Tamilnadu, India. <i>K. Sivakumar and A. Murugesan</i>	174
PP 114	Host-guest complex of 4-hydroxybenzophenone: β -cyclodextrin and its application for enhancing the UV protective ability of cotton fabric. <i>K. Sivakumar and A. Nalini</i>	174
PP 115	Supramolecular cocrystals of 18-crown-6 with 5-nitroisophthalic acid: solvent effect and optical nonlinearities. <i>C. Balakrishnan, M. Manonmani, SP. Meenakshisundaram and RM. Sockalingam</i>	175
PP 116	Fundamentals of Supercapacitors: based on nanomaterials for energy storage. <i>N. Soundarya, P. Muthukumar and P. Elumalai</i>	176
PP 117	Bent-Core liquid crystal alignment over a functionalised flexible substrate. <i>B. Sivaranjini, V. Ganesh and S. Umadevi</i>	177
PP 118	Hydrothermal synthesis of $NiMn_2S_4$ nanosheet arrays for high-performance of supercapacitor applications. <i>A. Srinivasan, M. Rajesh and Shakkthivel Piraman</i>	178
PP 119	The effect of ZrO_2 filler particle concentration on the ionic conductivity variation of PVP/PEO based gel polymer electrolyte <i>C. Subbu, M. Sundrarajan, M. Karunakaran</i>	179
PP 120	Synthesis, characterization of SrO/β -CD nanocomplex for biological application <i>R. Subhalakshmi, G. Banupriya M. Balaji, P. Nithya, V. Muthulakshmi, A. Mayakrishnan, J. Suresh and M. Sundrarajan</i>	180
PP 121	Green synthesis and characterisation of iron nanoparticle from green tea leaf extract and their waste water treatment <i>M. Suthi, R. Gowsalya Bharathi, B. AsmathaBeham and P. Indurani</i>	180

PP 122	Exploring the rhizobium <i>Leguminosarum</i> -Legume Root Nodule Associated Bacteria RL(LRNAB) as potential corrosion inhibitor on mild steel in acidic medium. <i>B. Tamilselvi and D. S. Bhuvaneshwari</i>	181
PP 123	Management of Cassava crop residues using termites. <i>A. Thamizharasan and S. Gajalakshmi</i>	182
PP 124	Preparation and characterization of PVP-ZnO-CuO composite for enhanced antibacterial activity <i>V. Umaiya Bharathi and S.Thambidurai</i>	183
PP 125	Mixed Metal Oxide nanocomposites of Ce/Ti/Mo-synthesis and characterization for supercapacitor application. <i>B. Uthiraselvi and Jessica Fernando</i>	184
PP 126	Iodine-catalyzed ring contraction rearrangement of tetraarylpiperidin-4-ones to 5-aryl-2-methoxy -2,4-diphenyl-1H-pyrrole-3-ones. <i>G. Vengatesh M. Sundaravadivelu and S. Muthusubramanian</i>	184
PP 127	Porous Organic Polymer derived Metal-free Carbon Composite as a Trifunctional Electrocatalyst for CO ₂ reduction and Water Splitting. <i>Venkatachalam Rajagopal, Murugavel Kathiresan, Vembu Suryanarayanan and David Velayutham</i>	185
PP 128	Facile Synthesis and <i>In Vitro</i> Microbial Exploration of Furyl Based 2-Cyanoiminodihydropyrimidines. <i>C. Vignesh and N. Ingarsal</i>	187
PP 129	Investigation on the Binding Interaction between 2,4-Dinitroaniline and γ -Cyclodextrin using Spectroscopic Techniques <i>Vigneshkumar Ganesan, Karthiyayini S and Stalin Thambusamy</i>	188
PP 130	Antibacterial activity, Structural, Optical and Morphological properties of Al doped ZnO nanoparticles synthesized by sol-gel method. <i>C. Vijayaraj, G. Nedunchezian and S. Sozhaveni</i>	188
PP 131	Spectral study of excited-state proton transfer process of 2-naphthol: α -cyclodextrin in inclusion complex and Cetyl trimethyl ammonium bromide <i>N. Vimalasruthi and T. Stalin</i>	189
PP 132	Biosynthesis of iron oxide nanoparticles by using <i>Acorus Calamus</i> extract and their DNA interaction studies <i>M. Rathimeena, G. Babu Raj, A. Palpandieswaran and K. M. Ponvel</i>	191

INVITED

TALK

IT 01

**ENGINEERING PURELY ORGANIC MATERIALS FOR LIGHT HARVESTING &
PHOTON UPCONVERSION**

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Abstract

Solar energy conversion represents a promising/alternative means for a sustainable/renewable energy technology. In recent years, photocatalysis and photovoltaics became the two mainstream techniques allowing to convert solar radiation into a useful and clean energy source. However, the materials which are engineered to harvest solar energy are limited to convert only a fraction of the solar spectrum into useful energy with various degrees of success. To overcome this limitation, scientists have been devising novel materials which can achieve non-linear photophysical processes allowing to maximize the efficiencies of solar energy conversion. In this picture, our research group has been working on engineering organic crystalline materials that are capable of transform low-energy radiation into higher energy photons (Fig.). This process is referred to as Photon Upconversion (UC). At the fundamental level, UC is a bi-molecular process requiring a light-harvesting triplet sensitizer (or donor) and an acceptor chromophore (emitter). Using advanced synthetic methods, we have designed donor and acceptor polyaromatic chromophores, which are structurally similar & complementary in a such a way that the rate of the donor→acceptor energy transfer (ET) competes with that of molecular diffusion. Notably, we demonstrated that the donor and acceptor chromophores could form supramolecular π - π aggregates, which favor ultra-fast ET. In this exploration, we synthesized novel organic quinoidal naphthalene triplet sensitizers that can efficiently harvest green radiation and then transfer the triplet

energy to polycyclic aromatic acceptors such as perylene. Subsequently, two triplet excitons of perylene annihilate to generate blue photons. We have also been successful in devising (crystalline) donor-acceptor dyads of our molecular systems, and we demonstrated that incident light with a power density in the microwatt regime was sufficient to perform UC in the solution phase and nanocrystalline suspension.

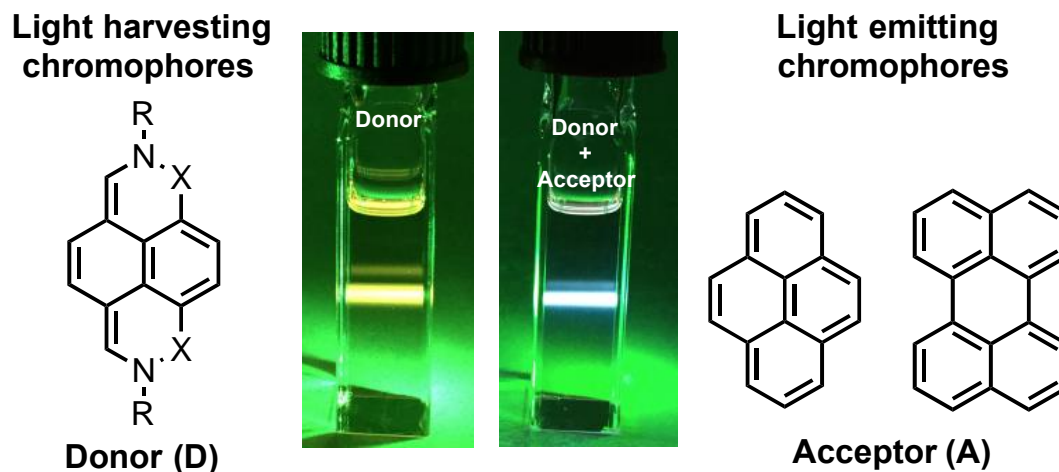


Fig. Illustration of UC with molecular systems which are developed in our lab

My presentation will navigate the synthesis of our organic donor-acceptor chromophores and the photophysics as well as the photo-kinetics of light-harvesting and excited state energy transfer. I will also describe our preliminary work and results regarding photon upconversion in the solid state.

IT 02

**DEVELOPMENT OF SOME DIAGNOSTIC AND ANALYTICAL TECHNIQUES
AIDED BY AND USING FLUORESCENCE SPECTROSCOPY**

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Abstract

Fluorescence spectroscopic techniques have the advantage of being sensitive, selective and compatible with in situ analytical procedures.[1] We have been looking at the fluorescence behaviour of complex multifluorophoric systems which has resulted in developing techniques for estimating petroleum fuel adulteration, composition of diesel-biodiesel and ethanol-petrol mix etc.[2] Our understanding of such systems also enabled us to develop facile methods for monitoring transformer oil degradation.[3] Our study of the network structure of polymeric hydrogels at the molecular level, using 8-Anilino-1-naphthalenesulfonic acid (ANS) (polarity sensitive probe), enabled us designing polyacrylamide-based tissue phantoms for ultrasonography and elastography applications. [4] Currently we are looking at the interesting problem of estimating faecal pigments in surface and drinking water sources using fluorescence. [5]

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IT 03

**HYBRID NANOCOMPOSITE-SUPPORTED METAL NANOCATALYSTS
FOR THE CATALYTIC REACTION**

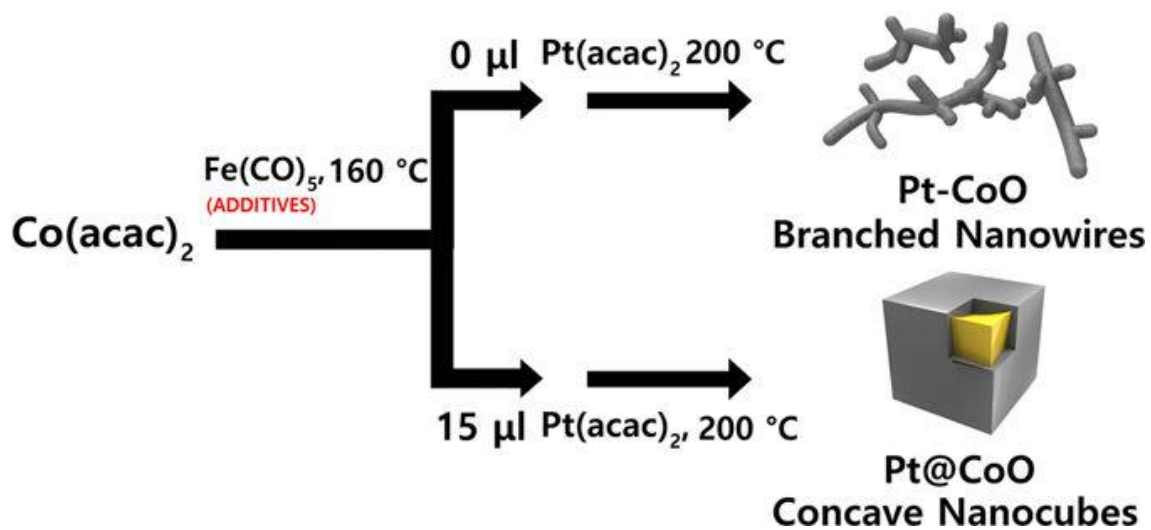
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Abstract

In recent years, numerous attempts have been made toward the design and synthesis of hybrid nanostructures with defined multicomponents by controlling the size and shape through solution-growth fabrication. Many studies have reported the incorporation of two or more distinct nano materials into one unit with increased functionality. The presence of multicomponent functions, combined with the enhanced chemical and physical properties, make hybrid nanostructures suitable for promising new applications. We report the effect of $\text{Fe}(\text{CO})_5$ additives in the synthesis of branched Pt-CoO nanowires (NWs) and core@shell concave nanocubes (NCs), in a one-pot system. Key to the success of this synthesis is control over the shape of the Pt seeds by controlling the quantity of $\text{Fe}(\text{CO})_5$ additive. In the absence of $\text{Fe}(\text{CO})_5$, branched Pt-CoO NWs were synthesized through the attachment of small Pt seed particles, followed by the growth of CoO by deposition. On the other hand, Pt@CoO concave NCs were obtained in the presence of $\text{Fe}(\text{CO})_5$ because of the stronger adsorption of Co on the Pt (100) surfaces than on the closely packed (111) surfaces. Also, various other conditions including the control of reducing agents, precursor concentrations, and stabilizing agents, were used to verify the effects of reaction kinetics on the synthesis of Pt-CoO nanoparticles. Compared to Pt/graphene oxide (GO) catalyst, branched Pt-CoO NWs supported on GO showed enhanced specific activity toward the oxygen reduction reaction (ORR).



IT 04

NANOSTRUCTURED NiPd/OMC: AN EFFICIENT BIFUNCTIONAL ELECTROCATALYST FOR HYDROGEN PRODUCTION VIA OVERALL UREA ELECTROLYSIS

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Abstract

Efficient catalysts for energy conversion from wastewater and energy storage are still existing. The effective hydrogen energy production through lower energy consumption is considering as a promising approach to access the world's clean energy demand. Herein, we demonstrate a facile strategy for preparation of nickel-palladium bimetallic nanoparticles incorporated on ordered mesoporous carbon support (Ni_(10%)Pd_(10%)/OMC) with controlled nanostructures. The resultant of Ni_(10%)Pd_(10%)/OMC electrocatalyst possess a well ordered mesoporous structure with highly dispersed tiny NiPd bimetallic nanoparticles (~2 nm), high-surface area (862.4 m² g⁻¹), a narrow pore size distribution (5.3 nm) and larger pore volume (0.91 cm³ g⁻¹). As a result, Ni_(10%)Pd_(10%)/OMC electrocatalyst can be used as an efficient bifunctional electrocatalyst for H₂ energy production (90-95% energy efficiency) at low overpotential via overall urea electro-oxidation reaction for the first time. Overall, the superior bifunctional ability of Ni_(10%)Pd_(10%)/OMC could be an appropriate energy efficient electrocatalyst to produce clean energy from wastewater treatment and fuel cell applications.

IT 05

HYBRID NANOMATERIALS FOR ADVANCED OXIDATION PROCESSES

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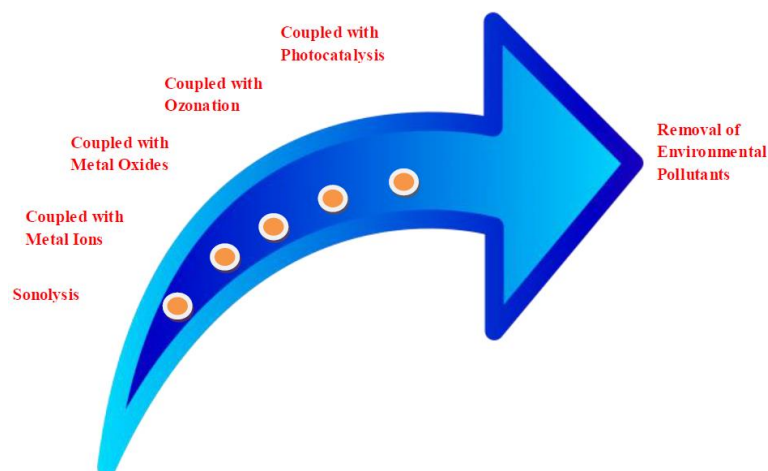
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Abstract

The creation of the modern world requires many industrial sectors, however, sustainability needs to be considered while developing industries. In particular, organic pollutants generated by many of these industries contaminate the environment leading to health and other issues. Many countries have adopted different oxidation/disinfection systems for the removal of pollutants for the remediation of an aqueous environment. Advanced oxidation processes (AOPs) have been introduced to remove organic pollutants present in wastewater. Sonolytic degradation of organic pollutants is considered as one of the AOPs, however, this process has its limitations. In order to overcome the limitations, hybrid techniques involving ultrasound other AOPs have been developed. Finally, highlights the advantages of using hybrid techniques involving ultrasound for the degradation of organic pollutants in aqueous solutions.



IT 06

RECENT DEVELOPMENTS IN COUNTER ELECTRODE MATERIALS FOR DSSCs

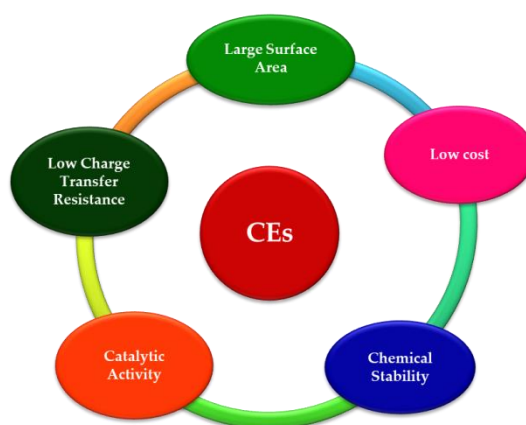
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Abstract

A dye-sensitized solar cell (DSSC) has been considered as a cost-effective alternative to silicon-based solar cell and achieved a maximum power conversion efficiency (PCE) of 13%. In order to enhance its power conversion efficiency, one of the essential ways is to improve the fill factor by modifying the counter electrode. The high cost of DSSC is mainly due to the high loading of Pt that required to catalyze the tri-iodide reduction reaction. In order to reduce the cost of DSSC, efforts have been made to find out cheaper alternative CEs for DSSC. This lecture gives a concise overview of alternative CE materials such as Pt-free alloys, graphene, carbon nanofibers, conducting polymers, chalcogenides and their nanohybrids.¹⁻⁵ Besides that the power conversion efficiency, cost and stability of their device are compared. This talk end-up with the conclusion and future prospects.



Desired Properties of Counter Electrodes

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IT 07

**THE PREPARATION OF NANOPARTICLES (NPS) BY TOP DOWN APPROACH
AND THEIR POTENTIAL INDUSTRIAL APPLICATION**

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Department of Physics, Faculty of Science, Mahidol University, Bangkok, Thailand.

Abstract

The preparation of nanoparticles (NPs) dispersed in aqueous and organic solvent from the agglomerate/agglomerate NPs by bead milling technique will be discussed. An example of the reduction of NPs with 0 dimension (0D), 1D and 2D will be shown along with the stabilization technique. The used of these NPs for a formation of clear hard coating on polymethy methacrylate are demonstrated. The used of these NPs as the nucleating agent for reducing the degree of supercooling in the phase change material (PCM) will also be discussed.

IT 08

HIGH ENERGY BATTERIES FOR DEFENSE APPLICATION

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Abstract

High Energy Batteries (India) Limited, was established in 1979. After Acquiring Transfer of Technology from Yardley Electric Inc., USA, the company started making sophisticated batteries for defense applications. The company has a very well equipped in-house R & D facility which has developed number of batteries for Naval and Air applications. The company also develops batteries for aerospace launch vehicle applications. The company established Sea water Activated Battery facility for under water applications in 2005 and Lead Acid Battery Plant which was established in 2009, with the facility equipped for making batteries for Automobiles, VRLA & Solar Battery applications.

The products and their applications are diversified into various technological fields like the Silver Zinc (Primary and Secondary) Battery which range from 0.5kW to 250 kW has applications in Aircraft Engine Starting, Satellite Launch Vehicles, Aerospace & Telemetry, and Underwater Propulsion & Detection. The Nickel Cadmium Battery which range from 4 Ah to 1000 Ah has its application in fields like Aircraft Engine Starting, Helicopter, UPS Back-up, and Battle Tanks. Also the Sea water Activated Battery which range from 30 kW to 250 kW has its areas of application being Under Water Propulsion, Flame float Smoke, and Sonobuoy.

The company develops batteries for torpedoes, missiles, aircraft, launch vehicle and automobile applications which vary in many shapes & sizes and with various chemistries involved. The company has got number of type approvals from agencies across India for those batteries. The company manufactures 2 types of batteries for each torpedo and missile

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application i.e., exercises version and combat version battery. The exercise version is secondary battery which is used for warfare simulations. These secondary batteries can be used for 6 to 8 cycles. The combat version is primary reserve battery which is used for real-time warfare scenario, as one-shot usage.

**ORAL
PRESENTATION**

OP 01

MWCNT COATED GLASSY CARBON ELECTRODE USED 2-HYDROXY-1,4-NAPHTHOQUINONE FOR OXYGEN REDUCTION

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Abstract

The electrochemical and catalytic behaviour of glassy carbon electrode modified by MWCNT in 2-hydroxy-1,4-naphthoquinone solution towards the reduction of oxygen were investigated by cyclic voltammetric, chronoamperometric and chronocoulometric techniques. The stability of the modified electrode was studied by cyclic voltammetry in acidic and neutral media. The influence of pH on the electrochemical and catalytic behaviour was studied and pH 7.0 was chosen as the optimum working pH by comparing the shift in oxygen reduction potential. The glassy carbon electrode modified by MWCNT with 2-hydroxy-1,4-naphthoquinone possesses good electrocatalytic ability for oxygen reduction with overpotential greater than that at a bare glassy carbon electrode. On increasing the scan rate, the peak separation also increases which shows the quasi-reversibility of the electron transfer process at MWCNT/GCE. The cathodic peak current (I_{pc}) increased linearly with scan rate (v), indicating adsorption controlled mass transfer for the reduction of 2-HyNQ at MWCNT/GCE.

The pH-potential diagram shows that at low pH (1 to 4) values, 2-HyNQ involves two-electron three-proton reduction process. In the intermediate pH range, it undergoes two-electron two-proton process and at pH above 10, the electrode surface reaction is a two-electron one-proton process. The cathodic peak reaches its maximum current with the maximum shift in oxygen reduction potential (ΔE) and the anodic wave was completely vanished in the presence of oxygen at pH 7.0. Hence pH 7.0 was chosen as optimum pH for oxygen reduction. The cathodic peak current, I_{pc} is linearly proportional to square root of scan rate, $v^{1/2}$ which confirms the diffusion controlled process for oxygen reduction. A larger potential shift (390 mV) was observed for 2-HyNQ combined with MWCNT/GCE than the bare GCE at its optimum pH 7.0.

OP 02

**DEVELOPMENT OF PROTON CONDUCTING POLYMER COMPOSITE
MEMBRANES FOR FUEL CELL APPLICATION**

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Abstract

Energy generation is one of the important factors that determine the overall sustainability of mankind. A steady depletion of fossil fuel reserves calls for an efficient, cost effective and sustainable technologies for energy conversion and power generation. Among which, proton exchange membrane fuel cell (PEMFCs) is regarded as a suitable alternative because it offers high efficiency and present a clean alternative to internal combustion engines. Broader applications of hydrogen fuelled PEMFCs are restricted in two ways: (i) the PEM has limited proton conductivity at high temperature and low relative humidity conditions, and (ii) the PEM exhibits poor durability in automotive environment due to inadequate mechanical stability upon swelling with water and shrinking when dried. To overcome the drawbacks, avenues of research includes development of variety of composite membranes.

This research focusses on the development of polymer composites using nano structured materials. Herein, polyvinylidene fluoride-co-hexafluoropropylene (PVdF-co-HFP) was sulfonated and the maximum sulfonation degree was found to be 2.7%. The sulfonated polymer composites were prepared by blending the polymer matrix with varying amount of a tri-metal oxide, barium strontium titanium oxide (BSTO). The casted composite membranes exhibited good ion-exchange capacity of 13.13 meq.g⁻¹. The composite membranes were thermally stable upto 400 °C and exhibited a lower impedance value of 0.7466 ohms than that of virgin polymer. Hence, polymer nanocomposites are good candidates for fuel cell application.

Keywords: Fuel cells, Proton exchange membrane, Polymer composite, Sulfonated PVdF-co-HFP, BSTO.

OP 03

IONIC LIQUID FUNCTIONALIZED HETERO ATOM DOPED PNF-MWCNT AND BNF-MWCNT AND ITS ENHANCED CATALYTIC ABILITY IN CLEAN ENERGY AND POLLUTION CONTROL APPLICATIONS

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Abstract

In recent times, heteroatom-doped carbon materials attracted much attention due to its low price and high stability in acidic and alkaline media compared with the noble metal catalysts (e.g., Pd or Pt). This work is focused on the preparation of B/P N, and F by self-assembling ionic liquids such as BMIM-PF₆ and BMIM-BF₄. The enhanced properties of the PNF-MWCNT and BNF-MWCNT were proved by XRD, FTIR, RAMAN, and XPS spectroscopy. Most interestingly, we observed that both the material displays bamboo-stick like morphology with the incorporation of heteroatoms in FE-SEM and HR-TEM analysis. Furthermore, the synthesized material exhibited the excellent catalytic activity in OER with an overpotential of 150 and 190 mV at a current density of 157 and 116 mA/cm² with prolonged stability over 12h. These results further confirmed by Tafel slope and EIS measurements. The smaller Tafel slope 88, 102 mV/dec and lower resistance 35Ω, 56Ω were obtained for PNF-MWCNT and BNF-MWCNT respectively. In addition, this catalyst showed exceptional catalytic activity toward the reduction of 4-NP. The PNF-MWCNT and BNF-MWCNT reduce the 4-NP within 2.83 and 3 min. The observed rate constant and TOF values are better than those of the previously reported graphene-based nonmetallic catalysts.

Keywords: Multi-walled carbon nanotube, Ionic liquids, Tri doped MWCNT, OER, 4-NP reduction.

OP 04

**SYNTHESIS AND CHARACTERIZATION OF MELAMINE CORE G1
GENERATION STARBURST DENDRIMERS USING 2,2-BIS(HYDROXYMETHYL)
PROPIONIC ACID AND THEIR POTENTIAL APPLICATION ANTIOXIDANT**

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Abstract

Synthesis of 2,2-bis(hydroxymethyl)propionic acid(bis-MPA) 2protected AB₂ type monomer was prepared and construct of melamine core to afforded G₁4 generation dendrimers for acetamide terminal groups. All the compounds were purified by column chromatography and characterized by using the spectral technique for FT-IR, ¹H & ¹³C NMR, HR-MS. G₁ generation dendrimers potential application of antibacterial, biofilm, and antioxidant was good activity present, so for further higher generation dendrimers used for biomedical application.

Keywords: Melamine, 2,2-bis(hydroxymethyl)propionic acid, 2,2-dimethoxypropane etc.,

OP 05

**ELECTROCHEMICAL PERFORMANCE OF Cr BASED LiCoO₂ NANOFIBRES AS
ELECTRODE MATERIAL FOR HYBRID SUPERCAPACITORS**

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Abstract

Nanofibrous LiCr_xCo_{1-x}O₂ was prepared successfully by electrospinning technique at the calcined temperature of 500°C for 4 hr. The morphology, phase transformation and crystal structure of the prepared LiCr_xCo_{1-x}O₂ nanofibres were studied using scanning
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electron microscope, FT-IR spectroscopy, thermal analysis and X-ray diffraction analysis, respectively. The crystalline phase of the sample was identified as a single phase with α -NaFeO₂ type structure and the peaks are indexed to the hexagonal system assuming the $R\bar{3}m$ symmetry. The morphology of LiCr_xCo_{1-x}O₂ material was nanofibrous with an average diameter of 45 nm. The electrochemical characteristics of the prepared LiCr_xCo_{1-x}O₂ nanofibres were investigated by cyclic voltammetry, AC-impedance and galvanostatic charge-discharge studies. The electrochemical measurements provided a maximum specific capacitance of 77.7 F/g with good stability over 1000 cycles. It revealed that the prepared LiCr_xCo_{1-x}O₂ nanofibres could be used as effective electrode material for high performance hybrid supercapacitors.

Keywords: Electrospinning, Nanofibres, X-ray diffraction, Scanning Electron microscope.

OP 06

ENHANCEMENT IN POWER CONVERSION EFFICIENCY OF ANGULAR LUMINESCENT SOLAR CONCENTRATOR EMPLOYING RE ION BASED POLYMER COMPOSITES

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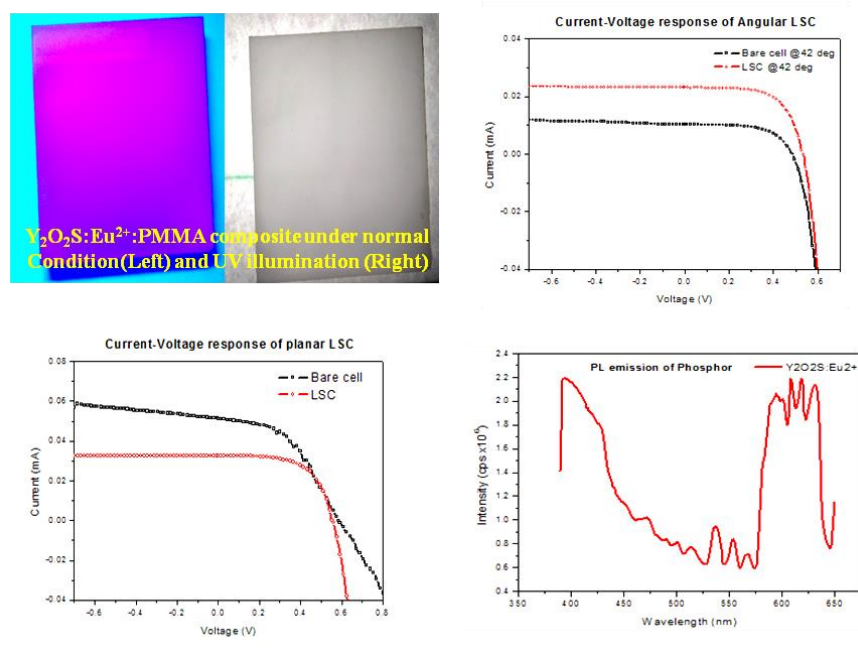
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Abstract

We report a phosphor:polymer composite in the form of a 5 x 5 x 0.5 cm square sheet for Luminescent Solar Concentrator applications. The phosphor, yttrium-oxysulphide activated with europium (Y₂O₂S:Eu) has been prepared through flux fusion method, which is then dispersed in the (poly)-methylmethacrylate (PMMA) matrix through water bath casting method. When excited at 365 nm, the photoluminescence emission of the phosphor shows an emission peak at 394 nm and four sharp peaks from 594 nm to 631 nm. As the composite's emission overlaps with the spectral response of a c-Si solar cell, the cell is coupled to one edge of the composite, forming an LSC. From the IV-measurements under a solar simulator at two different orientations, the LSC's power conversion efficiency (PCE) is found to outperform the bare c-Si cell at an angle of 42°. At planar orientation, the LSC retains 71% of the PCE of the bare c-Si indicating the absence of re-absorption loss. At the critical angle of PMMA, the escape cone loss is sufficed indicating a 152% enhancement of the LSC's PCE.

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OP 07

GREEN SYNTHESIS OF NOVEL 1,3-DITHIAZO FUSED HETEROCYCLIC COMPOUNDS AND THEIR ANTITUBERCULOSIS STUDIES

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Abstract

“Green synthesis” of fused heterocyclic compounds using Aromatic ketone as the starting material assisted with microwave irradiation. The structure and stereochemistry of the synthesized compounds was elucidated using one and two dimensional NMR, FT-IR, *Department of Industrial Chemistry, Alagappa University, Karaikudi.*

Mass Spectroscopy, Elemental analysis and Single crystal X-ray studies. The synthesized compounds were screened for their *in-vitro* anti-mycobacterium activity against *Mycobacterium tuberculosis* (MTB) H37Rv strain. The *in-vitro* cytotoxicity against these compounds was evaluated by RAW 264.7 cell line using (4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay. The fused heterocyclic compound was found to be the most active with minimum inhibitory concentration.

Keywords: Fused heterocyclic compounds, *Mycobacterium tuberculosis*, cytotoxicity.

OP 08

SYNTHESIS OF TRIPHENYLAMINE-BASED D- π -A MOLECULES FOR OFET APPLICATIONS

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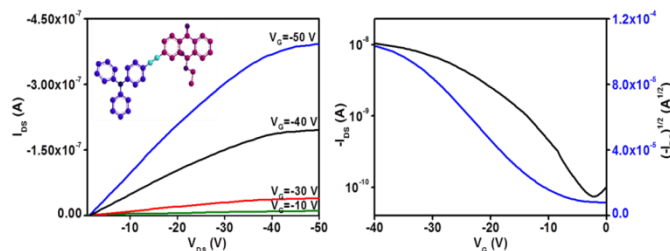
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Abstract

Research on organic field-effect transistors (OFETs) gained significant interest for their real life applications such as flexible large-area displays, RFID tags, and sensors. π -conjugated molecular materials with electron-rich (donor) and electron-deficient (acceptor) units in a fused manner are the focus in the emerging area of organic electronics. In this work, four conjugated D-A molecules with triarylamine or methoxyphenyl groups as donor and 2-benzoylbenzoate as acceptor and acetylene as π -spacer was synthesized for the application of OFETs. UV-vis absorption and fluorescence emission statistics shows that the introduction of triple bond red-shifted absorption maxima. Molecules with triarylamine donors exhibited high absorption and Stokes shift due to strong electron donating property. Synthesized molecules were thermally stable up to around 390 °C ensures the enhanced life-time and durability of the devices.

Devices fabricated by a cost-effective way by solution processing technique in Bottom Gate Top Contact architecture (BGTC). Thermal annealing at 80 °C for 30 min has improved the nature of the thin film to improve the device efficiency. Heavily n^{++} doped Si wafer served as gate and Ag contacts as source and drain electrode. The molecule with strong triarylamine donor were found to deliver the highest mobility up to $2.16 \times 10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and low V_{TH} of -3.2 V with higher On/Off current.



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OP 09

TETRANUCLEAR PALLADACYCLES OF 3-ACETYL-7-METHOXY-2H-CHROMEN-2-ONE DERIVED SCHIFF BASES: EFFICIENT CATALYSTS FOR SUZUKI-MIYaura COUPLING IN AQUEOUS MEDIUM

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Abstract

Organopalladium(II) complexes **1-3** have been synthesized by the complexation of 3-acetyl-7-methoxy-2H-chromen-2-one derived Schiff bases with potassium tetrachloropalladate $K_2[PdCl_4]$. Structural confirmation for the complexes has been attained by single crystal X-ray diffraction analysis which confirmed the tetrameric nature of the complexes. The ligands were found to bind with the palladium ion through azomethine nitrogen, thiolate sulphur and C4 carbon atom of the coumarin moiety subsequent to C-H activation. Computational study has been used to optimize the proposed molecular structures of the complexes. A systematic study on exploring their potential as catalysts in Suzuki-Miyaura coupling (SMC) has been done with different aryl halides and phenyl boronic acid in

aqueous medium. Optimization of the reaction indicated that the complex **2** has more efficiency than other complexes. An appreciable yield of the coupled products was observed with the minimum utility of the catalyst (μmol) and the C–C coupling has been confirmed by GC/GC-MS. Interesting scope of our catalyst is the coupling of four different chloroquinolines with phenyl boronic acid to afford the coupled products in good yields.

OP 10

STARBURST UNSYMMETRICAL TRIARYLAMINES FOR *p*-CHANNEL OFETs: IMPROVING DEVICE PERFORMANCE BY SOLVENT ENGINEERING

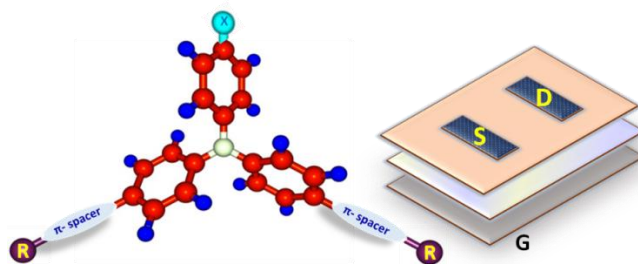
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Abstract

Organic small molecules have gained prominent attraction for scientific and technological inventions due to their defined structure which throws light on structure property relationship understandings. Triarylamines (TAA) are found to be suitable for electronics owing to their strong electron donating and hole transporting ability. We have designed a library of unsymmetrical triarylamines for organic field-effect transistor (OFET) applications to exploit their self-assembly, and optoelectronic properties without recasting their peculiar geometry. Unsymmetrical substitutions changed the bond angle and twist of the molecule and resulted in efficient molecular packing pattern which enhanced the charge carrier mobility. Introducing various electron donating and accepting substituents changed the frontier molecular orbitals of the molecule and offered optimum band gap. HOMO values is observed around 5.3 eV which is matching with widely used many hole transporting materials.



Further, improving the stability and extending the conjugation by diverse linkers gave huge impact in device performance and lifetime. The solubility of this molecules

informs that they are promising material for solution processing; economic and efficient method to attain high crystalline thin film in ambient conditions. TAA molecule OFETs are with field-effect mobility up to $1 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and ON/OFF ratio of 10^6 , expected to be a promising candidate for larger displays, logic switches, and sensors.

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OP 11

**TAILORED SULFONATED POLY (VINYLIDENEFLUORIDE-CO-
HEXAFLUOROPROPYLENE) NANOCOMPOSITE MEMBRANES USING POLY
(ETHYLENEIMINE) FUNCTIONALIZED REDUCED GRAPHENE OXIDE FOR
VANADIUM REDOX FLOW BATTERY APPLICATIONS**

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Abstract

Poly (ethyleneimine) functionalized reduced graphene oxide (PEI-RGO) embedded sulfonated poly (vinylidene fluoride-co-hexafluoropropylene) (SPVDF-co-HFP) nanocomposite proton exchange membranes (PEMs) are fabricated by solution casting method for vanadium redox flow battery (VRFB) applications. The functionalized GO and PEMs are characterized in terms of FT-IR, XRD, FT-Raman, surface morphology (FE-SEM and AFM), thermal and mechanical stability, proton conductivity and vanadium ion permeability. The characterization results confirmed that the successful preparation of PEI-RGO and fabrication of SPVDF-co-HFP/PEI-RGO nanocomposite PEMs. FE-SEM images of SPVDF-co-HFP/PEI-RGO PEMs obviously show a dense and homogeneous structure. Further the nanocomposite PEMs exhibited the highest ion exchange capacity and moderate water uptake. This is possibly due to the interfacial-formed acid-base pairs between PEI-RGO and SPVDF-co-HFP matrix effectively reduce the vanadium ion permeability and swelling ratio, increasing the proton conductivity of the nanocomposite PEMs. Moreover, the

dispersing ability of PEI-RGO content in the SPVDF-co-HFP matrix is enhanced the surface roughness, thermal and mechanical stability of the nanocomposite PEMs. Particularly, the SPVDF-co-HFP/PEI-RGO-0.75 PEM displayed the highest proton conductivity of 5.69 and $6.93 \times 10^{-3} \text{ Scm}^{-1}$ at 25 and 80°C respectively, the lowest vanadium ion permeability of $2.05 \times 10^{-7} \text{ cm}^2\text{s}^{-1}$ and the highest membrane selectivity of $25.52 \times 10^3 \text{ Scm}^{-3}\text{s}$. Overall results suggest that the SPVDF-co-HFP/PEI-RGO-0.75 nanocomposite PEM is found suitable alternative for commercially costly Nafion in VRFB applications.

OP 12

A NOVEL DUCKLING TOY MICROBIAL FUEL CELL FOR TREATING THE SEWERAGE WASTEWATER AND GENERATION OF ELECTRICITY FOR POWERING THE DANGER ZONE ALERT LAMP OVER THE SEWERAGE CANALS

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Abstract

In this novel work, for the first time the concept and the principles of Air-Cathode microbial fuel cells for treating the sewerage wastewater and production of electricity was incorporated for making a duckling toy microbial fuel cell. The MFC technology came into light at the earlier 19th century, but it was not popularised due to the lack of awareness, low power production even with the high fabrication costs. Later in the mid of the 21st century, due to the enforcement of the government laws towards the treatment and safe disposal of the generated wastewater from the industries and the households had made the researchers to rethink about the MFC technology for treating water and generation of electrical energy parallelly.

In the recent years, research on the MFC technology got tremendous growth and shown huge scope for the real time applications. The present work is a new attempt to employ the concepts of MFC technology in the duckling toy with the utilization of low cost ceramic separators for ion exchange, nitrogen doped α -Mn₂O₃ nano catalyst for high reduction potential at the cathode and finally the red colour LED bulb as a indicator to caution the people regarding the presence of the sewerage canal near the road sides. Notably,

this novel duckling toy MFC will result in the self-sustainable power generation for the cautioning red LED bulbs during the night time and also result in the removal of the organic pollutants in the sewerage canals.

OP 13

IN VITRO ANTIDIABETIC AND ANTIOXIDANT ACTIVITIES OF 2-(3,4-DIHYDROXYPHENYL)-3,5,7-TRIHYDROXY-4H-CHROMEN-4-ONE ISOLATED FROM THE METHANOLIC LEAF EXTRACT OF *ANDROGRAPHIS ECHIOIDES*

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Abstract

Objective: The present study was undertaken to determine anti-diabetic and anti-oxidant antimicrobial activity of the 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-chromen-4-one isolated from the methanolic leaves extract of *Andrographis echioides*.

Materials and methods: Antidiabetic activity of the isolated compound 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-chromen-4-one from the methanolic leaf extract of *Andrographis echioides* was studied for alpha amylase and alpha glucosidase inhibition using an in vitro model. Antioxidant activity was determined by DPPH free radical scavenging assay. The isolation was done using column chromatography using gradient elution with different mobile phase. Structural elucidation was carried out on basis of spectral analysis.

Results: The Isolated compound 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-chromen-4-one exhibited significant antioxidant inhibitory activities with an IC₅₀ value and well compared with standard ascorbic acid drug. As the concentration of 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-chromen-4-one increased from 20-100 µg/ml, the inhibitory actions of the isolated compound increased towards all the strains used in this study. In *vitro* study revealed that the isolated compound 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-chromen-4-one exhibited significant α-amylase and α-glucosidase inhibitory activities with an IC₅₀ value and 42.52± 45.03% respectively and well compared with standard acarbose drug.

Conclusion: Therefore, it is suggested that isolated compound 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-4H-chromen-4-one is a potential source for natural antidiabetic and antioxidant compounds and could have potential use in the management of diabetes mellitus.

KEY WORDS: *Andrographis echioides*, leaves, alpha amylase inhibitory activity, alpha glucosidase inhibitory activity, antioxidant activity.

OP 14

DEVELOPMENT OF RUTHENIUM DOPED GRAPHITIC CARBON NITRIDE FOR HIGHLY SENSITIVE NON-ENZYMATIC GLUCOSE SENSING

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Abstract

Development of a highly sensitive, selective and enzyme-free sensor for glucose determination is highly important for the diagnosis and management of diabetes. Here in, we have reported the novel ultra nano-molar sensitive and non-enzymatic sensor development by ruthenium doped graphitic carbon nitride (g-Ru-C₃N₄). The structural and morphological properties of the Ru doped g-C₃N₄ were characterized by X-ray diffraction (XRD), scanning microscopy (SEM), Ultra Violet-Visible spectroscopy (UVVis), Fourier transform infrared spectroscopy (FTIR) and energy dispersive X-ray (EDX) spectrum techniques. The prepared g-Ru-C₃N₄ was directly used as an electrochemical sensor for glucose determination, and its performance was evaluated by cyclic voltammetry (CV), differential pulsed voltammetry (DPV) and amperometric (CA) techniques. Fabrication of novel g-Ru-C₃N₄ modified electrode as a proficient nonenzymatic glucose sensor with high sensitivity (4.20×10^{-4} A mM⁻¹cm⁻²) over applied potential of + 0.30 V (vs. Ag/AgCl), fast response (5 s), and broad linear range (2–18 mM) coupled with lower limit of detection (5 nM). The constructed electrode provides good anti-interference ability with acceptable reproducibility and stability.

OP 15

**ROOM TEMPERATURE HYDROGEN SENSING PROPERTY OF
POLYPYRROLE/POLYANILINE CONDUCTING POLYMER BLENDS
SYNTHESIZED BY INTERFACIAL POLYMERIZATION**

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Abstract

Polypyrrole/Polyaniline conducting polymer (CP) blends for room temperature operated hydrogen gas sensor are synthesized using simple inexpensive interfacial polymerization method. Miscible and Immiscible polymer blends are synthesized and the sensing parameters are compared. The type of blend is confirmed by the Glass Transition Temperature (T_g) which is measured by Differential Scanning Calorimeter (DSC). Surface morphological studies are characterized by the Scanning Electron Microscope (SEM) and High Resolution Transmission Electron Microscope (HRTEM). Structural studies are done by the X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR) and UV-visible absorption Spectroscopy. The polymer blends showed selectivity towards hydrogen among oxygen and Liquid Petroleum Gas (LPG). It also exhibits improved sensor characteristics such as % sensitivity (79.1 %), response time (180 sec) and recovery time (280 sec). The lower limit of detection (LOD) of the electrode is determined as 5 ppm. The fabricated electrodes exhibit improved stability for the period of 50 days.

Keywords: Polypyrrole/Polyaniline Blends, Interfacial Polymerization, Hydrogen Gas, Sensitivity

OP 16

**LOW-COST AND ECO-FRIENDLY SYNTHESIS OF SILVER NANOPARTICLES
USING *TRIDAX PROCUMBENS* LEAF EXTRACT AND ITS LARVICIDAL
ACTIVITY**

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Abstract

Mosquitoes are a key threat for millions of people worldwide, since they act as vectors for devastating pathogens and parasites. In this scenario, vector control is crucial. Mosquito larvae are typically targeted victimization through organophosphates, insect growth regulators and microbial agents. Here, we are intended to target on some crucial challenges regarding eco-friendly control of mosquito vectors, mainly the improvement of behavior-based control strategies including green synthesized nanoparticles. The present study was carried out to screen the phytochemicals present in the leaf extract of *Tridax procumbens* by standard protocols. Synthesized silver nanoparticles were characterized by using UV-visible spectroscopy, FTIR, SEM and EDAX. The colloidal solution of silver nanoparticles was found to exhibit mosquito larvicidal activity against *Anopheles stephensi* malaria vector.

Keywords: *Tridax procumbens*, Phytochemical analysis, Silver nanoparticles, UV- visible analysis FTIR, SEM, EDAX and Larvicidal activity.

OP 17

SYNTHESIS OF ANCHORED NICOTINIC ACID HYDRAZIDE GRAPHENE OXIDE FOR EFFICIENT ELECTROCHEMICAL DETECTION OF CAFFEINE

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Abstract

A simple modified sensor based on glassy carbon electrode (GCE) was developed using nicotinic acid hydrazide-anchored graphene oxide. The synthesised anchored nicotinic acid hydrazide graphene oxide (NAHGO) was characterised by Fourier Transform Infrared spectroscopy (FTIR), Powder X-ray diffraction (PXRD), Raman spectroscopy, Scanning electron microscopy (SEM), Energy-dispersive X-ray spectroscopy (EDX) and thermogravimetric analysis (TGA). And we have also demonstrated the electrochemical

behaviour of GCE modified nicotinic acid hydrazide-anchored graphene oxide (NAHGO) for the determination of caffeine by employing voltammetric techniques. Modification of working electrode increases the electro oxidation of caffeine with increased current. The influence of parameters like scan rate, pH and concentration on the peak current of caffeine were studied. The studies showed that we could qualitatively determine caffeine in imol plus and ocean one 8 energy drink using NAHGO anchored graphene oxide.

Keywords: electrochemical sensor, caffeine, anchored nicotinic acid hydrazide.

OP 18

Cu₂NiSnS₄ NANOPARTICLES GROWN ONTO GRAPHENE AS AN EFFICIENT NANOHYBRID COUNTER ELECTRODE FOR HIGH-PERFORMANCE DSSC

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Abstract

In the present work, we prepared nanohybrid quaternary chalcogenide (Cu₂NiSnS₄) nanoparticles decorated graphene nanosheets to use as an efficient nanohybrid counter electrode for dye-sensitized solar cell (DSSC). The physical characterization of Cu₂NiSnS₄ nanoparticles, graphene, and Cu₂NiSnS₄/Graphene nanohybrid were characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM) and Raman spectroscopy. The ac - impedance spectroscopy, cyclic voltammetry (CV), and Tafel polarization studies demonstrate the positive synergetic effect between graphene and Cu₂NiSnS₄. Due to the exceptional electron-transfer pathway of graphene nanosheets and an excellent catalytic ability of Cu₂NiSnS₄ nanoparticles, the prepared nanohybrid exhibited excellent electrocatalytic activity towards tri-iodide reduction than individual Cu₂NiSnS₄ nanoparticles and graphene. Finally, DSSC was fabricated using Cu₂NiSnS₄/Graphene nanohybrid as a counter electrode has higher PCE of 7.92% than that of std. Pt (7.68%) and Cu₂NiSnS₄ nanoparticles CE(7.20%).

Keywords: DSSC, Quaternary chalcogenide, Cu₂NiSnS₄, Graphene nanosheets, Nanohybrid, Counter electrode.

OP 19

ASAFETIDA-RESIN STABILIZED MoO₃ NANOPARTICLES ENCRUSTED WITH RUTHENIUM BIPYRIDINE AN EFFECTIVE TRANSDUCER FOR ELECTROCHEMISTRY OF BUTEIN

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Abstract

Polyphenolic phytochemicals are well-known adjuvant in anti-cancer regime. However, difficulty in identification, extraction and quality control limits its potential application in health care domain. In this context, developing a rapid sensing platform to detect complex phytochemical is paramount importance for ease of extraction and quality control of final formulation. Current research progresses focused on developing a highly sensitive, selective and rapid sensing platform based on hybrid materials is highly promising due to its synergistic effect. Herein, asafetida resin mediated green synthesis of MoO₃ nanoparticles (*g*-MoO₃ NPs) were chemically adsorbed with Ru(II) and demonstrated for the direct electrochemical detection of clinically important herbaceutical, butein. The interaction between MoO₃ and Ru(II) in the hybrid nanocomposite is systematically validated using UV-Vis absorbance, photoluminescence, and Raman spectroscopy. The redox activity of fabricated *g*-MoO₃-Ru(II) modified on glassy carbon electrode is examined in presence of external redox mediator of methylene blue. The hybrid *g*-MoO₃-Ru(II) nanocomposite exhibits superior electrochemical activity in nanomolar range (50–1250 nM) of detection compared to that of pristine *g*-MoO₃. The improved electrochemical property with respect to the synergistic effect of hybrid is promising for sensor platform useful for herbaceutical fingerprinting. Furthermore, the developed optical and electrochemically active *g*-MoO₃-Ru(II) may find multifunctional applications in intracellular bio-imaging, antioxidant and electrochemical sensor studies.

OP 20

HIGH CAPACITY AND ENHANCED CYCLING STABILITY OF K⁺-DOPED LiNi_{1/3}Mn_{1/3}Co_{1/3}O₂ CATHODE MATERIALS FOR LITHIUM - ION BATTERIES

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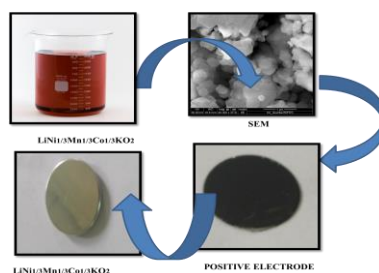
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Abstract

K⁺-doped LiNi_{1/3}Mn_{1/3}Co_{1/3}O₂ cathode materials are synthesized via sol-gel method. Lithium – ion coin cells were fabricated by using K⁺ - doped LiNi_{1/3}Mn_{1/3}Co_{1/3}O₂ positive electrode materials and LiPF₆ as electrolytes. The influence of K⁺ -doped on the structural and electrochemical properties of LiNi_{1/3}Co_{1/3}Mn_{1/3}O₂ positive electrode materials were characterized by XRD, SEM, TEM and electrochemical experiments. The results revealed that LiNi_{1/3}Mn_{1/3}Co_{1/3}O₂ with small amounts of K⁺ -doping keeps the α-NaFeO₂ layered structure. As the doping content increases, the lattice parameters increase and the random stacking happens. The average particle size is about 0.3-0.4 μm and the specific surface area decreases. The K⁺ -doping improved the discharge capacity of Li - ion cells. The battery with the Potassium-doped LiNi_{1/3}Mn_{1/3}Co_{1/3}O₂ materials has delivered a discharge capacity of 267.34mAh g⁻¹ and good capacity retention even after 100 cycles at a current density of 0.1 mA cm⁻² at room temperature.

Key words: Positive electrode materials, XRD, SEM, TEM, Charge/discharge



Synthesis of K⁺ - doped LiNi_{1/3}Mn_{1/3}Co_{1/3}O₂ positive electrode materials by sol-gel method

OP 21

**SYNTHESIS OF ZINC COMPLEX USING PYRIDOXAL BASED SCHIFF BASE:
FUNCTIONAL MIMICS OF HISTONE DEACETYLASE 6 ISOFORM**

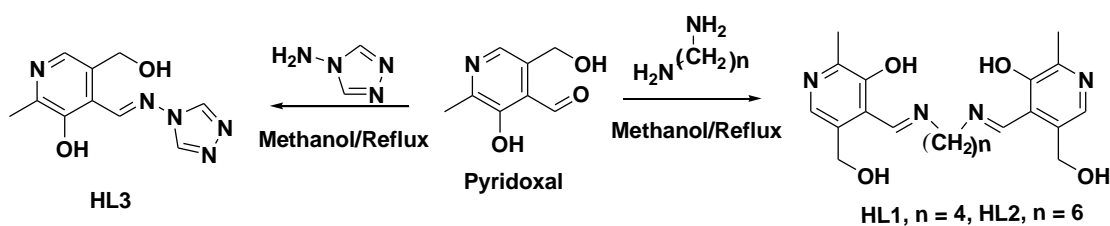
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Abstract

Histone deacetylases (HDACs) regulate myriad cellular processes by catalyzing the hydrolysis of acetyl-L-lysine residues in histone and nonhistone proteins. The Zn^{2+} dependent class II b enzyme HDAC6 regulates microtubule function by deacetylating α -tubulin, which suppresses microtubule dynamics and leads to cell cycle arrest and apoptosis.^[1] Acetylation and deacetylation of HDAC6 is balanced process. However, the balance is often upset in diseases such as cancer.^[2] Since the exact mechanism of HDAC6 isoform not clearly understood till days, the regulation process of HDAC6 is not controlled. The development of HDAC inhibitors is a milestone of research for curing diseases such as cancer and brain diseases. The known inhibitors are not selective for particular isoform and also produce some side effect.^[3] To understand the mechanism clearly, we try to mimic HDAC6 isoform. In this regard, Pyridoxal, the biologically important molecule, is chosen to make ligands. The pyridoxal-based zinc complexes has been developed and synthesized. The synthesized zinc complexes will be screened for HDAC activity.

Keywords *Histone deacetylases (HDACs), Pyridoxal, and Schiff base*



Scheme : Synthesis of Ligand HL1, HL2, HL3

Reference

- [1] Miyake Y.; Keusch, J. J.; Wang, L.; Saito, M.; Hess, D.; Wang, X.; Melancon, B. J.; Helquist, P.; Gut, H.; Matthias, P.; *Nature Chemical Biology*, **2016**, *12*, 748–754.
- [2] Hai Y, Christianson D. W.; *Nature Chemical Biology*, **2016**, *12*, 741–747.

[3] Nurul Islam, M.; Shahidul Islam, M.; Ashraful Hoque, M.; Kato, T.; Nishino, N.; Ito A.; Yoshida, M.; *Bioorganic & Medicinal Chemistry*, **2014**, *22*, 3862–3870.

OP 22

**PHOTOPHYSICAL AND SPECTRAL PROPERTIES OF BORON DIFLUORIDE
CURCUMIN COMPLEX DYE AND THEIR DERIVATIVES: A DFT STUDY**

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Abstract

The optical, electronic, and charge transport properties of Boron difluoride curcumin (BFC) complex have been explored with the various substitution like electron donor as well as electron acceptor by advanced Quantum chemical calculations. In this article, we show that BFC complex allow for additional electron donor/acceptor substituents to induce unexpected redshifts in the optical transitions of curcumin. For this purpose, BFC were analyzed with F, Cl, Br, CH₃, C≡N, OCH₃, C₆H₅, NO₂, NH₂, N(CH₃)₂ functional groups for these studies. The ground and excited state geometries of the BFC and their derivatives were optimized using Density Functional Theory. The Dipole moment, NBO charge, HOMO-LUMO energy gap, absorption and emission energies of the BFC complexes have been calculated. NBO charge analysis clearly shows that the charge transferred by the electron donor substitution on BFC complex. The absorption and emission spectra of substituted and unsubstituted BFC have been calculated using Time-Dependent Density Functional Theory (TD-DFT). The results of DFT calculations are in good agreement with available experimental results. The result shows that the absorption and emission of BFC has been highly influenced by the substitution of strong electron donor and electron acceptor. Both λ_{abs} and λ_{ems} of the BFC derivatives with electron donor fragments show bathochromic shifts compared with parent compound, while the corresponding values of the substituted derivatives with electron acceptor fragments are similar to those of parent compound BFC. Our results suggest that the substituted derivatives with Amino, Phenyl and N,N'-dimethyl amino substituents are expected to be promising candidates for fluorescent materials and also the electron/charge transport materials for OLEDs.

Keywords: Boron difluoride curcumin (BFC); Absorption; Emission; TD-DFT; Molecular Orbitals;

OP 23

NEW UNDERSTANDING ON SUSTAINABLE FABRICATION ENHANCED PHOTOCATALYTIC PERFORMANCE OF Pr₆MoO₁₂/g-C₃N₄ NANOCOMPOSITE FOR THE DEGRADATION OF ORGANOPHOSPHATE PESTICIDE (METHYL PARATHION)

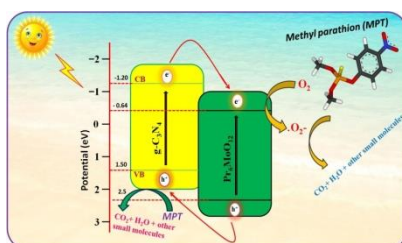
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Abstracts

In the present study, a novel Praseodymium molybdate/graphitic carbon nitride (Pr₆MoO₁₂/g-C₃N₄) nanocomposite were successfully fabricated by simple hydrothermal environment for the first time. The synthesized Pr₆MoO₁₂/g-C₃N₄ nanocomposites were used for the photocatalytic degradation of methyl parathion (MP) under visible light irradiation. The Pr₆MoO₁₂/g-C₃N₄ nanocomposite was demonstrated that superior crystalline nature with 22.8 nm, the surface morphology studies were confirmed the large scale formation of flower-like Pr₆MoO₁₂/g-C₃N₄ nanocomposite with typical size were observed from 20-30 nm. More importantly, the various physicochemical parameters including such as concentration of MP solution, catalyst dosage and scavengers was obtained as an optimized condition for the best photocatalytic experimental results. According to the trapping experiments using various scavengers showed that the reactive hydroxyl radical (•OH) and •O₂⁻ play the major role in the photocatalytic degradation process. On the basis of the result, a plausible mechanism has also been reported. This study provides an efficient and ideal approach to construct the new strategy to develop g-C₃N₄-based architected photocatalyst for poisonous wastewater treatment in the near future.

Keywords: Photocatalyst, Pr₆MoO₁₂, g-C₃N₄, Pesticide, Scavengers



OP 24

**POSSIBLE MECHANISM OF THE MPT DEGRADATION UNDER VISIBLE LIGHT
IRRADIATION OVERVIEW OF MODIFIED CARBON PASTE ELECTRODE
WITH CHITOSAN COMPOSITE**

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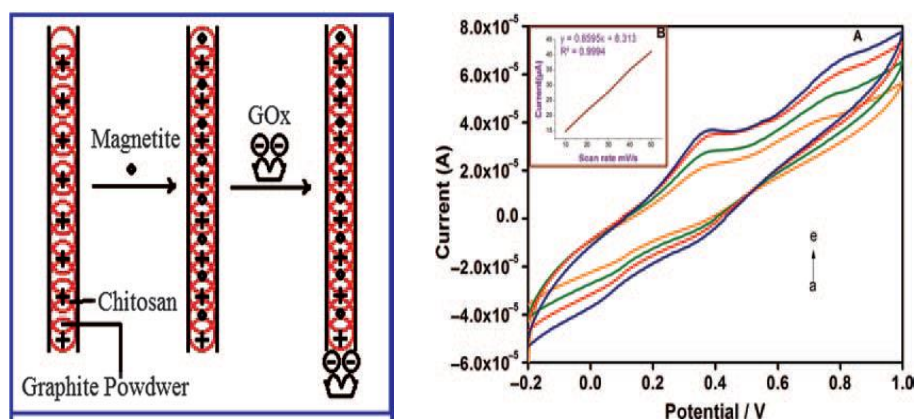
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Abstract

Graphene/graphene oxide(GO) and its nanocomposites have been utilized for improved performance of biosensors, attributed to synergistic effect of graphene and accompanying material in the nano composite. GO dispersed in a polymer matrix like chitosan (CH) have been reported to enhance electrochemical performance, ease of immobilization, biocompatibility and favorable micro environment for fabrication of enzymatic biosensors. Chitosan is commonly used to disperse nano materials due to its excellent capability of film formation, non toxicity, biocompatibility, mechanical strength and good water permeability. Accordingly, a variety of materials with ability to promote electron transfer between Glucose oxidase enzyme(GOD) and electrode (e.g. carbon nanotubes (CNTs), Chitosan (CH) have been adopted as the matrix to immobilize GOD. CNTs with properties of excellent electricity, metal and semiconductors, especially the biocompatibility, have become suitable candidates for the promotion of heterogeneous electron transfer. They are one of novel nano material components to improve the electrical contacting of enzymes with electrode. The attractive benefits of modifying electrodes is their improved electrocatalytic response which includes reduction in over-potentials and large voltammetric signals allowing low detection limits and high sensitivities. The proposed modified carbon paste electrode will enhance the electrochemical performance of metal/metal nanoparticles which would be a next generation, low cost and biosensing applications.

Keywords: Carbon paste, metal nanoparticles, graphite, biosensor, Modified electrode, Composite.



Proposed mechanism of carbon paste bioelectrode containing magnetite-CH-GOx

OP 25

ELECTROCHEMICAL AND SPECTROSCOPIC APPROACH FOR IODIDE ION SENSING BY FERROCENE BASED SCHIFF BASE RECEPTOR (Fc-AEP)

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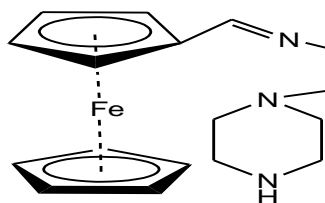
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Abstract

The ferrocene based receptor **Fc-AEP** was synthesized by one pot condensation reaction of ferrocene carboxyaldehyde and 1,2-aminoethylpiperazine. The physico-chemical characterization and purity of the synthesized compound was verified by ^1H NMR, ^{13}C NMR, ESI Mass, FTIR, UV-Visible and cyclic voltammetry. Anion-binding properties of receptor **Fc-AEP** (cyclopenta-2,4-dien-1-yl(2-(((2-(piperazin-1-yl)ethyl)imino)methyl)cyclopenta-2,4-dien-1-yl)iron, bearing piperazine group connected to the ferrocene unit via Schiff base condensation was evaluated by both UV-Visible spectral and electrochemical analysis. The results revealed that the receptor was highly selective towards the I^- ion in the presence of other anions (Cl^- , Br^- , F^- , AcO^- and HSO_4^-) due to the fact that, the H-bond donor unit (receptor unit, N-H) is directly attached to the signaling unit (ferrocene unit) and the H-atom of the N-H group may relatively be more acidic due to enhanced ICT transition and thus interacts strongly with the I^- ion. The 1:2 binding stoichiometry was observed using jobs plot and the corresponding binding constant was determined by the analysis of the spectral titration data, $K_a = 8.22 \times 10^5 \text{ M}^{-1}$ for I^- anions. The electrochemical studies shows cathodic shifts in Receptor- I^- anion binding because the oxidation process became easier in the presence of the negatively charged ion as a consequence of electrostatic stabilization. Hence, Department of Industrial Chemistry, Alagappa University, Karaikudi.

I⁻ ion can be detected even at low concentrations (10⁻⁶ M). There was no significant response of receptor upon addition of other anion and metal ions. Thus, the receptor **Fc-AEP** is a selective chemosensor for I⁻ anion (as its TBA⁺ salt).

Keywords: Iodide anion, Ferrocene based Schiff base receptor, chemosensor, electrochemical analysis.



Fc-AEP

Reference: 1. Fabiola, C. Antonio, E. Arturo, T. Alberto and M. Pedro, *J. Org. Chem.*, 73, 2008, 4034–4044.

OP 26

FLUOROGENIC MERCURY ION SENSOR BASED ON PYRENE-AMINO MERCAPTO THIADIAZOLE UNIT

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Abstract

The present work describes a highly selective and sensitive determination of Hg²⁺ in water samples with bioimaging applications in living cells using a fluorogenic pyrene-amino mercapto thiadiazole (PYAMT) probe. The probe PYAMT exhibited three absorption peaks at 333, 348 and 394 nm and emission maxima at 378, 388 and 397 nm ($\lambda_{ex}=348$ nm). It showed significant fluorescent quenching (96%) with $I/I_0=0.051$ upon the addition of 2.5 μ M Hg²⁺ ion in CH₃CN:H₂O (1:1, v/v; pH 7.2), whereas its fluorescence remained unaltered in the presence of other metal ions. The quenching phenomenon is attributed to the heavy atom effect of Hg²⁺ ion followed by electron transfer. The fluorescence intensity decreased linearly against a wide range from 100 nM to 2.5 μ M Hg²⁺ ($R^2 = 0.9937$) with a limit of detection as low as 0.35 nM (S/N=3). The binding stoichiometry ratio of PYAMT-Hg²⁺ is proved to be 1:1 by fluorescence and DFT measurements. The sensor possesses high association constant with Hg²⁺ ion in the order of 9.08×10^5 M⁻¹ and it is also capable of reversibly detecting

cysteine with OFF-ON mechanism. Finally, the proposed method is successfully applied to selectively detect Hg^{2+} ion in real water samples and bioimaging studies in live cells.

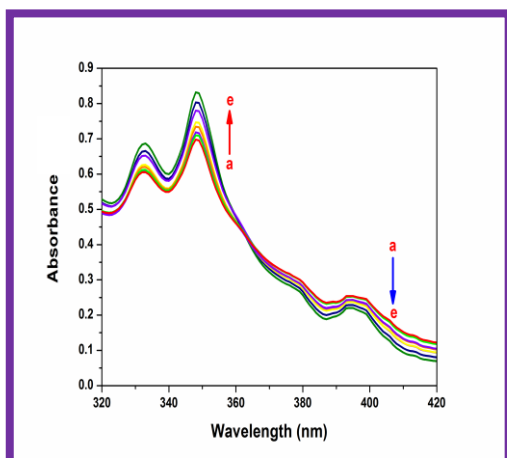


Fig.1. Absorbance spectra on Hg(II) addition
(increasing concentrations of 0.5 mM)

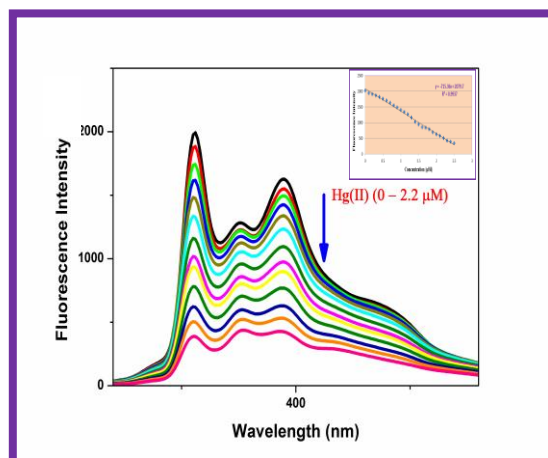


Fig.2. Fluorescence spectra on Hg(II) addition

Reference

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OP 27

MECHANISM PROPOSED FOR THE PREPARED CHITOSAN-ZNO NANOCOMPOSITE

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Abstract

Chitosan–ZnO composite was prepared by direct addition of dissolved chitosan with different ratio of zinc nitrate and sodium hydroxide at 80°C. The formation of chitosan-ZnO composite was confirmed by FTIR analysis. XRD patterns, determined the hexagonal structure of ZnO. Maximum of 82% zinc ions was noticed by Energy dispersive x-ray analysis. The SEM images revealed that ZnO particles were dispersed within the chitosan matrix. The antibacterial activities of chitosan-ZnO composites were measured in terms of zone of inhibition by disc method. A highest zone of inhibition about 60 mm against Gram-positive *S. aureus* and 53 mm against Gram-negative *K. aerogenes* bacteria were obtained

with prepared chitosan-ZnO composite. The mechanism was proposed for the formation of Chitosan-ZnO composite based on the literature studies and own studies.

Keywords: Chitosan-ZnO composite, FTIR, XRD, SEM, Antibacterial activity.

OP 28

A CONVENIENT ELECTROCHEMICAL METHOD FOR THE PREPARATION OF BROMOHYDRIN USING NaBr AS ELECTROLYTE

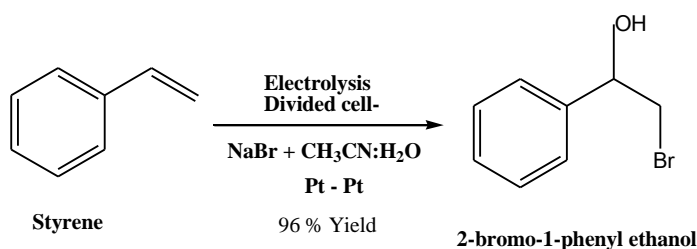
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Abstract

A convenient electrochemical method for the preparation of bromohydrin is reported using bromide as a mediator. A yield of 75 - 94% is obtained for cyclic and acyclic alkenes in a divided cell using a solvent mixture of CH₃CN: H₂O (1:1). Acyclic alkenes substituted with aromatic ring (styrene) gives better yield than the cyclic compounds (cyclohexene). The effect of electro chemical parameters like current density, charge, electrodes were studied in detail and reported. At optimum experimental condition, a yield of 96% styrene bromohydrin is obtained using platinum electrodes with 80% current efficiency. Bromohydrins are useful intermediates having reactive functional groups like Br and hydroxide.



OP 29

PREPARATION OF PALLADIUM NANOPARTICLES IN A MICROEMULSION AND THEIR APPLICATION FOR THE HECK REACTION

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Abstract

Microemulsion is an optically isotropic, transparent and thermodynamically stable system formed by two or more immiscible liquids which are stabilized by a surfactant (1-3). Microemulsions are considered as convenient and economic templates for preparing nanoparticles. Herein we employed a microemulsion consisting of water, triton X-100 and an imidazolium based ionic liquid crystal (H₂O/TX-100/ILC) for the *in situ* preparation of palladium (Pd) nanoparticles. The Pd nanoparticles were characterised using UV-Vis spectroscopy and transmission electron microscopy (TEM) studies and employed as a catalyst for ligand free heck reaction. Conventionally, higher temperature, longer time, polar solvents such as dimethylformamide, dimethylacetamide and phosphine ligands are essential to enhance the product yield in heck reaction. In contrary, herein, we propose an environmental benign strategy for the ligand free heck reaction using microemulsion stabilized Pd nanoparticles. The catalytic efficiency of the Pd nanoparticles was analysed for the two coupling reactions involving i) iodobenzene, butyl acrylate and ii) iodobenzene, styrene systems. The coupling reactions were completed in a shorter period with good yields. Further, the Pd nanoparticles were recycled and showed good activity till 3rd cycle.

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OP 30

SYNTHESIS OF NITROGEN-DOPED RGO/BaWO₄ NANOCOMPOSITES WITH HIGHLY ENHANCED PHOTOCATALYTIC ACTIVITY

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Abstract

Novel nitrogen-doped reduced graphene oxide/barium tungstate (NRGO/BaWO₄) nanocomposite has been synthesized by microwave method. A series of nanocomposites with varying composition with respect to NRGO was synthesized and well characterized by *Department of Industrial Chemistry, Alagappa University, Karaikudi.* 41

using different techniques. The prepared nanocomposites are tested for its performance to the photodegradation of methylene blue (MB) dye in 120 minutes under visible light irradiation. The observed results suggest that the 2.5%-NRGO/BaWO₄ nanocomposite showed maximum photocatalytic efficiency. Hence, the synergistic effect makes NRGO/BaWO₄ nanocomposites can be a potential candidate material as high performance photocatalyst under visible light irradiation.

Keywords: NRGO/BaWO₄ Nanocomposites; Microwave Irradiation; Photocatalyst; Degradation

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OP 31

ELECTRODEPOSITION OF Pd-Ni FROM A DEEP EUTECTIC SOLVENT SYSTEM: EFFECT OF ADDITIVES AND HYDRODYNAMIC CONDITIONS

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Abstract

Palladium alloy nanostructure is deposited using deep eutectic solvent namely choline chloride/Ethylene glycol (Ethaline mixture) by direct electrodeposition *in situ* over carbon paper using palladium(II) chloride and Nickel chloride as precursors. Influence of temperature, composition of metal precursors and electrodeposition parameters are studied systematically as well their electro catalytic activity towards ethylene glycol and glycerol are evaluated. Influence of surface morphology of electrodeposited palladium alloy upon their electro catalytic response is assessed through Tafel Analysis and Chronoamperometry. SEM, TEM and EDAX studies are performed to understand physico-chemical properties of Pd-Ni deposit. It is inferred that thickness, surface characteristics and electrocatalytic

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properties of Pd-Ni deposits could be influenced pointedly by electro-deposition parameters such as current density, time period and temperature. Microstrure with improved roughness and higher surface area is obtained when optimum experimental conditions are maintained. Changes in the microstructure of the deposits is evident when precursor composition is changed. It is possible to improve electro catalytic activity of Pd-Ni using appropriate electrodeposition conditions.

OP 32

SULFUR-DOPED CARBON QUANTUM DOTS INCORPORATED IRON OXIDE NANOPARTICLES FOR A SENSITIVE ELECTROCHEMICAL DETERMINATION OF ANTIPSYCHOTIC DRUG OLANZAPINE

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Abstract

Herein, we report the synthesis of sulfur-doped carbon quantum dots (S-CQDs) chemically incorporated with iron oxide nanoparticles (S-CQDs/Fe₂O₃) using hydrothermal synthesis strategy. The as-synthesized nanocomposite was characterized using powder X-ray diffraction, Fourier transform infrared spectroscopy, transmission electron microscope, thermogravimetric analysis, and energy dispersive X-ray spectroscopy. We have analyzed the clear electrochemical kinetics of the S-CQDs/Fe₂O₃ nanocomposite modified glassy carbon electrode. Addition to this, electrochemical sensing property of S-CQDs/Fe₂O₃/GCE towards the detection of antipsychotic drug olanzapine (OLZ) was explored. Remarkably, S-CQDs/Fe₂O₃/GCE has shown the good electrocatalytic activity for OLZ oxidation and also exhibits a very low detection limit and sensitivity of about 0.006 μM and 0.88 μA μM⁻¹ cm⁻² respectively. The excellent performance of the nanocomposite was emerged from the synergistic effect of their constituents. Thus, the proposed sensor has further applied for the detection of OLZ in urine samples.

Keywords: Carbon quantum dots, Iron oxide, Hydrothermal synthesis, Olanzapine, Electrochemical sensor.

OP 33

HIGHLY PHOTOACTIVE Ag-ZO/Fe₂V₄O₁₃ (AZF) NANOCOMPOSITE FOR EFFECTIVE ENVIRONMENTAL REMEDIATION

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Abstract

Facile fabrication of Ag-ZnO/Fe₂V₄O₁₃ (AZF) nanocomposite via sol-gel and photo-deposition methods. The photocatalytic efficiency of the AZF catalyst was monitored by mineralizing Reactive Orange 4 (RO 4) under natural UV-A light irradiation. The Prepared Ag-ZnO/Fe₂V₄O₁₃ nanocomposites were characterized by XRD, FTIR, FE-SEM-EDS, Colour mapping, HR-TEM and UV-DRS. The photodegradation of RO 4 using AZF was found to be maximum efficiency at pH 7. The nanocomposite is stable and reusable for multiple runs for five consecutive cycles. The complete mineralization was confirmed by COD measurements.

OP 34

SYNTHESIS AND CHARACTERIZATION OF MN DOPED CuCo₂S₄ FOR SUPERCAPACITOR APPLICATIONS

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Abstract

Nowadays, Transition metal Sulfide was emerged as a promising electrode material for the supercapacitors. Among them, mixed transition metal sulfide has the merits of rich redox activity, strong positive synergic effect and higher electrical conductivity. These factors play a vital role for the enhanced electrochemical performances. Especially, ternary metal sulphide has revealed excellent electrochemical performance than the binary metal sulfide since their abilities to deliver multiple oxidation states for wealthier redox reactions. In this present

work, successfully prepared the pristine and Mn doped CuCo_2S_4 electrode materials by Microwave method. The crystallinity and the phase of the as prepared electrode materials were confirmed by XRD analysis. The nanostructured morphology of the bare and Mn doped CuCo_2S_4 revealed SEM images. The pseudocapacitance and reversibility behaviour of the electrodes were notorious by cyclic voltammetry analysis. The GCD results exposed that the calculated areal capacitance of the CuCo_2S_4 , $\text{CuCo}_{1.50}\text{Mn}_{0.5}\text{S}_4$ and $\text{CuCo}_{1.0}\text{Mn}_{1.0}\text{S}_4$ are 1188.3, 2370.6 and 3166 F/cm^2 respectively at a current density of 1 A/cm^2 . Electrochemical Impedance Spectroscopy agrees the improved capacitance of the Mn doped CuCo_2S_4 electrode materials. It clearly indicating that, the increasing the manganese ratio in the composition, leads to the enhanced electrode/electrolyte interactions. From the above electrochemical results, strongly proposed that the $\text{CuCo}_{1.0}\text{Mn}_{1.0}\text{S}_4$ electrode is suitable candidate for the for high performance supercapacitor applications.

Keywords: Microwave Synthesis; Mn doped CuCo_2S_4 ; Supercapacitor.

OP 35

CONSTRUCTING A g- $\text{C}_3\text{N}_4/\text{MnV}_2\text{O}_6$ p-n HETEROJUNCTION PHOTOCATALYST FOR ORGANIC POLLUTANT DEGRADATION

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Abstract

g- $\text{C}_3\text{N}_4/\text{MnV}_2\text{O}_6$ heterostructured composites were synthesized by facile hydrothermal method. The obtained pure and composite photocatalysts with different ratios were characterized by X-ray diffraction (XRD), Scanning electron microscope (SEM), and UV-Visible Diffuse reflectance spectroscopy (UV-Vis DRS) for the investigation of crystalline, morphology, and band gap respectively. XRD analysis confirms the both g- C_3N_4 and MnV_2O_6 material present in the composite. Under visible light irradiation 1:1 g- $\text{C}_3\text{N}_4/\text{MnV}_2\text{O}_6$ composite exhibited the best photodegradation performance than pure g- C_3N_4 and MnV_2O_6 for the degradation of methylene blue and Indigo carmine. It was found that the methylene blue and Indigo carmine dye degradation was 95% and 94% respectively in the presence of 1:1 g- $\text{C}_3\text{N}_4/\text{MnV}_2\text{O}_6$ composite. Simultaneously, the generated reactive species during the photodegradation process were analyzed by radicals trapping experiments and it was proposed that the hole plays a major role in methylene blue degradation.

Keywords: Heterojunction, Photodegradation, MnV_2O_6 , Indigo Carmine.

OP 36

**COMPARISON OF CORROSION INHIBITION PERFORMANCE OF A
SYMMETRICAL SCHIFF BASE IN ACID MEDIA**

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Abstract

The Schiff base, 1,3-bis(2-aminobenzilideneimino)ethane has been synthesized and its inhibition effect on the corrosion of mild steel in 1.0M HCl and 0.5M H_2SO_4 was studied by electrochemical methods. It has been observed that the inhibition efficiency increases with inhibitor concentration and exhibits higher corrosion inhibition efficiency in 1.0M HCl solution than in 0.5M H_2SO_4 solution. Tafel polarization curves showed that the Schiff base was mixed type inhibitor. The adsorption of the compound on the mild steel surface obeyed Langmuir adsorption isotherm. The potential of zero charge was measured to find corrosion inhibition mechanism in these media.

Keywords: Schiff base, corrosion inhibition, electrochemical studies, adsorption isotherm, potential of zero charge.

OP 37

**EXPERIMENTAL AND THEORETICAL STUDIES OF THE INCLUSION
COMPLEX BETWEEN BIPHENYL THIOL DERIVATIVES AND β -
CYCLODEXTRIN**

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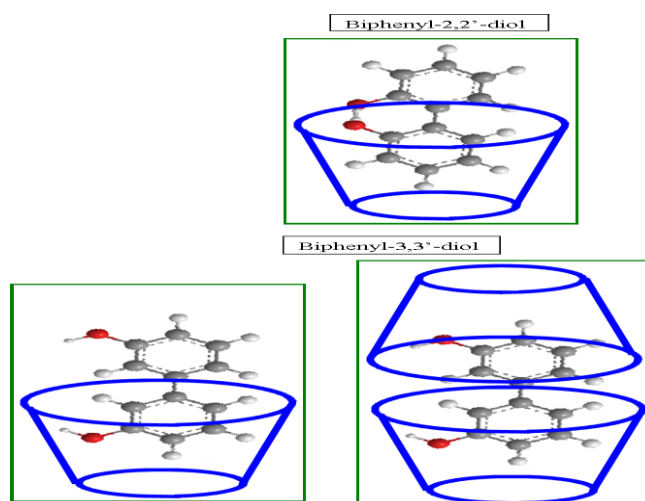
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Tiruppattur, Sivaganga, Tamil Nadu, India.

Abstract

The inclusion complex formation between Biphenyl-2,2'-diol (22-DHBP) and Biphenyl-3,3'-diol (33-DHBP) and β -cyclodextrin (β -CD) in aqueous state were studied by *Department of Industrial Chemistry, Alagappa University, Karaikudi.* 46

UV spectroscopy, Fluorescence spectroscopy and electrochemical study (cyclic voltammetry, CV). The solid state complex between β -CD and 22-, 33-DHBP was characterized by FT-IR, XRD techniques and SEM morphological studies. And molecular docking technique (using PatchDock server) used to study on virtual state. The β -CD: 22-, 33-DHBP inclusion complexes obtained by molecular docking studies are in good correlation with the results obtained through experimental methods. The binding constant of β -CD: 22-, 33-DHBP inclusion complexes was calculated using Benesi–Hildebrand plot at 303 K. Thermodynamic parameter (ΔG) involved in the complex formation also calculated for to find the thermodynamic spontaneous and exergonic reaction. The point energy, stabilization energy upon complexation, frontier molecular orbitals, and hydrogen bonds were obtained. The calculation results correlates well with the docking and experimental observations.



OP 38

SYNTHESIS AND CHARACTERIZATION OF COBALT BASED METAL-ORGANIC FRAMEWORK FOR ASYMMETRIC SUPERCAPACITOR PERFORMANCE

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Abstract

Metal-Organic frameworks (MOFs) have recently attract tremendous interest, due to their potential application in the energy storage field. In this work, Cobalt metal-organic framework (Co-TDPAT) was synthesized through a simple solvothermal route. Cobalt-based MOF shows an excellent high specific capacitance and good cycling stability. Its maximum specific capacitance is 653.67 F g^{-1} at a current density of 0.5 A g^{-1} and the capacitance retention is about 87.5% after 2000 cycles. Moreover, an asymmetric supercapacitor assembled using Co-TDPAT and activated carbon electrode as positive and negative electrode respectively. The fabricated asymmetric capacitor exhibited a specific capacitance of 386.8 F g^{-1} at a current density of 0.5 mA and provided a maximum energy density of $53.72 \text{ W h kg}^{-1}$ at 200 W kg^{-1} . The excellent electrochemical property may be ascribed to the intrinsic nature of Co-TDPAT, enough space available for the storage, tailored pore size and efficient capability for ion insertion.

Keywords: Metal-Organic frameworks, asymmetric supercapacitor, energy storage

OP 39

HYDRAZINE BASED SCHIFF BASE FERROCENE DERIVATIVE AS OPTICAL AND ELECTROCHEMICAL SENSOR FOR THE DETECTION OF COPPER(II) AND IODIDE IONS

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Abstract

Ferrocene derivatives are ideal platforms for development of cations, anions and neutral molecules recognition. Schiff bases are one of the most important and widely explored organic species because of their potential applications as catalysis corrosion inhibitor, enzymatic agent and chelating ligands. Schiff bases have become one kind of most popular fluorescent chemosensors to detect metal ions. Fluorescent chemosensors have many advantages such as high selectivity, rapid response, easy operation, and high sensitivity. In the current study we designed and synthesized ferrocene schiff base derivatives using acetyl ferrocene (L_1) and ferrocene carboxaldehyde (L_2). The synthesized receptors were

characterized by ^1H NMR, ^{13}C NMR, ESI-Mass, FTIR and UV spectroscopy. The sensing behavior of synthesized receptor was studied using spectral and electrochemical techniques. The acetyl ferrocene Schiff base derivative showed very high fluorescent response to Cu^{2+} and I^- ion. Ferrocene carboxaldehyde schiff base showed fluorescent response only to I^- ion. The probe L_1 and L_2 exhibited $4.45 \times 10^6 \text{ M}^{-1}$, $3.42 \times 10^6 \text{ M}^{-1}$ and $3.62 \times 10^5 \text{ M}^{-1}$ binding constant values for $\text{L}_1 + \text{Cu}^{2+}$, $\text{L}_1 + \text{I}^-$ and $\text{L}_2 + \text{I}^-$ ions respectively. The detection limit of the probe L_1 and L_2 towards $\text{L}_1 + \text{Cu}^{2+}$, $\text{L}_1 + \text{I}^-$ and $\text{L}_2 + \text{I}^-$ was found to be $0.16 \mu\text{M}$, $0.04 \mu\text{M}$ and $0.05 \mu\text{M}$. Other ions, including Hg^{2+} , Pb^{2+} , Al^{3+} , Zn^{2+} , Co^{2+} , Ni^{2+} , Mg^{2+} , Mn^{2+} , K^+ , Cd^{2+} , Cr^{2+} , Cu^{2+} , Fe^{2+} , Fe^{3+} and Cl^- , SCN^- , Br^- , F^- , HSO_4^- , I^- , BH_4^- and CH_3COO^- had nearly no influence on the sensing behavior.

Keywords: Ferrocene derivatives, Chemosensor, Optical sensor, Electrochemical sensor, Bio-imaging sensor application.

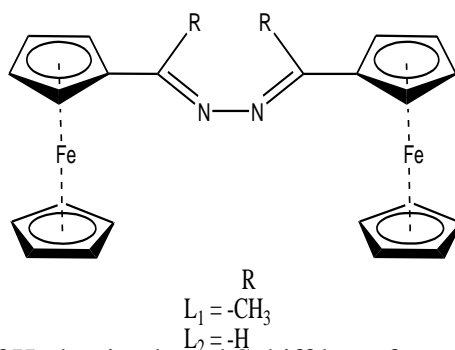


Figure 1: Chemical structure of Hydrazine based Schiff base ferrocene derivative

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OP 40

CERAMIC MEMBRANES FOR PHOTO-CATALYTIC DYE DEGRADATION

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Abstract

Color removal of the dye from the effluent is a difficult environmental problem faced by the textile finishing, dye manufacturing, pulp and paper industries. Many investigators studied various techniques e.g., physicochemical flocculation, nano-filtration, micellar enhanced ultrafiltration, and adsorption on suitable adsorbents, etc for removal of colored dye

from wastewater. Here, color removal of methyl orange dye was investigated in photo-catalytic reactor. We synthesised the ceramic membranes by impregnation of cerium oxide on TiO₂ thin film. The ceramic membranes has been characterised with FTIR, UV-Vis, XRD, SEM and CV analysis. The removal efficiency of methyl orange by ceramic membranes photo-catalytic process was investigated. The effects of free radical scavengers were studied to determine the role of hydroxyl free radical in catalytic process. Results showed that it could effectively remove about 90-95% color of methyl orange. Thus ceramic membranes based photo-catalytic process offered an excellent economical and feasible method for dye remove. Moreover, developed reactor can be efficiently used for the degradation of other dye effluent.

Keywords: Water treatment, Methyl orange, Ceramic membranes, Photo-catalytic process

OP 41

PREPARATION AND CHARACTERIZATION OF TiO₂ THIN FILM BY ARTIST SPRAY GUN PYROLYSIS METHOD FOR PEROVSKITE SOLAR CELL APPLICATIONS

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Abstract

In the present investigation, TiO₂ thin film is deposited by artist spray gun (ASG) pyrolysis using polyvinylpyrrolidone (PVP) as a binding agent. The influence of distance between substrate and spray gun nozzle at the optimized substrate temperature of 300°C on the formation of TiO₂ thin film was also studied. This thin film has better photovoltaic performance due to the formation of finer nanoparticles on the substrate with improved contact than other conventional spray pyrolysis method. The formation of pure anatase phase of TiO₂ thin film was conformed by X-ray diffraction study. The band gap of this thin film was measured by UV-Vis analysis and it was found to be 3.19 eV. The emission spectrum, charge separation and carrier dynamics of the films were analysed by photoluminescence and life time measurement studies. They exhibited emission spectrum at 390 nm and the average lifetime of the film was ~30 ns. The scanning electron microscope also confirmed that the

film deposited at the distance of 15 cm was uniformly deposited over the substrate with fine nanoparticles. According to Raman mapping spectra, the variation in the intensity, peak position and full width half maximum (FWHM) of TiO₂ anatase high intensity Eg peak indicates the uniform deposition on the glass substrate. These results revealed that TiO₂ thin film obtained by artist spray gun pyrolysis method could be used as a potential electron transport layer for perovskite solar cell applications.

Keywords: Artist spray gun pyrolysis, TiO₂ thin film, Perovskite solar cell, Polyvinylpyrrolidone.

OP 42

ORIENTATION AND ENERGY BASED STABLE SUPRAMOLECULAR INTERACTION OF 3-HYDROXYFLAVONE AND QUERCETIN WITH NATIVE AND MODIFIED β -CYCLODEXTRINS

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Abstract

In a recent days, because of the limitation of the experimental methods, molecular modeling approach is very popular and most required in supramolecular chemistry with cyclodextrin [1-3]. The inclusion complexes of two selective flavonols such as 3-Hydroxyflavone (HF), Quercetin (QRC) on β -Cyclodextrin (β -CD) and 2-Hydroxypropyl- β -Cyclodextrin (2HP- β -CD) have been analyzed by using docking and natural bond orbital approach. The guest molecules, HF and QRC with β -CD and 2-HP- β -CD has been organized by PM3 method. The complex is constructed by introducing the guest into 2HP- β -CD according to A or B orientation. The formed complex is optimized by PM3 method. We have calculated the donor-acceptor interactions and their stabilization energies $E^{(2)}$ at B3LYP/6-31G method. With the help of NBO analysis and its energy parameters (ΔE), the structure of complex between guest (HF and QRC) and host (β -CD and 2HP- β -CD) is proposed. The results indicated that these inclusion complexes are highly stable media.

Keywords: 3-Hydroxyflavone; Quercetin; Cyclodextrins; Supramolecular Assembly; NBO analysis; PM3

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OP 43

TITANIUM DIOXIDE NANOCATALYST FOR PHOTOCATALYTIC DEGRADATION OF ACID RED DYE UNDER SOLAR IRRADIATION

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Abstract

Titanium dioxide nanocatalyst was synthesized by simple chemical precipitation technique and characterized by Fourier Transform Infra Red Spectroscopy, X-ray Diffraction analysis, Scanning Electron Microscopy, Energy Dispersive X-ray analysis and Transmission Electron Microscopy. The synthesized TiO₂ catalyst is evaluated for its photocatalytic activity towards the degradation of Acid red-94 dye under solar irradiation. The parameters such as catalyst dosage, initial dye concentration, and pH were optimized for the effective photocatalytic dye degradation. The photodegradation rates of acid red dye reached 98% within 60 minutes of reaction time. The reaction rate followed pseudo-first order kinetics obeying Langmuir-Hinshelwood kinetic model and the rate of dye degradation was found to be enhanced by air oxidation using TiO₂ catalyst under sunlight.

Keywords: TiO₂, air oxidation, Acid red dye, pseudo-first order kinetics.

OP 44

DEVELOPMENT AND PERFORMANCE EVALUATION OF PANI PIGMENTED HYBRID ORGANIC COATING AS AN ALTERNATIVE TO CHROMATE PRIMER

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Abstract

Due to the carcinogenic nature of chromate coating, alternate polyester polyol-melamine formaldehyde-based hybrid organic coatings with and without anticorrosive pigments such as polyaniline (PANI) has been developed. The coating performance was studied by using physical, mechanical, structural and electrochemical studies. Polyaniline pigment has been prepared by chemical oxidation synthesis method and confirmed by Raman spectroscopy. The surface morphology studies of hybrid coating with and without anti-corrosive pigments have been studied by using SEM analysis and it's showing that the pigment has been uniformly distributed over the substrate without any cracking. The corrosion resistance performance of the hybrid organic coating has been evaluated by using electrochemical impedance and salt spray analysis. The electrochemical impedance studies in 3.5% NaCl solution shows that the coating resistance (R_c) of polyaniline pigmented hybrid organic coating has in the range of $10^6 \Omega \text{ cm}^2$. Whereas, mild steel coated without anti-corrosive pigment shows that R_c value in the range of $10^4 \Omega \text{ cm}^2$. Besides, salt spray test demonstrated that the paint with polyaniline coated mild steel sample showed no significant effect on corrosion in salt spray test even after 500 hr of exposure.

Keywords: *Polyester polyol, Melamine formaldehyde, Polyaniline, Hybrid organic coating, Anti-corrosive paint.*

OP 45

NORTRIPTYLINE AND NORTRIPTYLINE:β-CYCLODEXTRIN LOADED ON ELECTROSPUN PAN NANOFIBERS AS A CARRIER FOR ANTIBACTERIAL ACTIVITY

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Abstract

With the consideration of uniqueness and promising characteristic features of nanofibrous mats (NFMs) and cyclodextrins (CDs) that possessing a significant opportunities and plying a vital role in anti-bacterial activities. Generally, CDs are used to enhance the antibacterial activities through the improvement of solubility, stability and so on to any molecule which can carry inside the CDs cavity through the formation of inclusion complexes. In this research paper, the nortriptyline (NP) is chosen as a reference drug molecule and electrospun Polyacrylonitrilenanofibrous mat (esPAN NFM) as a carrier for the antibacterial activity. NP is interacted with β-Cyclodextrin (β-CD) to form an inclusion complex (NP:β-CD-IC). The PAN NFMs are allowed to soaking in it to incorporate the complexed NP on the fibrous surface. The soaking of PAN NFM in NP solution without β-CD is also carried out. The characterization of nanofibrous mat of NP/PAN and NP:β-CD/PAN NFMs are analyzed by UV-visible, emission, FT-IR, Raman, XRD and SEM studies. Selective stretching frequencies of NP has been largely shifted in the soaked NFMs evident that the encapsulation of NP into β-CD cavity on the surface of NFM. SEM image showed that the NP and NP:β-CD are mostly occupied on the surface of PAN NFM. The antibacterial activity of NP and NP:β-CD have been tested against positive control tetracycline by zone of inhibition method. As a result, the activity has been improved for NP: β-CD /PAN NFMs over NP/PAN NFMs due to the solubility enhancement of NP by the complexation of β-CD.

Keyword: Nortriptyline, Cyclodextrin: Supramolecular assembly, PAN Nanofiber, Anti-bacterial activity

OP 46

**SUGARCANE JUICE CLARIFYING CAPACITY OF GREEN SYNTHESIZED
NANO CaO**

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Abstract

The sugarcane is grown as an industrial crop for the production of sugar, food and bio-energy. The main challenge during the production of sugar is attaining purity with high yield. Clarification is a key step during the production of sugar. Hence, there is always a need to look the best clarifying agents. The main objective of this research was aimed to evaluate the clarifying potential of nano CaO (as CaO NPs) compared with existing lime (as N-CaO) for raw cane juice and also to produce raw sugar using them. In this study, sugarcane variety B52-298 was used and extracted the juice and its juice percentage was calculated as 76.9 %. Here in this study, CaO NPs was prepared by green approach using papaya leaf extract as reducing agent, and the prepared CaO NPs is used as a clarifying agent. The amount of calcium, crystal size, and morphology of CaO NPs was characterized through flame atomic absorption spectroscopy (FAAS), x-ray diffraction (XRD), and Scanning electron microscope (SEM) respectively. The extracted cane juice was clarified by using N-CaO and CaO NPs. The physicochemical characterization of raw cane juice, clarified cane juice and the produced sugar was carried out. The process parameters were optimized by varying conditions, then the optimized parameters such as amount of clarificants (0.05 g), clarification time (80 min.), pH (8), volume of juice (100 mL) and temperature (95⁰C) were recommended based on the least turbidity and mud volume, and maximum settling rate. The best optimized clarified cane juice was sulphited using SO₂ and crystallized into sugar. The characterization of CaO NPs clarified and sulphited juices were carried out and measured the turbidity (1268 IU), moisture content (85.03%), and color (8381.7 IU). The sugar was produced upon crystallization, which was analyzed in the fact of turbidity (1193 and 1421IU), purities (96.75 % and 93.49 %), moisture content (0.08 % and 0.083 %) and color (653.4 and 936.7 IU) by employing CaO NPs and N-CaO respectively. The clarification

efficiency among the presently studied clarificants CaO NPs has better clarifying potential than N-CaO.

Keywords: Cane Juice, Clarification, Extraction, Nanoparticles, Sugarcane.

OP 47

THERMAL STABILITY AND ANTIBACTERIAL PROPERTIES OF CHITOSAN-MAGNESIUM OXIDE NANOCOMPOSITE

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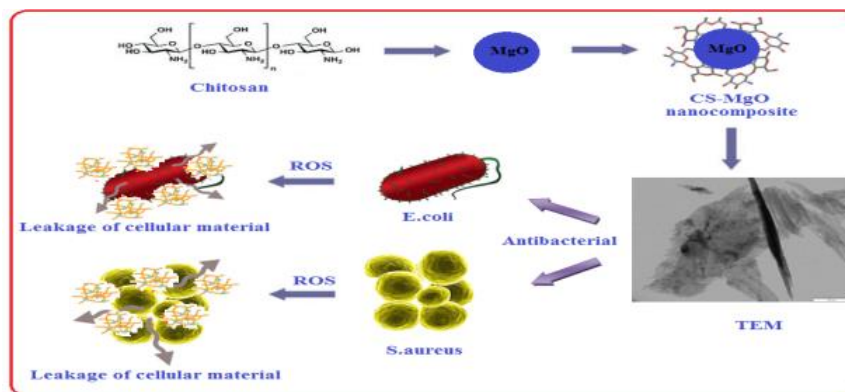
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Abstract

In the present study, biopolymer-inorganic material of chitosan-magnesium oxide (CS-MgO) nanocomposite was synthesized by simple precipitation method. The nanocomposite thereby obtained was characterized by different analytical techniques. Fourier Transform Infrared (FTIR) spectroscopy is used for analysing the functional groups which is involved in the reaction, UV-Visible spectroscopy (UV-Vis) for to analyse the absorption patterns, X-Ray Diffractometer (XRD) for crystalline nature, Higher Resolution Scanning Electron Microscope (HR-SEM) and Transmission Electron Microscope (TEM) for morphological studies and Thermo gravimetric (TGA) analysis for to study thermal stability. From the HR-SEM and TEM analysis, CS-MgO nanocomposite shows small grain and rod like structure respectively. Thermo gravimetric analysis showed that CS-MgO nanocomposite has higher thermal stability than chitosan matrix. Gram positive organism *Staphylococcus aureus* and Gram negative organism *Escherichia coli* were used to test the antibacterial activity of synthesized nanocomposite CS-MgO. The nanocomposite CS-MgO has promisingly inhibited the bacterial growth when compared with as-synthesized chitosan. In conclusion, nanocomposite obtained in this study showed enhanced antibacterial activity. We believed that the enhanced physical properties of nanocomposite achieved by incorporating MgO in the chitosan matrix could be beneficial in various applications.

Keywords: Chitosan, MgO, XRD, SEM, Antibacterial activity.



OP 48

EFFICIENCY ENHANCEMENT OF METHYLAMMONIUM TIN IODIDE PEROVSKITE SOLAR CELL USING BENZYLTRIMETHYL AMMONIUM IODIDE AS AN ADDITIVE

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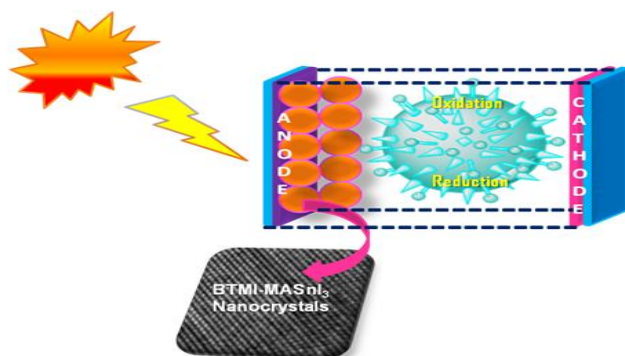
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Abstract

In the present investigation, try to enhance the efficiency of methylammonium tin iodide (MASnI_3) perovskite solar cell using benzyltrimethyl ammonium iodide (BTMAI_2), it is used as an additive. BTMAI_2 based methylammonium tin iodide is prepared by the Two-step solution process. The surface morphology of the formation of perovskite has analysed by HR-TEM, the image appears in nanocrystalline. XRD pattern is observed in the crystalline nature of BTMAI-MASnI_3 . The present functional group of BTMAI-MASnI_3 is identified by FT-IR spectral analysis. The absorption maxima 710 nm is observed by the UV-Visible spectra analysis. Finally, the perovskite solar cells is fabricated that the presence and absence of BTMAI_2 . The presence of BTMAI_2 perovskite solar cell gives 6.89% of sunlight into electrical energy conversion efficiency.

Keywords: Benzyltrimethyl ammonium iodide, Methylammonium lead iodide, Perovskite solar cell, Efficiency.



OP 49

**FLUOROMETRIC AND COLORIMETRIC “OFF-ON-OFF” RELAY SENSOR FOR
CN⁻/Cr³⁺ IN RAW264.7 CELLS**

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Abstract

Innumerable increase of industry around the globe enhanced the water pollution immensely and hence apparently stands out to be a threat to the eco-system. Among all deadly pollutants, cyanide is paramount in quantity, as cyanide is a ubiquitous element in widespread applications like metallurgy, mining, electroplating and polymer synthesis^[1-3]. Some of the deleterious consequences of cyanide include complications of vascular, visual, central nervous, cardiac, endocrine and metabolic systems^[4-11]. According to the WHO guideline, the optimum tolerance limit of cyanide is 0.07mg/lit in drinking water and about 0.5–3.5 mg/kg of cyanide to an adult is lethal^[12]. Alongside cyanide, transition metal ions are also ingredient of pollutants which have significant impact on day-to-day life. So it is of ample significant to develop an indicator for real time application to detect selectively the noxious analytes. On this note, a tailor-fit, novel molecular framework has been designed and synthesised for naked eye detection of deleterious analytes (CN⁻/Cr³⁺) in real-time condition. The receptor shows specificity and selectivity towards CN⁻ anion among a library of toxic anions in semi-aqueous medium. Upon introduction of CN⁻, the receptor solution turn into intense red colour with an absorption maxima at 500 nm and a ‘turn on’ emission with emission maxima at 564 nm. On addition of all transition metal ions, only Cr³⁺ is selectively sensed by receptor-CN⁻ adduct by quenching the orange emission. The detection limit for CN⁻ and Cr³⁺ are 15 nM and

8.6 μM respectively. The receptor is capable in real-time application in strip test and effectively can image in vivo CN^- by confocal fluorescence imaging in RAW264.7 cell line.

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OP 50

CORROSION INHIBITION STUDY OF A NEW SYNTHETIC SCHIFF BASE DERIVED FROM DRUG COMPOUND ON MILD STEEL IN ACID MEDIUM

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Abstract

A new class of corrosion inhibitors namely drug based Schiff bases was synthesized and its inhibiting action on the corrosion of mild steel in 1N sulphuric acid and 1M HCl at 30°C was investigated by various corrosion monitoring techniques. A preliminary screening of the inhibition efficiency was carried out using weight loss measurements. Potentiodynamic polarization studies showed that the Schiff bases were mixed type inhibitors. The potential of zero charge (PZC) at the metal–solution interface was determined for both the inhibited and uninhibited solutions to provide the mechanism of inhibition. The inhibitor formed a film on the metal surface through chloride or sulfate bridges depending upon the medium. The value of the activation energy (E_a) calculated showed that the inhibition film formation on the metal surface occurred through chemisorption. The thermodynamic parameters such as the

adsorption equilibrium constant (K_{ads}) and the free energy of adsorption were calculated and discussed.

Keywords: Schiff base, Impedance, polarization, corrosion potential, double layer capacitance, charge transfer resistance.

OP 51

SYNTHESIS AND CHARACTERIZATION OF TRIAZINECORED IMIDAZOLE POLYMERS

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Abstract

Carbon dioxide Capture and Storage (CCS) is the most promising and emerging technology, as a tool for the development of different variety of porous adsorbent materials. Some of new kind of sorbents such as porous carbons, metal organic frameworks (MOFs), porous organic polymers, Covalent Organic Frameworks (COFs), nitrogen doped carbeneous materials, N-rich imine polymers, Covalent triazine frameworks (CTFs), charged porous organic polymers, Poly-ionic liquids (PILs) and N-heterocyclic carbene based co-ordination polymers have shown promising carbon dioxide capture capacity.¹ It is well known that imidazolium cations with neighboring bases are effective nucleophiles for binding with CO₂. Various attempts have been made for the incorporation of imidazolium motif into porous materials such as polymers and metal organic frameworks (MOFs). However, to the best of our knowledge, only few studies have reported the incorporation of imidazolium motifs into covalent triazine frameworks (CTFs), especially those with neighbouring bases.² Herein, we report the synthesis of triazine cored imidazole polymers (PTIM and PTIMPH) via imidazole alkylation method. The synthesized polymeric materials are examined using FT-IR, PXRD, SEM and TGA analysis. The surface morphology provides micrometer sized spherical morphology for PTIM-1 and small agglomerated spherical particles for PTIM-2. The attempt towards CO₂ capture will be made using these polymeric networks.

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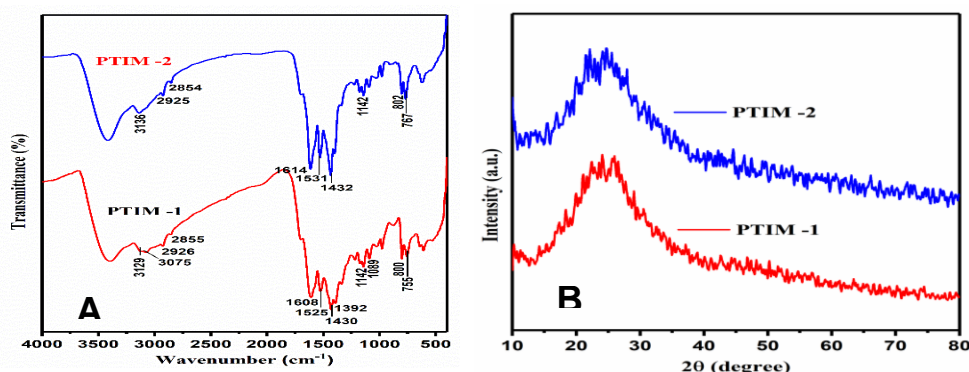


Figure 1. FT-IR (A), Powder XRD pattern (B) of PTIM-1 and PTIM-2.

OP 52

RUTHENIUM CATALYZED INTERMOLECULAR HYDROACYLATION OF UNACTIVATED ALKENES: RUTHENIUM HYDRIDE-XANTPHOS AS A PRE-CATALYST FOR AN INTERMOLECULAR MARKOVNIKOV SELECTIVE HYDROACYLATION REACTIONS

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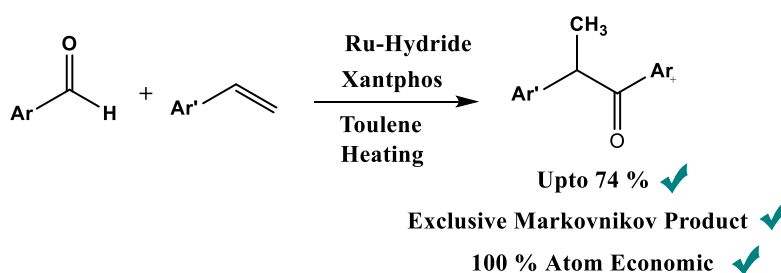
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Abstract

The transition-metal-catalyzed hydroacylation reaction constitutes a highly sustainable protocol for introducing acyl group to unsaturated organic substrates because of its inherent 100% atom efficiency.[1] For the hydroacylation of olefins, the intramolecular version of the reaction has been effectively used to form cyclic ketone products.[2] Since the pioneering reports on the intermolecular hydroacylation of olefins,[3] a number of late-transition-metal catalysts have been found to mediate anti-Markovnikov hydroacylation of alkenes to form the linear ketones.[4–6] One of the most challenging problems on the olefin hydroacylation reaction resides in competing decarbonylation of aldehyde substrates, which often leads to the deactivation of metal catalysts. A number of clever strategies have been implemented to circumvent the decarbonylation problem. One successful approach has been to employ aldehyde substrates with a heteroatom chelate group to promote the hydroacylation reaction.[4] Employing aldimines as a synthetic equivalent to aldehydes[5] and using activated olefin substrates[1,6] have also been shown to be effective strategies for promoting regioselective hydroacylation reaction while limiting the decarbonylation side reaction.

Because most of these catalytic methods generally exhibit anti-Markovnikov selectivity in forming linear ketone products, much research effort has been directed to develop Markovnikov-selective hydroacylation reaction to form the branched ketone products.[7] Even though the Markovnikov-selective asymmetric hydroacylation reaction has been achieved under intramolecular conditions relatively few examples of intermolecular Markovnikov-selective hydroacylation methods have been reported.

Designing highly effective and generally applicable Markovnikov-selective hydroacylation technology remains a largely unsolved problem in the homogeneous catalysis field. Therefore, our effort is to design a practically convenient protocol that uses an air stable ruthenium-hydride pre-catalyst with commercially available ligands such as Xantphos which is very well known for pincer like ligands with large bite-angle.[8] Initial screening by exploring the coupling reaction of aldehydes with olefin substrates. Herein, we disclose a highly Markovnikov selective intermolecular hydroacylation of styrene to yield branched ketone products in good yield (Scheme.1). The catalytic method provides an atom-economical acylation protocol for styrene derivatives without employing any reactive reagents or directing groups. The product mixture was analyzed by NMR methods.



Scheme. 1 Ruthenium-hydride Xantphos catalyzed intermolecular Markovnikov selective Hydroacylation of aldehydes with unactivated olefins.

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OP 53

FABRICATION OF 2D-MoWS₄||MXene ASYMMETRIC SUPERCAPACITOR AND ITS SUPERCAPACITIVE PERFORMANCE STUDIES

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Abstract

In the present work, 2D-molybdenum tungsten sulfide (MoWS₄) nanosheets were prepared by a simple solvothermal method and 2D MXene (Ti₃C₂) was prepared by a selective chemical etching method. The prepared MoWS₄ nanosheets and MXene were characterized by X-ray diffraction, Raman spectroscopy, scanning electron microscopy and High-resolution transmission electron microscopy. Further, MoWS₄ nanosheets based electrode was fabricated and used as a cathode and MXene based electrode was fabricated and used as an anode and its supercapacitive behaviour in 6M KOH electrolyte was studied in detail. It is observed that MoWS₄ electrode exhibited the maximum specific capacitance of 126 F g⁻¹ at a current density of 0.2 Ag⁻¹. The electrochemical impedance studies for MoWS₄ gives high internal resistance and incomplete semicircle line at the high-frequency region that corresponds to the redox behaviour of the cathode material and high oxidation state of MoWS₄. Finally, the ASC device, MoWS₄||MXene was fabricated using 6M KOH as the electrolyte and measured its specific capacitance and it was found to be 62.88 F g⁻¹ at the current density of 2 Ag⁻¹.

Keywords: MoWS₄ nanosheets, MXene, Asymmetric supercapacitor, Specific capacitance.

OP 54

SYNTHESIS AND CHARACTERIZATION OF TRIAZINE BASED POROUS POLYMER

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Abstract

Carbon dioxide (CO₂) is one of the major greenhouse gases, it is emitted largely from the human activities (thermal power plant, transports and industrials). There are numerous technologies developed towards CO₂ capture. Porous organic polymers are promising materials, because these polymers consist of abundant micropores and high surface areas.¹⁻³ Herein, we have developed the triazine based porous polymers by one-pot polycondensation reaction with melamine and TRIPOD. Synthesized polymer is characterised by FT-IR, powder-XRD. The surface morphology of the polymer is examined by SEM analysis. Textural property of polymer is studied by N₂ adsorption isotherm at 77 K. From FT-IR analysis, the aminal linkage is confirmed peak at 2918 cm⁻¹ and the triazine ring (C-N stretching vibration) confirmed by peak at 1552 cm⁻¹, 1480 cm⁻¹ and 1360 cm⁻¹.⁴ The amorphous morphology of the synthesized polymer is confirmed by XRD analysis.

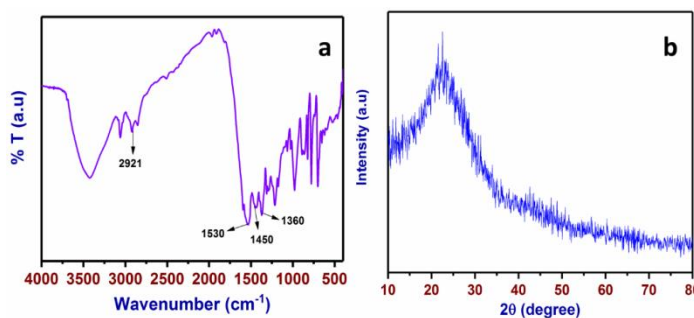


Figure 1. FT-IR spectrum (a) and XRD pattern of polymer

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OP 55

REDOX-ADDITIVE MEDIATED ELECTROCHEMICAL ACTIVITY OF INVASIVE WEED DERIVED ONION-LIKE POROUS CARBON FOR SUPERCAPACITOR APPLICATION

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Abstract

The eradication of invasive weeds is always challenging and ungovernable. Therefore the production of activated carbon from such eco-threats appears to be an alternative management technique to convert them into a productive, profitable, and sustainable resource of energy. And hence, the present work gives away the preparation of onion-like porous carbon derived from the pods of *Prosopis juliflora*. Initially, the hydrothermal carbonization was carried out, and the hydrochar was subjected to chemical activation using KOH. The desired porous carbon was obtained by optimizing the activation temperatures. The optimized porous carbon shows a unique morphology of onion-like nanostructures with a significant specific surface area of $967 \text{ m}^2 \text{ g}^{-1}$. The electrode delivers a sensible specific capacitance of 274 F g^{-1} at 1.3 A g^{-1} in H_2SO_4 electrolyte. Thus, a symmetric EDLC was fabricated, and the performance of the device is effectually enhanced by adding KI as redox additive. Interestingly, an increased cell voltage (1.4 V) and improved cell capacitance (588 F g^{-1}) are attained. Ultimately, a superior energy density of 35.7 Wh kg^{-1} at an enhanced power density of 971 W kg^{-1} is also obtained in the redox additive based aqueous electrolyte. A detailed investigation of the surface charge storage mechanism of redox-mediated electrochemical activity is discussed in detail. Moreover, the stability of the prepared supercapacitors is also demonstrated for about 10,000 cycles. Thus, the *P. juliflora* is successfully reformed into an efficient electrode material for the supercapacitor application.

OP 56

SYNTHESIS AND CHARACTERIZATION OF CADMIUM SULFIDE QUANTUM DOTS AND ITS ANALYTICAL APPLICATION IN THE PHOTOCATALYTIC DEGRADATION OF RHODAMINE B UNDER SOLAR LIGHT

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Abstract

Cadmium sulfide (CdS) quantum dots were prepared precipitation method using cadmium chloride, and sodium sulfide using β -cyclodextrin as a reducing agent. UV-DRS and photoluminescence spectroscopy is used to determine the optical property of CdS quantum dots. The formation of CdS quantum dots were confirmed using photoluminescence, XRD, FTIR and SEM characterization techniques. Photocatalytic degradation of CdS was tested on the degradation of Rhodamine B dye under solar light with good recycling ability.

OP 57

ELECTROCHEMISTRY AND ELECTROCHEMILUMINESCENCE OF LUMINOL/DCHA

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Abstract

In Electrochemiluminescence (ECL), the light emission is generated at the electrode electrolyte interface by applying energy in terms of either current or potential and used as an electroanalytical probe for the detection of various biomolecules and environmentally important analytes. Though, Luminol is one the best luminophore in ECL, only hydrogen peroxide is widely used as co-reactant for generation of ECL and it always limits applications because of short time reactive radicals which are playing a crucial role in enhancing the stability of ECL. Dicyclohexylamine (DCHA) is a class of alicyclic amine, found its major application in the synthesis of corrosion inhibitors, organic pesticides, insecticides, rubber
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chemicals, dyestuff and etc. The present work, we identified DCHA as a new efficient anodic co-reactant in ECL for luminol molecule. The systematic electrochemistry and ECL studies were conducted and discussed the possible reaction mechanism behind the ECL of luminol- DCHA system on glassy carbon electrode surface.

OP 58

**POLY (ETHER IMIDE) ULTRAFILTRATION MEMBRANES TAILORED WITH
POLY (HEXAMETHYLENEBIGUANIDE) WOVEN COPPER OXIDE
NANOPARTICLES FOR WATER TREATMENT APPLICATIONS**

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Abstract

Herein, the copper oxide nanoparticles (CuO NPs) are synthesized *via* a facile wet chemical precipitation technique and coated with the poly (hexamethylene biguanide) hydrochloride (PHMB). The surface properties of the resulting poly (hexamethylene biguanide)-CuO (P-CuO) are probed by field emission scanning electron microscopy (FESEM) and X-ray diffraction spectroscopy (XRD). In order to facilitate the improvement in permeation, anti-organic fouling and antibacterial characteristics, P-CuO nanoparticles are incorporated into poly (ether imide) (PEI) ultrafiltration (UF) membrane matrix *via* a phase inversion technique. The morphological and hydrophilicity investigations are confirmed that the influence of P-CuO is improved the macrovoids, porosity (15.2%), and water permeation ($192.8 \text{ Lm}^{-2}\text{h}^{-1}$) of the PEI UF membrane. The rejection and flux recovery ratio of the PEI/P-CuO membranes are found to be > 97% towards foulants such as bovine serum albumin (BSA), humic acid (HA) and motor oil demonstrated its excellent separation and antifouling ability. Antibacterial activity of PEI/P-CuO membranes are probed against *Escherichia coli* and *Staphylococcus Aureus* and showed that the wider inhibition zone. Results are confirmed that the PEI/P-CuO nanocomposite UF membranes provided outstanding permeation, anti-fouling and antibacterial performance than the pristine PEI membrane and promising for an effective water treatment applications.

OP 59

**ONE-POT MULTICOMPONENT SYNTHESIS OF SPIRO BIS PHENYL
PYRAZOLONE PIPERIDIUM SALT DERIVATIVES**

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Abstract

An effortless and fast synthetic approach for the synthesis of Spiro bis phenyl pyrazolone piperidium salt derivatives by one-pot four-component reaction between aromatic aldehyde, 3-methyl-1-phenyl-1H-pyrazole-5(4H)-one and piperidine in ethanol is described. The reaction was expected to give the products 3,5-dimethyl-1,4,7-triphenyl-4,7-dihydro-1H-pyrano[2,3-c:6,5-c']dipyrazole or 4,4'-(*phenylmethylene*)bis(3-methyl-1-phenyl-1H-pyrazole-5-one) when piperidine acts only as organocatalyst. But surprisingly the reaction proceeded via Knoevenagel condensation followed by piperidine bond formation to give the organic salt as the sole product where piperidine acted as a reactant as well as a catalyst. The products are formed in good yield for different aldehydes containing electron withdrawing and electron donating group in mild reaction conditions and shorter reaction time with easy isolation of products without column chromatography. The structures are confirmed by IR, ¹H, ¹³C, DEPT 135, NMR and mass spectrometer.

Keywords: Organic salt, Aldehyde, 3-methyl-1-phenyl-1H-pyrazole-5(4H)-one, Knoevenagel condensation,

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OP 60

SYNTHESIS AND CHARACTERIZATION OF N-CHLOROPICOLINAMIDE: A NEW, MILD, STABLE, EFFECTIVE AND EFFICIENT OXIDANT FOR ORGANIC SUBSTRATES

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Abstract

N-Halo compounds are being used in kinetics, analytical, organic structural investigation and in synthesizing organic substrates. The new oxidant N-Chloropicolinamide (NCP) is synthesized by the chlorination of picolinamide using trichloroisocyanuric acid. The physical constant, formal redox potential and spectra characterization (IR, UV, ¹H-NMR, C¹³ –NMR and mass spectrum) confirms the presence of nitrogen-halogen bond. It is prepared by a simple method giving high yield in a short period of time. It is found to be a mild and stable oxidant and formal redox potential of N-chloropicolinamide shows that it can be used as an effective source of positive halogen.

Keywords: N-Chloropicolinamide, oxidant, Kinetics Mechanism, N-halo compound.

OP 61

PREPARATION AND CHARACTERIZATION OF NOVEL ELECTROSPUN ALUMINA/POLY(VINYLPYRROLIDONE) NANOFIBROUS MATS WITH ANTIBACTERIAL AND ANTIOXIDANT PROPERTIES FOR PROTECTING CELLS FROM OXIDATIVE STRESS

Suganya Bharathi Balakrishnan and Stalin Thambusamy*

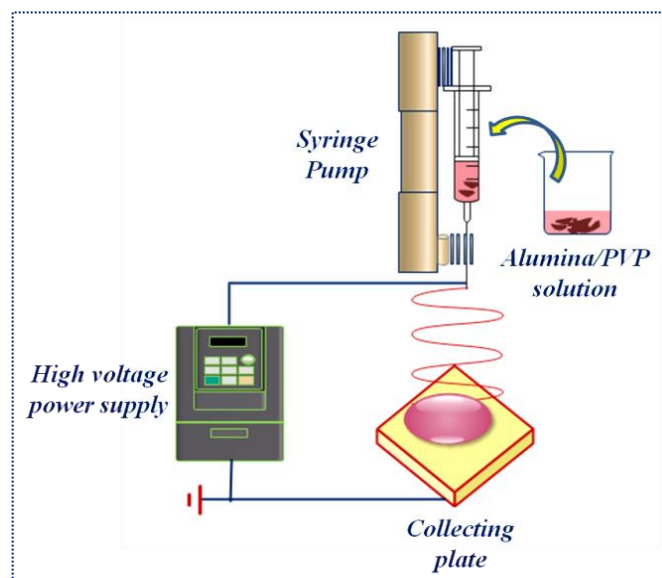
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Abstract

In the present study, a strategy for fabrication of the alumina nanoparticles implanted poly(vinylpyrrolidone) (PVP) nanofibers is presented. The addition of alumina nanoparticles to PVP nanofiber may assist to combat the oxidative stress induced by PVP as a biomaterial. The prepared nanofibrous mats are characterized by DSC, AFM and TEM analysis. The nanofibrous mats exhibit smooth surface with a fiber diameter of 260~330 nm indicating the miscibility of PVP and alumina matrix in nanoscale. The antibacterial activity was significantly improved for the composite nanofibrous scaffolds. Furthermore, the antioxidant assay proves that the scavenging capacity enhanced with the presence of alumina nanoparticles. Thus, our studies suggest that the developed nanofibrous mats hold great potential to be used as a biomedical scaffold for protecting cells from oxidative stress conditions. Here, the free radicals are produced by various biochemical pathways in the living system, causing severe oxidative stress to the biomolecules leading adverse disease conditions.

Keywords: *Nanofibrous mats, Poly(vinylpyrrolidone), Alumina nanoparticles, Oxidative stress*



Schematic representation for the fabrication of Alumina/PVP nanofibrous mat

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OP 62

**HIGHLY EFFICIENT RECYCLABLE Cu-(I)-SBA CLAY CATALYST FOR
CONVERSION OF NITROARENES TO AMINOARENES**

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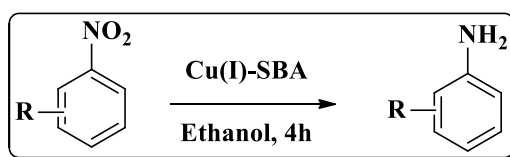
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Abstract

Conversion of nitroarenes to aminoarenes is of great importance since amines are among the vital intermediates essential for dyestuffs, pharmaceuticals, etc. in the industrial chemistry. The preparation of Cu (I)-SBA clay material by alcothermal strategy has been described in this study and characterized by FT-IR, XRD, SEM, XPS and BET analysis. The synthesized clay material is efficient in reduction of nitro aryl compounds to corresponding aniline in presence of LiAlH₄ and achieved in short time with high catalytic turn over number (TON) which retained good activity and stability after five cycles. The various nitroarenes were subjected for Cu(I)-SBA mediated reduction that provided the selective reduction of the nitrogroup even in the presence of other reducible functionality. This protocol affords the desired aminoarenes in excellent yields within short reaction times, when the reactions are performed at room temperature in the presence of LiAlH₄.



Keywords: Cu-(I)-SBA clay- alcothermal strategy- Aminoarenes - LiAlH₄- reduction

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OP 63

**FABRICATION AND CHARACTERIZATION OF NANOSTRUCTURED
Cd_{0.5}Zn_{0.5}S BASED SENSITIZER FOR PHOTOVOLTAIC APPLICATIONS**

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Abstract

Exploration of ecologically clean alternate energy resources is need of hour to meet outenergy demands. Renewable energy such as sunlight is believed to be the most ideal to fulfill our energy requirement but it needs new advancement to harvest more incident photons with more efficiency. Dye sensitized solar cells (DSSCs) have attracted much attention compared to conventional solid-state/ inorganic solar cells due to their low-cost, eco-friendly and high power conversion efficiency. Ruthenium complexes/ organic dyes based sensitizersexhibit power conversion efficiency of up to 11%. In recent days these semiconductor chalcogenides such as CdS, ZnS, PbS, CdSe, and InAs areengaged as sensitizers due to their size quantization effect, spectral tunability,and high extinction coefficient, superior thermal and photochemical stability. Since CdS and ZnS are promising sensitizers, the combined effect of these two sensitizers may helpful to harvest more light in the entirevisible region. Herein, we report a new convenient route to fabricate CdZnS nanostructure sensitized ZnO thin filmstowards photovoltaicapplications.

Keywords: Semiconductor Chalcogenide, CdZnS sensitizer, light harvesting property and Photovoltaic application.

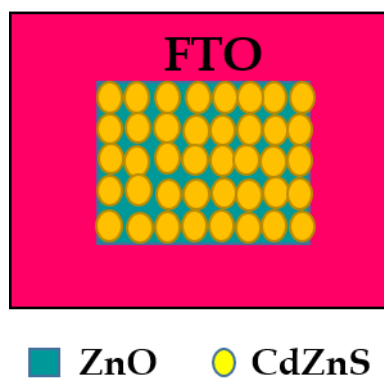


Fig. 1. Schematic representation of Prepared CdZnS sensitized ZnO Photoanode

PP 64

**DIMETHYL DIOXIRANE AND ZnO NANOCATALYST ASSISTED
PHOTOCATALYTIC DEGRADATION OF METHYLENE BLUE DYE**

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Abstract

Zinc oxide nanocatalyst was successfully synthesized by a facile single step sol-gel method using water as medium and used for the photodegradation of methylene blue dye. The synthesized zinc oxide nanoparticles were characterized using high resolution transmission electron microscope (HR-TEM), scanning electron microscope (SEM) with energy dispersive X-ray analysis (EDX), X-Ray diffraction (XRD), and fourier transform infrared spectroscopy (FTIR). Photocatalytic degradation under dark condition at room temperature was investigated with variation of pH, catalyst dosage, initial dye concentration and initial concentration of oxidizing agent. Dye degradation efficiency of methylene blue was increased by addition of dimethyl dioxirane and ZnOnanocatalyst. The kinetic studies were also done for the photocatalytic degradation of the dye. The effect of pH and initial dye concentration were also investigated.

Keywords: Zinc oxide; Methylene blue; Photocatalysis; Degradation; kinetics; Dimethyl Dioxirane.

OP 65

ELECTROCHEMICAL BIOSENSOR FOR AFLATOXIN B1 IN WHEAT FLOUR

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Abstract

Humans are exposed to toxins by consuming foods contaminated with products of fungal growth throughout life time. Since prevention of fungal growth in foods is difficult, such exposures are not easy to be avoided. Foodborne illness caused by microorganisms is a large and growing public health problem. It is estimated that about 4.5 billion people are chronically exposed to Aflatoxins. Since it is impossible to reverse its carcinogenic effects, the identification and prevention of human exposure to aflatoxins have become a major research topic in the area of food science. Due to the warm and favourably humid climate of India, the wheat is one of the most important crops. The high toxicity of aflatoxins and its effects on public health, determination of aflatoxin level in Wheat flour samples was investigated. Aflatoxin B1 (AFB1) is considered the most toxic and is produced by both *Aspergillus flavus* and *Aspergillus parasiticus*. Therefore, effective detection of AFB1 in food products is indispensable for ensuring that the products offered meet regulatory and market requirements. We have therefore investigated to develop an electrochemical immunosensor for the detection of AFB1. In this work screen-printed gold electrodes was used. Aflatoxin B1–BSA conjugate immobilized onto gold nanoparticle by self-assembled monolayer of 3-mercaptopropionic acid. The screen printed nanoelectrode based biosensor is an indirect competitive immunoassay. The AFB1 quantitatively determined in the 5ng/mL range. The developed sensor was found to be highly sensitive and exhibited a remarkably low limit of detection (LOD; 3 ng/mL). This method is accurate and more sensitive when compared with conventional AFB1 detection methods, and is highly applicable in food analysis to screen the mycotoxins in wheat.

Keywords: Electrochemical Biosensor, Immunosensor, Aflatoxin B1, wheat

OP 66

ANTIOXIDANT POTENT DIIMINES

G. Thirunarayanan

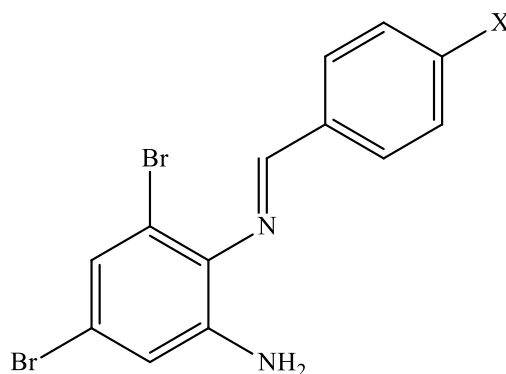
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Abstract

About six numbers of (*E*)-4,6-dibromo-*N'*-(4-substituted benzylidene) benzene-1,2-diamines were synthesised by more than 8 h refluxation of mixture of equi-molar quantities of 2-amino-4,6-dibromobenzaldehyde and 4-substituted aniline in ethanol medium(I). This condensation gave more than 85% yields. These diamines were characterised by their physical constants, analytical and spectroscopic data. The antioxidant activity of these diamines was evaluated by DPPH radical scavenging activity using L-Ascorbic acid as standard. From the experimental results, the methoxy substituted diimine showed satisfactory antioxidant activity against the standard. The order of observed antioxidant activity of these diimines are $\text{OCH}_3 > \text{CH}_3 > \text{Br} > \text{Cl} > \text{F} > \text{H}$. The parent compounds show least antioxidant activity. The +R effect of OCH_3 group favourably showed the antioxidant activity than the CH_3 group. The +I effect of halogens including F shows less antioxidant activity. The parent compound ($\text{X}=\text{H}$) shows least antioxidant activity.

Keywords: 1, 2-Diimines, IR and NMR spectra, Antioxidant activity



$\text{X}=\text{H}, \text{Br}, \text{Cl}, \text{F}, \text{OCH}_3, \text{CH}_3$ (I)

**POSTER
PRESENTATION**

PP 01

**PLANT-EXTRACT ASSISTED GREEN SYNTHESIS OF SILVER
NANOPARTICLES USING NYCTANTHES ARBOR-TRISTIS FLOWER AT ROOM
TEMPERATURE**

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Abstract

Plant-mediated green synthesis of nanomaterials has been increasingly gaining popularity due to its eco- friendly nature and cost – effectiveness. In the present study, we synthesized silver nanoparticles (AgNPs) by using an aqueous solution of Nyctanthes arbor-tristis plant extract as a bioreducing agent. The size and shape of AgNPs synthesized were depending on the initial extraction temperature employed and the PH of the reaction medium. The synthesized AgNPs were corroborated by XRD and SEM with EDAX, FTIR, UV-Visible spectra analyses. The different peaks in XRD were indexed to the face-centered cubic (fcc) phase of silver. The SEM images of AgNPs showed spherical shape for 60°C extraction. UV-Vis absorbance spectra of synthesized silver nano colloidal solutions showed surface Plasmon resonance (SPR) at wavelength of 423nm for 60°C extraction. FT-IR spectra indicate that synthesized AgNPs were capped with phytochemical present in the extract. This procedure is expected to be a new pathway for green chemical, low cost and shape controlled synthesis of AgNPs.

Keywords: AgNPs, Nyctanthes arbor-tristis flower, Green synthesis, FT-IR.

PP 02

SYNTHESIS AND CHARACTERIZATION OF GROUNDNUT-ZnO COMPOSITES

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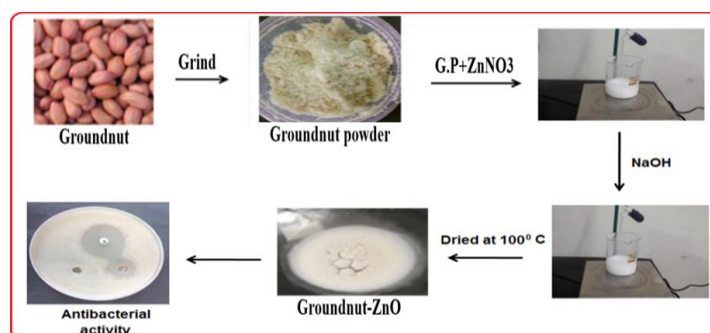
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Abstract

In this work, Groundnut-ZnO Composites was isolated from Groundnut in biomaterials. The Groundnut-ZnO Composites are prepared by simple precipitation method. The composites were prepared by using Groundnut as biomaterial, zinc nitrate as a source material and NaOH as a precipitating agent. The prepared composite was characterized and the functional groups confirmed by Fourier transform infrared spectroscopy (FT-IR). The optical properties of composite are studied by UV-Vis DRS spectroscopy. The crystalline structure of the composite was characterized by X-ray diffraction (XRD) and surface morphology of the composite observed by Higher resolution-scanning electron microscopy (HR-SEM). The Groundnut-ZnO composite exhibited antibacterial activity against gram-positive (*S.aureus*) as well as gram-negative (*E.coli*) microorganisms. The Groundnut-ZnO composite material showed excellent antibacterial activity. The enhancement of antibacterial of the composites revealed the composite would be a suitable candidate for implant application in biomedical field.

Keywords: Groundnut, ZnO, Composite, Antibacterial activity.

Graphical abstract



PP.03

PLANT MEDIATED GREEN SYNTHESIS OF TiO₂ AND MgO NANOPARTICLES USING ABUTILON INDICUM FLOWERS EXTRACT AND THEIR ANTIBACTERIAL ACTIVITY

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Abstract

Greener synthesis of Ti and Mg oxide nanoparticles (NPs) using *Abutilon indicum* flowers extract by hydrothermal method at low temperature. The synthesized metal oxide NPs characterized by various properties such as structural, spectral, optical, morphological, and biological studies. Powder X-ray diffraction studies confirmed that TiO₂ and MgO NPs crystallize and average crystalline size was shown 34 and 36 nm. FTIR spectroscopy confirmed the O-Ti-O, Mg-O and some functional groups. The O-Ti-O stretching vibration band attributed at 470 cm⁻¹ and Mg-O stretching vibration band attributed at 617 cm⁻¹. The optical property of TiO₂ and MgO NPs was characterized by ultra violet- diffuse reflectance spectroscopy (UV-DRS). The optical band gap energy of TiO₂ and MgO nanoparticles observed at 3.23 eV and 3.7 eV. The morphological and particle size determination were investigated by SEM with EDX spectra and TEM with SAED analyses. The agglomerated particles of hexagonal, spherical, and rod shape were observed from TEM images. TiO₂ and MgO NPs have good biological activities regarding antibacterial activity which could be utilized in different biological applications to the food and biomedical industries. A TiO₂ and MgO nanoparticles has a higher range of zone of inhibitions.

Keywords: MgO nanoparticles, plant extracts, *Abutilon indicum*, Antibacterial activity.

PP 04

CYCLIC VOLTAMMETRIC STUDIES ON NEW NITRO CHALCONES

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Abstract

Chalcone is an aromatic ketone that forms a central core for a variety of important biological compounds, which are collectively known as chalcones. They possess different activities like antibacterial, antifungal, anti-inflammatory and anti-tumor etc depending on the substitution made on them. At present investigation of New Nitro Chalcone derivatives were synthesized from 4-Nitroacetophenone by Claisen–Schmidt condensation with different aromatic aldehydes in ethanol in the presence of Sodium Hydroxide. The structures of chalcones were confirmed by UV, IR, ¹H-NMR and ¹³C-NMR Spectral Studies. All the synthesized 4-Nitro Chalcones were studied using cyclic voltammetry in an aqueous medium
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has been performed. The effects on the first reduction potential (E) were analyzed with the help of Hammett Equation and the ρ values were evaluated for various substituents.

Key words: Nitro Chalcones, Cyclic Voltammetry

PP 05

STRUCTURAL, PHOTO-PHYSICAL AND BIOMEDICAL APPLICATIONS OF CURCUMIN-BASED NOVEL CONJUGATED TRIAZINE CENTRED METAL COMPLEXES

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Abstract

Cancer is one of the major causes of death worldwide, and minimal progress has been accomplished in reducing its morbidity. Curcumin is a highly pleiotropic molecule found in the rhizomes of *Curcuma longa* (turmeric) and proves to inhibit the proliferation of cancer cells and to be of use in preventing or treating a number of diseases. In view of the antioxidant and metal ion-chelating activities of curcumin, the neuroprotective effect of its metal complexes indicates the great advantages of curcumin as a promising anti-cancer agent. Curcumin has been shown to modulate multiple cell-signaling pathways simultaneously, thereby preventing many different types of cancers, including multiple myeloma and colorectal, pancreatic, breast, prostate, lung, head, and neck cancers, in both animal models and humans. The current research focuses on diverse molecular targets modulated by curcumin that contribute to its efficacy against human oral and gastric cancer. Keeping in mind the literature review, transition metal complexes of curcumin based ligand of the type ML [where M = Co(II), Cu(II), Ru(III); L = PPTIDM] have been synthesized and characterized using various physico-chemical methods including C,H,N elemental analysis, melting point determination, molar conductivity measurement, IR, ^1H NMR, UV-Vis, Mass, CV, XRD, SEM-EDAX and photophysical studies. Spectroscopic and other analytical data of the complexes suggest octahedral geometry to the molecules. All the synthesized compounds may serve as potential photoactive materials as indicated from their characteristic fluorescence properties. Among the synthesized metal complexes, Ru-PPTIDM has been screened for its *in-vitro* biomedical applications and it exhibited a significant reduction in cell

viability towards *M. Tuberculosis* cell-line H37Rv and oral cancer cell-line H357 respectively for which considerable percentage of cell-death was obtained at 250µg/ml.

PP.06

**SELECTIVE SENSING OF DOPAMINE ON Mn₂O₃-TiO₂-GRAPHENE NANO
STRUCTURED ELECTRODES**

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Abstract

Composite nano particles recently attract paramount interest to develop electrocatalytic surfaces for sensors to be applied in medical and environmental field and that too raising a selective and sensitive platform for sensing of specific analyt draws special attention for using composites of carbon with metal and metal oxides with minimal pre-treatment of biosample. Dopamine is an important neurotransmitter whose decreased concentration in the physiological fluid leads several neurological disorders like Parkinson's disease, Huntington's disease etc. In this work, nano composites of TiO₂ and Mn₂O₃ were prepared by simple Sol-gel method and anchored on the graphene (Gr) sheets for selective sensing of dopamine (DA) in the presence of interfering components in Phosphate buffer saline. The interaction between the metal oxides and graphene was evaluated using characterization techniques like FE-SEM, TEM, XRD, FT-IR, and Raman spectra. Comparative electrochemical study using Electrochemical impedance spectroscopy (EIS) and Cyclic voltammetry (CV) techniques indicate higher activities for pristine graphene based metal oxide composites than the composites obtained using GO, observed for conventional redox probe K₃[Fe(CN)₆] as well as the neurotransmitter dopamine at pH 5. The composite is validated for DA sensing in blood and urine real samples by standard addition method and observed good selectivity and signal recovery. The transducer exhibits two different linear ranges viz., 1 nM – 900 nM and 0.02 nM – 0.09 nM with the lowest detection 0.026 nM. Developing this approach is less expensive and could act as a sensitive sensor in biological system and in environmental applications.

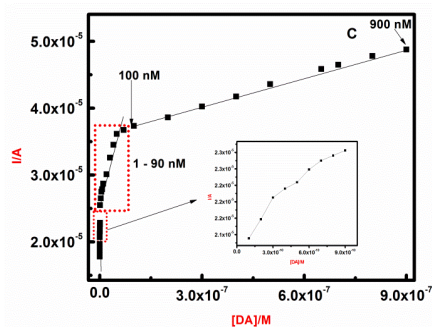


Fig.1 - Calibration plot. Wide linear range of concentration from 0.02 nM – 900 nM.

PP 07

EFFECT OF pH ON THE PHYSICAL AND NLO BEHAVIOR OF AMMONIUM DIHYDROGEN PHOSPHATE CRYSTALS (ADP) CRYSTALS

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Abstract

The influence of pH of the growth medium from pH = 2.5 to 12.5 on the physical and non linear optical properties of ammonium dihydrogen phosphate (ADP) crystals has been described. The reduction in the intensity observed in powder X-ray diffraction (XRD) of the specimens and slight shifts in vibrational frequencies (FT-IR) confirms minor structural variations. Surface morphological changes due to the change of pH in growth conditions are confirmed by scanning electron microscopy (SEM). The thermogravimetry and differential thermal analysis curves show the purity of the materials and no decomposition up to the melting point is observed. Changing the pH of the growth medium of ADP enhances the second harmonic generation (SHG) efficiency to a significant extent.

Keyword: ammonium dihydrogen phosphate, nonlinear optical properties, pH, growing from solution

PP 08

**CORROSION INHIBITION OF CARBON STEEL IN 1M HNO₃ SOLUTION BY
AUBUTILON X HYBRIDUM YELLOW EXTRACT/POWDER AS AN ECO-
FRIENDLY INHIBITOR USING WEIGHT LOSS METHOD**

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Abstract

Aubutilon X Hybridum Yellow Extract/Powder were studied as a sustainable and eco-friendly corrosion inhibitor in 1M HNO₃, using weight loss technique. The plant extracts reduced corrosion rate of carbon steel in the corrosive medium, thereby exhibiting corrosion inhibition property. The corrosion inhibition effect is attributed to the extract molecules being able to get absorbed to the metal surface creating a barrier between the acid and the carbon steel. The study indicates that as acid concentration increases corrosion rate increases. The corrosion inhibition efficiency increases with increase in concentration of extract/powder. The result obtained revealed that *Aubutilon X Hybridum Yellow* Extract/Powder act as an efficient inhibitor. Corrosion is an unavoidable but a controllable process. Due to the issues of toxicity of substances like organic and inorganic inhibitors, there is an increasing interest in exploration and utilization of eco-friendly inhibitors, which are also known as green inhibitors. The significance of this area of research is primarily due to the fact that natural product are environmentally friendly and ecologically acceptable. Maximum inhibition was attained 94% (1/2 h)/94% (3h) at the concentration of 1g for *Aubutilon X Hybridum Yellow* Extract/Powder.

Keywords: Plant corrosion inhibitor, Carbon steel, *Aubutilon X Hybridum Yellow*, 1M HNO₃ and Weight loss methods

PP 09

**RELATION BETWEEN BIOMARKER ENZYME AND TISSUE DAMAGE OF
CLAM, DONAX FABA EXPOSURE TO LEAD**

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Abstract

Lead (Pb) is one of the most widely distributed metals in the marine ecosystem. The acute toxicity tests of *D. faba* exposed to lead under acute Continuous Flow Through (CFT) method was conducted. After 24 h exposure, 100% survival of test animal was in all five lead exposed concentrations and after 48 h exposure, mortality was observed in the concentrations - 1.7, 3.4, 6.8 and 13.6 mg.l⁻¹ and as compared to control animal, sudden reduction in protein level was noticed in the lowest concentration (0.85 mg.l⁻¹) 52% and in the highest concentration (13.6 mg.l⁻¹) the reduction was 69%. More damage of gill and foot tissue was observed in Pb exposed *D. faba*. In the highest concentration of 13.6 mg.l⁻¹, coagulated gill filaments with disintegrated secretory vesicles found along the margin and also within the gill membrane. In the lowest concentration (0.85 mg.l⁻¹), the activation of enzyme was only 17%, however the activation was 172% when *D. faba* was exposed in the highest concentration (13.6 mg.l⁻¹). This present study indicates that *D. faba* is a marine bivalve molluscs species deserving of greater attention in future. Meanwhile, this could be regarded as a suitable bio indicator of Cd, Cu, Pb and Mn exposure by measuring Protein and LPO as biomarkers. LPO was considered to be an important feature in cellular injury. The reactive oxygen forms (O₂, H₂O₂, OH) which are produced during oxidative stresses potentially damaging cells and tissues.

Keywords: Lead, Accumulation, Tissue, Lipid peroxidation, Histology.

PP 10

A NOVEL SCHIFF BASE LIGAND AND ITS COMPLEXES FOR SENSOR APPLICATION

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Abstract

The versatile ligational behaviour of Schiff base compounds had evoked considerable interest in the past. It is our aim to synthesize new azo methine derivative and expected to
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exhibit variety of characteristics such as biological and catalytic properties. We have demonstrated that metal ions acting as modulators (or inputs, in digital design parlance) can generate absorbance changes in accordance with the operation of a half-adder. It was also obtained exploiting differential binding affinities of metal ions for different ligands. The present work focuses on the synthesis of ligand HPBABF and its complexes of copper, zinc, cobalt and nickel. All the synthesized compounds were characterized using various physical and chemical methods of analysis such as UV-Vis, FTIR, NMR, fluorescence, CV, TG, SEM, XRD and elemental analysis.

Keywords: Hydroxypyrimidine, antimicrobial, metal complexes.

PP 11

SYNTHESIS AND ELECTROCHEMICAL CHARACTERIZATION OF HIGH VOLTAGE CATHODE MATERIAL ($\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$) FOR LITHIUM ION BATTERIES

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Abstract

Cathode material $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ was successfully synthesized by a sol-gel method. The cathode material was calcinated at different temperatures: 120 °C, 600 °C, 900 °C. The XRD result reveals a spinel compound of $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ for 600 °C-12 hrs. $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ for 600 °C-12 hrs is well crystallized and lattice parameter, space group, cell volume is evaluated. The surface morphology, particle size and elemental analysis were analyzed by SEM and EDAX spectrum. SEM result shows the smooth morphology and less particle size and EDAX shows weight percentage elements is better for $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ at 900 °C -5hrs compared to $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ at 600 °C -12hrs. The oxidation state is analyzed by XPS and the highest binding energy occurs for $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ at 900 °C -5hrs compared to $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ at 600 °C -12hrs. Half cells were assembled and tested at C/10 rate. The maximum discharge capacity of around 106 mAh/g was obtained for the sample $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ at 900 °C -5hrs. The charge transfer resistance value of $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ at 900 °C -5hrs is 411.341 Ω also better compared to 600 °C at 12 hrs.

sample. The cyclic Voltammeters experiment does not reveal the complete reversibility of the electrodes. Charging and discharging range for CV 3 to 5v. The $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ at 900 0 C -5hrs give better voltage 3.30 to 4.57V come from $\text{Mn}^{3+}/\text{Mn}^{4+}$ and $\text{Co}^{3+}/\text{Co}^{4+}$ compared than $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ at 600 0 C -12hrs. Charge discharge studies were carried out by applying constant current. This study gives the specific charge capacity and specific discharge capacity from charging and discharging capacity. Specific discharge capacity and capacity retention gives the actual performance of the cell.

Keywords: Spinel, sol-gel method, Metal ion-doped spinel, Cyclability, charging and discharging capacity, Lithium secondary battery

PP 12

PHOTOPHYSICAL STUDIES ON DONOR-ACCEPTOR BLENDS OF PICENE – PTCDI

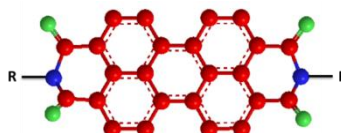
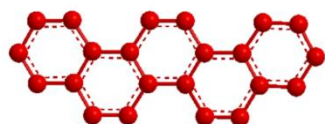
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Abstract

Blending two different organic molecules with opposite electron affinity open up new perspectives for developing high-performance luminescent materials for optoelectronic devices. Donor and acceptor molecules have been exploited for their self-assembling ability towards various applications. However, few reports on the role of D-A molecules in device fabrications are available. In this context, we have chosen picene as donor and perylene tetracarboxylic diimide (PTCDI) as acceptor to evaluate their photophysical aspects in various solvents. In addition, we have studied in mono and binary mixtures of solvents with different polarities. The specific DA dyad exhibited interesting behavior in binary mixture of chloroform and methanol. These two solvents are considered as good and poor solvent for both the components. λ_{max} of picene was blue shifted in the binary mixture which shows formation of h aggregates accompanied by hyperchromic shift in UV-vis absorption spectra. Interestingly, in equimolar D-A combination, a new peak was observed at 572 nm is may be due to intermolecular charge transfer (ICT).



Molecular self-assembly and non-covalent interactions are crucial in defining the morphology. This dyad architecture can be utilized for photovoltaic, light emitting display, sensor, and transistor applications.

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PP 13

HYDROTHERMAL APPROACH OF NANO SILVER DOPING ON THE CuO NANOMATERIAL AND STUDY OF ITS PHOTOCATALYTIC ACTIVITY UNDER UV-LIGHT

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Abstract

We report superficial and hydrothermal product of bare CuO (X) and reduced Ag-CuO (AX) nanostructured materials. The nanostructured materials are investigating with dual properties of photocatalytic degradation and antibacterial activity against (gram positive +^{ve} and gram negative -^{ve}) bacterial strain. This synthesized nanostructured materials were confirmed through HR-TEM and XRD analysis. HR-TEM results shown the particle size become 1.5 1/nm. The nanoparticles are crystallite in nature with average size 23 nm. The direct bandgap energy was suitable for AX catalyst. Pseudo first order reaction was followed in the Kinetic process. Better dye degradation result was shown along with Methylene blue (MB) in few hours under Uv-irradiation process. The complete mineralization of MB dye suspension also carried out by COD techniques. XRD, FT-IR, HR-SEM, HR-TEM, XPS, PL, CV and UV-DRS Spectroscopic and microscopic results have been discussed for confirmatory of nanostructures.

Key Words: Nanostructured materials, Bacterial strain, HR-SEM;CV;COD;

Department of Industrial Chemistry, Alagappa University, Karaikudi.

PP 14

**SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL ACTIVITIES OF
POLY (N-TERT-AMYLACRYLAMIDE-CO-ACRYLAMIDE-CO-2-ACRYLAMIDO-
2-METHYLPROPANE SULPHONIC ACID SODIUM SALT) ZINC OXIDE
NANOCOMPOSITE HYDROGELS**

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Abstract

Poly(N-tertiary amyl acrylamide -co-acrylamide-co-2-acrylamido-2-methylpropane sulphonic acid sodium salt) Zinc oxide (ZnO) nanocomposite hydrogels were synthesized by *in situ* free-radical copolymerization in aqueous methanol medium at 60 °C using N,N'-methylenebisacrylamide (MBA) as a crosslinker and ammonium per sulphate (APS) as the initiator. The N-tert-amyl acrylamide (NTA) and acrylamide (AM) monomers were fixed as 1:1 w/w and the amount of sodium salt of the 2-acrylamido-2-methylpropane sulphonic acid (AMPSNa) was varied. Characterization of the polymer composite by FT-IR, SEM/EDX and XRD indicated the presence of ZnO nanoparticles in the polymer matrix. The ZnO nanocomposite hydrogels showed potent antimicrobial activity on pathogenic bacteria *Escherichia coli* and *Staphylococcus aureus* and fungi *Candida albicans*.

Keywords: Hydrogels, Nanocomposites, Antimicrobial activity.

PP 15

**IONIC LIQUID ASSISTED SYNTHESIS OF TRI-DOPED N, P, F AND N, B,F-
MWCNT AND THEIR PREVENTION ACTIVITIES OF BACTERIAL BIOFILM-
ASSOCIATED WITH ORTHOPEDIC IMPLANTATION**

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Abstract

The multifunctional biological active material design for bone tissue engineering is essential to induce osteoblast cell proliferation and attachment. Adhesion of bacteria on biomaterials to produce biofilms can be major contributors to the pathogenesis of implant material associated infections. This research work focuses on NPF & NBF elemental doping and functionalization of MWCNT using an imidazolium-based ionic liquid such as BMIM PF₆ and BMIM BF₄ by hydrothermal method. The resulting tri doped reduced MWCNT (NPF-MWCNT and NBF-MWCNT) composite was further used as a scaffold for bone tissue engineering and anti-biofilm activities. The observation of the effect of NPF-MWCNT and NBF-MWCNT on the morphology, adhesion and cell proliferation of human osteo sarcoma (HOS) cell was investigated. Moreover, the tridoped composite tested its antibiofilm properties against *B. subtilis*, *E. coli*, *K. pneumoniae*, and *P. aeruginosa* pathogenic bacteria. *In-vitro* studies clearly show the effectiveness of N, P, B, and F doping promoting the rGO mineralization, biocompatibility, and destruction of bacterial biofilm formation. The result of this study suggests that NPF-MWCNT and NBF-MWCNT hybrid material will be a promising scaffold for bone re-aeration and implantation with a minimal bacterial infection.

Keywords: Ionic liquid, MWCNT, 1-butyl 3-methyl imidazolium hexafluorophosphate, 1-butyl 3-methyl imidazolium tetrafluoroborate.

PP 16

EFFECT OF DIFFERENT CHEMICAL TREATMENT ON THERMAL, MORPHOLOGICAL AND MECHANICAL PROPERTIES OF SHORT PINEAPPLE FIBER REINFORCED WITH UNSATURATED POLYESTER/CERAMICS POWDER/NANOSILICA FILLED HYBRID NANOCOMPOSITES FOR AUTOMOTIVE APPLICATION

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Abstract

Natural fibers have recently become attractive to researchers, engineers and scientists as an alternative reinforcement for fiber reinforced polymer (FRP) composites. Due to their low cost, fairly good mechanical properties, high specific strength, non-abrasive, eco-friendly and bio-degradability characteristics, they are exploited as a replacement for the conventional fiber, such as glass, aramid and carbon. Nanocomposites show considerable applications in different fields because of larger surface area, and greater aspect ratio, with fascinating properties. Being environmentally friendly, applications of nanocomposites offer new technology and business opportunities for several sectors, such as aerospace, automotive, electronics, and biotechnology industries. The tensile properties of natural fiber reinforce polymers (both thermoplastics and thermosets) are mainly influenced by the interfacial adhesion between the matrix and the fibers. Several chemical modifications are employed to improve the interfacial matrix–fiber bonding resulting in the enhancement of tensile properties of the composites. The effect of chemical treatment on pineapple fiber, nanosilica, ceramic powder and its interaction with polyester resin were studied. The aim of present research work was focused with enhancing the mechanical strength, thermal stability and less % of water absorption.

A systematic study was carried out to investigate the effect of different chemical treatment on thermo mechanical properties of short (2 cm) length of pineapple fibre reinforced thermosetting unsaturated isothalic polyester nanocomposites fabricated by the compression moulding technique. The influence of chemical modifications of pineapple fiber and effect of nanosilica/ceramics powder polyester(PE)/ pineapple fiber/nanosilica/ceramics powder hybrid nanocomposite fabricated by compression moulding technique was investigated by thermo gravimetric (TGA), FESEM, water absorption, tensile strength, compression, flexural analysis. Before making composite, pineapple fiber were subjected to different chemical treatment such as formic acid (HCOOH), sodium hydroxide (NaOH), permanganate (KMnO₄), hydrogen peroxide (H₂O₂), and acetic anhydride (Ac₂O). The use of chemically treated fibers caused an increase in thermo physical properties of composite irrespective of the chemical treatment. The various chemical treatments such as alkaline (NaOH), acid (HCOOH), acetic anhydride (Ac₂O), peroxide (H₂O₂) and permanganate (KMnO₄) treated were to improve the interfacial adhesion between the fibre/matrix interfaces compare with the untreated pineapple fiber. Of the various treatments HCOOH, NaOH and

KMnO₄ treated fiber nano composites showed highest values of thermal and mechanical properties. This treatment is to improve the interfacial bonding with matrix. Fibre/matrix compatibility were increases and also increases in thermal (TGA/DTG) stability, mechanical properties of tensile strength, bending, compression strength, and impact strength. Lower water absorption was also observed due to the surface treatment and addition of nanosilica. FE-SEM image and FT-IR study were identified with untreated and treated pineapple fibre. In our study, the alkaline (NaOH), acid (HCOOH) treatment was better than other treatment were perfectly interperated by morphological and FT-IR study. Meanwhile, the thermal stability and mechanical strength were increases in the HCOOH treatment. Both chemical treatment and nanosilica were significantly increases the thermal, mechanical properties of nanocomposite and less water absorption.

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PP 17

SYNTHESIS OF ZIRCONIA DOPED ZINC OXIDE NANOPARTICLES AND EVALUATION OF INTERACTION BETWEEN NPs AND CALF THYMUS DNA

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Abstract

Nanotechnology has become increasingly important in the biomedical and pharmaceutical areas as alternative antimicrobial strategy due to re-emergence infectious

Department of Industrial Chemistry, Alagappa University, Karaikudi. 91

diseases and the appearance of antibiotic-resistant strains especially within Gram-negative microorganisms. Inorganic antibacterial agents such as metal and metal oxides are advantageous compared to organic compound due to their stability. Among these metal oxides, ZnO has attracted a special attention as antibacterial agent. For instance, ZnO inhibits the adhesion and internalization of enterotoxigenic *E. coli* (ETEC) into enterocytes. In addition, ZnO nanoparticles exhibit antibacterial activity and can reduce the attachment and viability of microbes on biomedical surfaces. ZnO is listed as “generally recognized as safe” (GRAS) by the U.S. Food and Drug Administration (21CFR182.8991). As a food additive, it is the most commonly used zinc source in the fortification of cereal-based foods. Because of its antimicrobial properties, ZnO has been incorporated into the linings of food cans in packages for meat, fish, corn, and peas to preserve colors and to prevent spoilage. Nano zirconia is also one of the widely used metal oxides for potential applications like biosensors, cancer therapy, implants and dentistry due to its high mechanical strength and less toxicity. *In vitro* cytotoxicity of ZrO₂ nanoparticles reveals 58% of cell death in *vero* cell line. However, scanty reports are available on the evaluation of toxic behavior of zirconia nanoparticles with respect to cytotoxicity, antioxidant and bioactivity.

The purpose of this research is to synthesis and evaluate the antibacterial activity of Zircona doped ZnO nanoparticles and also examining the mode of interaction through the utilization of UV-visible, Fluoresces and as well as advanced molecular spectroscopy methods finds the mechanism.

Keywords : CT-DNA, Nano particles, Doped nano metal oxide, DNA binding

PP 18

SURFACTANT ASSISTED SYNTHESIS OF ZnS FOR SUPERCAPACITOR APPLICATIONS

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Abstract:

Nowadays, it is essential for us to design and fabricate efficient and cost-effective electrode materials for energy conversion and storage systems. Nanostructures are remarkable electrode material which exhibit large surface area and large number of active sites. Herein we have *Department of Industrial Chemistry, Alagappa University, Karaikudi.* 92

successfully synthesised via solvothermal method surfactant free and surfactant assisted Zinc sulphide (ZnS) electrode materials under microwave (MW) condition. The electrodes were prepared by slurry-coating method using Ni-foam as a current collector. Surfactants such as TRITON, CTAB, SBDS were used to increase surface area, which results in a better electrochemical performance compared to bare Zinc sulphide (ZnS). To study the morphology changes and nanostructures the resulting samples were characterized by X-ray Diffraction and SEM, the electrochemical performance of the supercapacitor (SC) electrode were examined by cyclic voltammetry, galvanostatic charge-discharge, electrochemical impedance spectroscopy. The CTAB assisted Zinc Sulphide (ZnS) electrode shows outstanding electrochemical performance in SCs with a specific capacitance of 1255 F/g at a current density of 1 A/g which is superior than 626.5 F/g for bare ZnS at a current density of 1 A/g. Increasing the current density from 1 to 10 A/g, the discharge capacitance was drastically decreased to 311 F/g for ZnS-CTAB, the electrodes were poorly participated in the electrochemical reactions, it leads to the poor rate capability as well as poor capacitance. The facile synthesis surfactant assisted Zinc sulphide (ZnS) especially CTAB-ZnS showed outstanding performance (1255 F/g), large surface area, well define surface morphology, synergetic effect and low cost makes the Surfactant assisted Zinc sulphide (ZnS) an ideal material for electrochemical energy storage devices.

Keywords: Supercapacitors (SCs), Surfactant, Zinc sulphide (ZnS), slurry-coating, CTAB-ZnS.

PP 19

FORMULATION AND CHARACTERIZATION OF WATER BORNE RUST CONVERTER COATING

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Abstract

Corrosion protection and prevention are remarkably important, since considerable part of the gross national products are consumed annually for corrosion and corrosion prevention. The rust was converted to a compact black protective rust-conversion film with this rust converter. HALOX® RC-980 is a low-odor, water-soluble rust converter. Water-based anticorrosion coating was prepared by applying a mixture of HALOX® RC-980 and

Department of Industrial Chemistry, Alagappa University, Karaikudi. 93

other additives to form polymer composites on the rusty mild steel plates. The formulated water borne rust converter was studied to investigate the anticorrosion performance on mild steel substrates in neutral and acid media. The electrochemical techniques such as electrochemical impedance spectroscopy and potentiodynamic polarization was used to analyze the corrosion rate of both coated and uncoated mild steel plates. Corrosion protection efficiency was also analyzed by the Tafel polarization curves and EIS studies. The formulated rust conversion paint shows high corrosion resistance capacities. The film forming mechanism of conversion layer was studied by FT-IR and SEM results.

Keywords: Rust converter, Potentiodynamic Polarization, Electrochemical Impedance Spectroscopy

PP 20

CARBAZOLE ENCAPPED COMPARTMENTAL COPPER (II) COMPLEXES FOR ANTIBACTERIAL AND THEORETICAL OPTOELECTRONIC STUDIES

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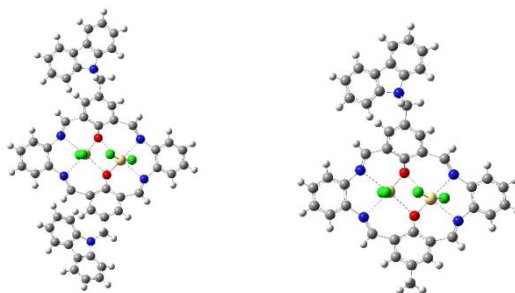
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Abstract

Macrocyclic chemistry is an astonishing field where more number of investigations are carried out even after years of its saturation in coordination chemistry. Vary many macrocyclic complexes are synthesized and investigated for their potential activity against a broad spectrum of gram positive and gram negative bacteria's. Carbazoles and its derivative are yet another class of alkaloids which is used as antibiotics. It has found applications also in fields such as optoelectronics¹, CO₂ trappers², MOF's³, etc.,

Fusing these molecules together give raise to unique complexes which has the combination of both properties. The current study involves in identifying a potential candidate for antibacterial activity and to find whether these complexes can be used for multiple applications. Cu(II) compartmental complexes are synthesized using diformyl ligand and it is tether on the methyl group of the compartmental ligand. It is screened for its potential antibacterial activity against *Staphylococcus Aureus* (Gram Positive bacteria) and *Klebsiella pneumonia*(Gram Negative bacteria). The molecules are characterized using UV,

FT-IR, and ESI-MS. Theoretical Gaussian was also carried out for these molecules to determine the HOMO-LUMO energy gap of these molecules.



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PP 21

SYNTHESIS, CHARACTERIZATION AND ELECTROCHEMICAL STUDIES OF BENZALAZINE SUPPORTED POLYANILINE AND COPPER(II) CHLORIDE NANO SIZED COMPOSITE

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Abstract

Composite of polyaniline containing copper (II) chloride supported by benzalazine was synthesized by oxidation polymerization of aniline in the presence of 10 weight percentage of copper(II) chloride and benzalazine. UV-Visible and infrared spectral studies confirmed the formation of this composite. X-ray diffraction studies revealed the partial crystalline nature of the composite. The percentage of crystallinity of this composite was 14%. SEM images showed spherical shaped particles in nanometer range. Surface morphology of composites carried out through atomic force microscopic. The surface was

flat with agglomerated particles. Redox nature of the synthesized composite was studied at different pHs by using cyclic voltammetry. This composite showed good redox behavior at acidic pHs. Electrochemical impedance spectroscopy studies were also carried out at different pHs. This composite showed very good specific capacitance at pH 1. Chronocoulometric studies were also done in different pHs. Double layer capacitance calculated from chronocoulometric studies was high at pH 1.

Key words: Polyaniline, Benzalazine, Specific capacitance. Nanocomposites

PP 22

ISATIN BASED RATIOMETRIC PROBE: SELECTIVE SENSORS FOR Cu²⁺ AND Hg²⁺ IONS IN AQUEOUS SAMPLES

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Abstract

Development of new chemosensors for selective and sensitivity detection of hazardous divalent metal ions with biological applications, is attracting more attention nowadays. Copper is one of the important elements in humans, excess concentration of Cu²⁺ can cause Alzheimer's disease.¹ Mercury, a potentially toxic heavy metal ion that can damage cardiovascular systems.² So far, isatin based derivatives have not been explored for sensing metal ions. Here we synthesized a novel isatin probe B for the selective detection of Cu²⁺ and Hg²⁺ ions to explore its cation – sensing ability. In the presence of Cu²⁺ & Hg²⁺, the chemosensor B provided a red shift (≈ 90 nm) with easily detectable color change from colorless to Yellow (Cu²⁺) and brick red (Hg²⁺), whereas other metal ions remain colorless. Moreover, this ratiometric probe forms 1:1 complex with a detection limit of 3.371×10^{-7} M and binding constant was found to be 6.96×10^{10} M⁻¹ & 1.40×10^{11} M⁻¹ for Cu²⁺ and Hg²⁺ respectively. Further, Addition of mercaptoethanol to B-Cu²⁺ and B-Hg²⁺ provides a complementary means to differentiate Cu²⁺ from Hg²⁺, which was also been confirmed by theoretical DFT calculations. We expect that the highly efficient, cost-effective probe will serve as a practical tool for detecting toxic ions in the environmental samples.

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PP 23

SYNTHESIS, SPECTRAL, X-RAY CRYSTALLOGRAPHY AND BIOLOGICAL PROPERTIES OF *N*-HETEROCYCLIC MIXED LIGAND CO(III) COMPLEXES CONTAINING 1,10-PHENANTHROLINE AND SODIUM AZIDE

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Abstract

The reactions of 6-methyl-2-chloroquinoline-3-carboxaldehyde-4(*N*)-thiosemicarbazones (H_2L^{1-3}) with cobalt(II) nitrate hexahydrate along with the co-ligands such as 1,10-phenanthroline and sodium azide. The ligands (H_2L^{1-3}) and new complexes $[\text{Co}(\text{phen})_2(\text{N}_3)_2] \cdot \text{NO}_3$ (**1a**), $[\text{Co}(\text{H-6MQtsc-Me})_3] \cdot \text{DMF}$ (**1b**), $[\text{Co}(\text{H-6MQtsc Et})(\text{N}_3)_2(\text{phen})] \cdot \text{DMF}$ (**2**) and $[\text{Co}(\text{H-6MQtsc-Ph})(\text{N}_3)_2(\text{phen})] \cdot \text{DMF}$ (**3**) were synthesized and characterized by various spectral analysis. While, **1a** was confirmed by ¹H NMR and mass spectral analysis. From the crystallography, it has been found that the complex **1b** has ML_3 type coordination of the ligand. However, the structure of the complexes (**2** and **3**) were also confirmed by X-ray analysis, there complexes (**2** and **3**) were coordinated to metal centre as bidentate monobasic ligand by using four nitrogen atoms from co-ligands such as 1,10-phenanthroline and two azide units. All the complexes were subjected to study their binding potential with calf-thymus DNA (CT-DNA) and Bovine Serum Albumin (BSA) by absorption and emission spectral measurements. Antioxidant and cytotoxic potential of the

complexes were examined and found to exhibit significant activity. Morphological changes of the complexes **1-3** assessed by acridine orange and ethidium bromide staining revealed that the cell death occurred through apoptosis.

PP 24

SYNTHESIS AND CHARACTERIZATION OF POLY (3,4-ETHYLENEDIOXYTHIOPHENE)–NICKEL OXIDE NANOCOMPOSITES FOR SOLAR CELL APPLICATIONS

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Abstract

Development of alternative energy to fossil fuels is one of the most important global issues caused by climate change and global warming. Among various types of renewable energies, photovoltaic cells are becoming an increasingly appealing option for energy production. The proposed research described the fabrication of Poly (3,4-ethylenedioxythiophene)-Nickel oxide nanocomposites solar cells. Nickel oxide nanoparticles and Poly (3,4-ethylenedioxythiophene) were synthesized through chemical and oxidative polymerization methods respectively. Five different percentages of NiO nanoparticles introduced nanocomposites were prepared. The metal oxide and nano-composites were characterized by UV-Vis, FT-IR, AFM, FESEM and electrochemical behaviour. The surface morphology was characterized by AFM and FESEM. UV-vis spectra of PEDOT-NiO NCs exhibit the absorption peak from 405 nm to 497 nm is assigned to the π to π^* transition of the thiophene ring and it can be seen that the intensity of π - π^* transition peak and bipolaron subgap transition peak slightly increased with increasing the percentage of NiO. FT-IR spectra of PEDOT-NiO NCs revealed that the composites contained all the main characteristic transmittance bands and slight shifting of peaks were indicates significant interaction between the polymer and the NiO nanoparticles. Poly (3,4-ethylenedioxythiophene)-Nickel oxide solar cell exhibits power conversion efficiency of 5.8%.

Keywords: Nanocomposites, AFM, FESEM, Electrochemical, Solar cell

PP 25

**ANTIBACTERIAL AND ANTIOXIDANT PROPERTIES OF VITAMIN B₃-
POLY(METHYL METHACRYLATE) / α -CYCLODEXTRIN ELECTROSPUN
NANOFIBERS**

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Abstract

In this work, we prepared the vitamin B₃-Poly (methyl methacrylate) (PMMA)/ α -Cyclodextrin (α -CD) nanofibers for biological activities. Here, PMMA which is acted as a polymer matrix for the fabrication of vitamin B₃-PMMA/ α -CD, due to its bioavailability and non-toxic nature. Furthermore, α -CD is widely used for the biomedical applications because of its hydrophobic and hydrophilic behavior. Vitamin B₃ is also known as niacin, which is essential for the metabolism of carbohydrates and fats. Therefore, we prepared vitamin B₃-PMMA/ α -CD nanofibers for biological evaluation. The surface morphology, functional behavior, and optical properties were confirmed by SEM, FT-IR, UV-Visible and emission Spectra, respectively. The bacterial efficiency of the prepared nanofibers was studied by the disc diffusion method. Moreover, the free radical scavenging activity of the prepared nanofibers was investigated by DPPH radical scavenging assay.

Keywords: Poly (methyl methacrylate), α -Cyclodextrin, Vitamin B₃, Antibacterial activity, Antioxidant activity.

PP 26

***SOLANUM PROCUMBEN* LEAVES EXTRACT MEDIATED GREEN SYNTHESIS
OF Ag-Pd/Mn₃O₄ NANOPARTICLES AND ITS ANTIBACTERIAL ACTIVITY**

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Abstract

In the present work, we reported hydrothermal method for the green synthesis of Mn_3O_4 , Ag/Mn_3O_4 , Pd/Mn_3O_4 and $Ag-Pd/Mn_3O_4$ NPs using *Solanum procumbent* leaves extract. Biosynthesized NPs were analyzed UV–Vis DRS, FTIR, XRD, MICRO RAMAN and SEM with EDX that the NPs were needle in shape. The surface morphology of Mn_3O_4 nanoparticles shows hexagonal shaped grains distributed uniformly. After doping of Ag and Pd into Mn_3O_4 the morphology changed into sponch and spherical and needle like structures which contributes enhanced biological activity. EDX analysis confirmed that the Ag and Pd ion is fully doped into Mn_3O_4 sample. The results of the antibacterial tests demonstrate that both pure Mn_3O_4 , Ag/Mn_3O_4 , Pd/Mn_3O_4 and $Ag-Pd/Mn_3O_4$ NPs show viable reduction of both *E. coli* and *S. aureus* strains. The sample $Ag-Pd/Mn_3O_4$ revealed enhanced and synergistic antibacterial activities for both Gram-negative and Gram-positive bacteria. From the result Gram-negative bacteria more liable compared with Gram-positive bacteria.

Keywords: $Ag-Pd/Mn_3O_4$ NPs, *Solanum procumbent*, Antibacterial activity.

PP 27

SYNTHESIS AND CHARACTERIZATION OF METAL OXIDE NANOPARTICLES

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Abstract

Nano particles research is currently an area of passionate scientific research, due to a wide variety of potential applications in biomedical, sensing, optical, and electronic fields. They exhibit a number of interesting characteristics including unique physical, chemical, optical, magnetic and electrical properties. Nano particles are of great scientific interest as

they are effectively a bridge between bulk materials and atomic or molecular structures. The properties of materials change as their size approaches the nano scale. Nano materials often show unique and considerable change in physical, chemical and biological properties compared to their macro scaled counterparts. Metal oxide nano particles represent an industrially important class of nano materials. They exhibit a number of interesting characteristics including unique physical, chemical, optical, magnetic and electrical properties. Metal oxide nano particles have great potential for electronic, magnetic, optical, and photo catalytic applications. Metals highly dispersed on nano support surfaces show active catalysts for a variety of reactions. The numerous methods have been documented in the recent reviews for the synthesis of a broad range of metal oxide nano particles. Among them, wet chemical method using microwave reaction system has fascinated many researchers in contemporary science owing to the advantages of simple process, easy scale-up and low cost. A work of fiction attempt has been made to synthesize and characterize some of the metal oxide nano particles. Iron oxide, Titanium dioxide, cerium oxide and thorium oxide are prepared by chemical methods using microwave reaction system. The prepared nano particles are characterized by using analytical techniques such as FT-IR, XRD, FE-SEM and UV-Vis (DRS) analysis.

Keywords: Nano particles, microwave reaction system, thorium oxide and FE-SEM.

PP 28

**PHYSICO CHEMICAL CHARACTERISTICS AND COMPOSITIONAL STUDIES
OF PALM KERNEL OIL**

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Abstract

Proximate, physico-chemical and elemental analysis of palm Kernel nut were determined to contain fat/oil 42%, Crude Protein 7.01%, Moisture 6.5%, crude fibre 11.09% and Carbohydrate (by difference) 33.40%. The elemental composition (mg/100g) included Na (37.00 ±0.40), K (39.51±0.22) mg (3.60 ±0.1), ca (19.0 to 0.42), Fe (20.04 ± 0.28) zn (2.82 ± 0.30), p (3.4 ± 0.00). The result of the physico- chemical Properties of the palm

kernel oil are: saponification value (232.815 mg KOH/g), refractive index (1.453), iodine value (41.24g/100g), acid value (11.60 mgKOH/g) and Peroxide value (1.70 Meo/kg)

Keywords: crude fibre, moisture, carbohydrate acid value.

PP 29

SYNTHESIS, CHARACTERIZATION, BIOLOGICAL STUDIES AND FLUORIDE SENSING OF SALICYLALDEHYDE SCHIFF BASE DERIVATIVE

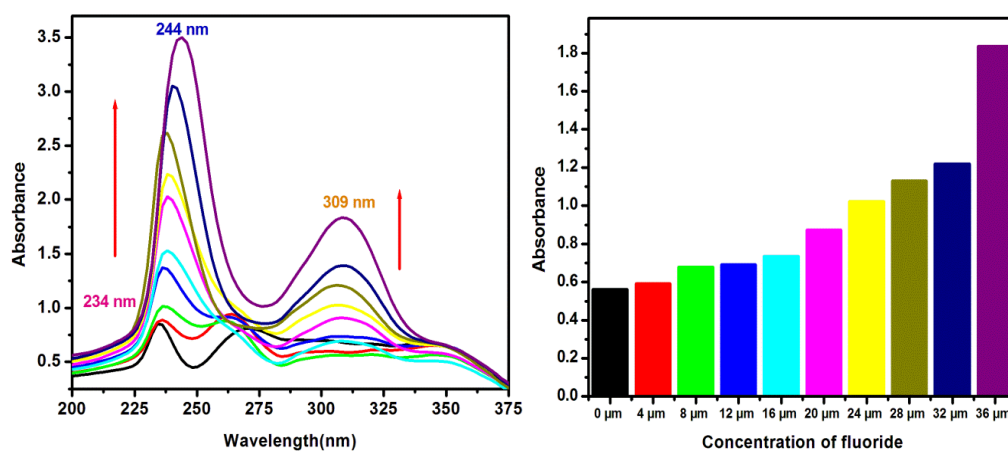
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Abstract

In this article we study the biological and sensing properties of Schiff base derivative. The Schiff base derivative prepared from salicylaldehyde and sulfanilamide. The derivative characterized by ESI-MASS, FT-IR, UV-visible absorption and fluorescence spectral studies. Interacting behavior of this derivative with Cl^- , Br^- , NO_3^- , AcO^- , H_2PO_4^- , I^- , F^- , SCN^- and ClO_4^- anions are studied by UV-visible absorption experiments. The Binding ability of fluoride with various concentration in THF medium is calculated by using Bensi-Hidebrand equation with the help of UV-Visible absorption spectral changes. The Schiff base act as a good sensor in the selective recognition for F^- with highest significant binding constant value. The Schiff base derivative also studied by anti-microbial studies using three bacteria and two fungus. The maximum level of zone inhibition was observed the schiff base derivative against the *Bacillus cereus*.



Key words: Fluoride Sensing, Anti- Bacterial and Fungal Studies.

PP 30

**SYNTHESIS AND EVALUATION OF TRIAZINE BASED CHEMOSENSOR FOR
THE DETECTION OF Co²⁺ ION**

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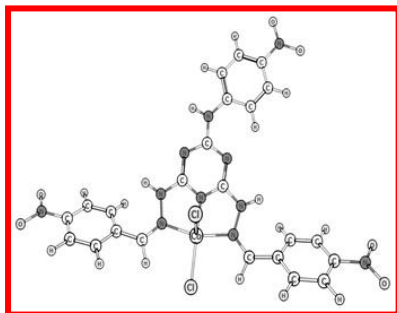
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Abstract

The present work investigates the synthesis of triazine Schiff base (BNHNTA) for the selective and sensitive determination of Co²⁺ ion using both colorimetric and electrochemically. Selectivity studies were carried out with different metal ions and found that the proposed chemosensor has high selectivity towards the detection of Co²⁺ with the colour change from yellow to blue due to the formation of complex with Co²⁺. Hence, the selectivity was also confirmed by the change in the optical properties of the sensor. It can be used as a robust ‘Naked- eye’ sensor for the selective detection of Co²⁺ ion due to colour changes in the visible region, which has a detection limit of 0.05 μM. In addition to that, amperometric studies were carried out and it reveals the selective electrochemical sensing of Co²⁺ ion by BNHNTA and the detection limit was found to be 0.03 μM. The density functional theoretical (DFT) study provides the structural insights about Cobalt (II) complex, which confirms the square pyramidal geometry of the formed complex. DFT studies confirm the formation of 1:1 receptor-metal ion complex in detecting Co²⁺ ion. It is confirmed by the high resolution mass spectrometry (HRMS) which is supported by the Job’s plot measurements. These results indicate that the as synthesized BNHNTA shows an excellent selectivity and sensitivity towards the detection of cobalt ion environmental applications.

Keywords: Cobalt, Triazine, Colorimetric sensor, Electrochemical sensor, DFT study.



PP 31

**PRECIPITATION SYNTHESIS AND CHARACTERIZATION OF CADMIUM
DOPED WO₃ NANOPARTICLES**

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Abstract

Cd doped WO₃ nanoparticles have been synthesised by chemical precipitation method. It is a simple method to prepared nanoparticles. The prepared samples were characterised by using UV-Vis, FTIR spectroscopy, Field Emission Scanning Electron Microscope (FESEM) with EDAX spectroscopy. Synthesised nanoparticles also characterized by Photoluminescence studies. From UV –Visible spectra of Cd doped WO₃ nano particles exhibited absorption at 320 nm and 380 nm. FT-IR spectral results revealed that the presence of metal oxide band. FTIR spectrum is applicable to confirm the presence of constituents qualitatively or quantitatively. The FESEM images exhibit the crystalline size of WO₃ nanoparticles, Cd doped WO₃ nanoparticles also in nanometer range. The elemental constitution of WO₃ nanoparticles are found to have atomic percentage 76 of W and 23 of O which confirms the formation of WO₃ nanoparticles. The PL intensity of the Cd-doped sample was significantly higher than that of undoped WO₃.

Keywords: Nanoparticles, FTIR, FESEM, EDAX

PP 32

**SYNTHESIS, SPECTRAL CHARACTERIZATION AND BIOLOGICAL
ACTIVITIES OF METAL (II) COMPLEX FROM MANNICH BASE LIGAND**

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Abstract

New Mannich base was synthesized from nicotinamide, formaldehyde and morpholine. And its metal(II) complexes were synthesized from prepared Mannich base ligand. The prepared ligand and its metal(II) complexes have been characterized by diverse spectral and analytical techniques. These results show that metal(II) complexes have square planar geometry. Moreover, the prepared ligand and its metal(II) complexes were tested against some microorganisms for their antimicrobial activity.

Key words: Mannich base; metal(II) complexes; spectroscopic; antimicrobial study

PP 33

A HIGHLY SELECTIVE AND SENSITIVE COLORIMETRIC AND FLUORESCENT TRIAZOLE SENSOR FOR Ni(II) ION

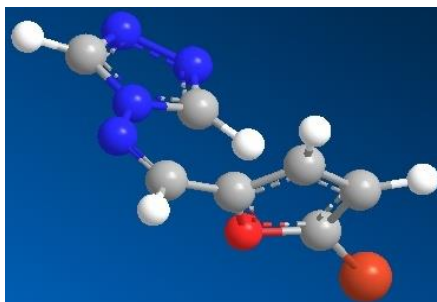
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Abstract

A novel and selective colorimetric and fluorescent triazole sensor for Ni²⁺ ion was synthesized by conventional method. In order to broaden the scope and to expose the novelty in the field of sensing, a novel fluorophore was synthesized using 5-bromo-2-furaldehyde and 4-amino-1,2,4-triazole. It was characterized using FT-IR, ¹H NMR and ESI-MS studies. There was no significant spectral changes were observed in the presence of other competing metal ions for the receptor indicating that the UV-Vis spectral response of probe is highly specific and selective detection of Ni²⁺. The obtained photo-physical changes are due to the process of the ligand to metal charge transfers (LMCT) after addition of Ni²⁺ to the receptor. Absorbance at 420 nm from that of the receptor at 320 nm clearly confirms the selectivity towards Ni²⁺ which is also confirmed by the colour change from colourless to pale yellow.

Keywords: Ni²⁺ ion, colorimetric, Schiff base, triazole.



PP 34

**FACILE CONSTRUCTION ELECTROCHEMICAL SENSING OF ATENOLOL BY
SYNTHETIC POLYMERIC RECEPTOR**

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Abstract

Hypertension is a growing disease of medical concern. Tremendous increase in the use of antihypertensive medications such as beta-blockers points toward an increasing number of hypertension cases in last decade. 4-(2-hydroxy-3-isopropylaminopropoxy)phenylacetamide, commercially known as atenolol, a beta-adrenoreceptor blocking agent, is used as an antihypertensive drug. In this present work, the Atenolol imprinted polypyrrole polymer thin film on glassy carbon electrode (GCE) was used for the electrochemical sensor for atenolol. Molecular imprinting allows the creation of artificial recognition sites in synthetic polymer. These sites are tailor-made in-situ by electro-polymerization of functional monomer around the template molecules. The electrochemical response of atenolol on the imprinted electrode was determined using differential pulse voltammetry. The dynamic range for the atenolol determination was found to be 10^{-3} M to 10^{-8} M. The LOD is found to be 10^{-8} M. These results show that the proposed sensor can be applicable to clinical analysis, quality control and a routine determination of Atenolol in pharmaceutical formulations.

Keywords; Molecularly Imprinted Polymers, Atenolol, voltammetry.

PP 35

**OF A SUPRAMOLECULAR ORGANIC FRAMEWORK USING NAPHTHYL
VIOLOGEN GUESTS AND CB[8] HOST VIA CHARGE-TRANSFER
COMPLEXATION**

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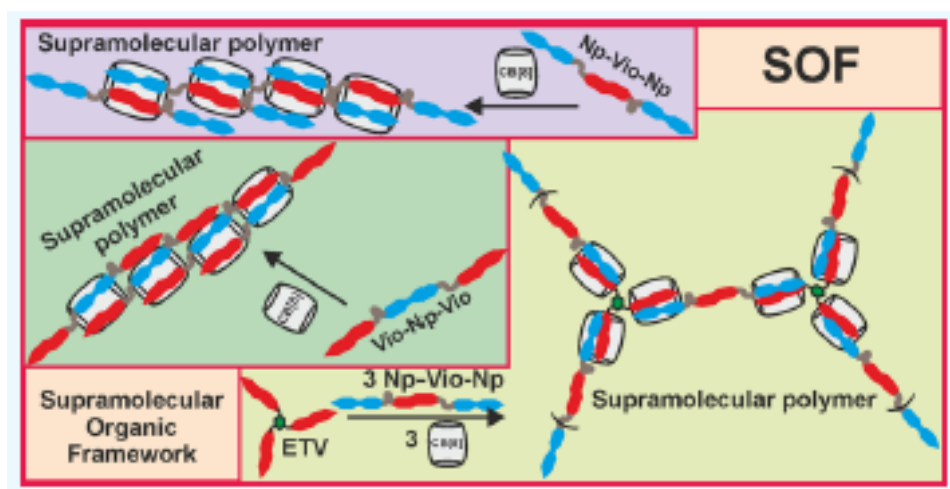
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Abstract

Herein, we report the synthesis of guest–host systems comprising naphthyl–viologen–naphthyl (Np–Vio–Np) and viologen–naphthyl–viologen (Vio–Np–Vio) guest molecules and their subsequent supramolecular polymerization in the presence of a CB[8] host in water.¹⁻² In addition, the guest complexation of ethyl-terminated trimeric viologen (ETV) with Np–Vio–Np and CB[8] was investigated. As a result of supramolecular interactions, 2D supramolecular organic frameworks with high internal periodicity were constructed. ¹H NMR studies clearly demonstrated the formation of a host-stabilized charge-transfer complex via folding back (Np–Vio–Np and Vio–Np–Vio) in the presence of CB[8]. In the case of ETV + Np–Vio–Np + CB[8], a large polymeric network was formed as indicated by the NMR titrations. UV–vis and fluorescence studies clearly confirm the formation of an inter/intra molecular CT complex upon complexation with cucurbit[8]uril. The size obtained using the dynamic light scattering (DLS) method pinpoints the formation of larger supramolecular aggregates in the order of μm through host–guest assembly, which is further complemented by FESEM and TEM. SAXS measurements indicate the formation of a 2D supramolecular polymer/polymer aggregate with longrange order.



Reference

- [1] Tian, J.; Chen, L.; Zhang, D.-W.; Liu, Y.; Li, Z.-T. *Chem. Commun.* 2016, 52, 6351–6362.
- [2] Zhang, C.-W.; Ou, B.; Jiang, S.-T.; Yin, G.-Q.; Chen, L.-J.; Xu, L.; Li, X.; Yang, . *Polym. Chem.* 2018, 9, 2021–2030.

PP 36

**FIRST PRINCIPLES CALCULATIONS OF THE PHASE STABILITY OF
RUTILE SnO₂**

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Abstract

In this work, we have performed the first principles calculation of rutile SnO₂ through density functional theory using GGA approximation of pseudo potentials for determining the crystal structures, bulk moduli, relative stability and cohesive energy. The calculated ground state properties such as equilibrium lattice constants and bulk modulus of rutile were found to be in agreement with the experimental data. Also the band structure, band gap and density of states of the rutile phase were identified. Further the phonon dispersion relations are realized by performing the lattice dynamic calculations. In addition, by fitting the pressure – volume data to the third order Birch - Murnaghan equation of state, the mechanical stability of the SnO₂ rutile phase has also been analyzed in detail. All of the above theoretical predictions agree well with experimental values.

Keywords: Rutile-SnO₂, Phonon, Lattice dynamics, BM-equation.

PP 37

**THERMAL STUDIES OF CYCLOHEXANE, SULFONE AND MALEIMIDE
CONTAINING POLYBENZOXAZINE HYBRID MATRICES**

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Abstract

The different types of bi-functional hybrid polybenzoxazine matrices were prepared via in-situ polymerization using skeletal modified functionalities namely Cyclohexane (PCBs), Sulfone (PSBs), and Maleimidophenyl (PBMPBs) benzoxazines. The thermal properties of the skeletal modified polybenzoxazines have been studied and compared with each other. The glass transition temperature, curing behavior, thermal stability, char yield and flame resistance of the hybrid polymer matrices were analyzed using DSC and TGA. The influence of amines with different substituent groups on thermal properties has also been studied. The DSC results showed that the onset temperature of the exotherm for curing the PSBs matrices was higher when compared to that of PCBs and PBMPBs matrix systems. The nature and reactivity of bi-functional amines made significant changes in the curing of polybenzoxazine hybrid matrices. The enhancement in the char yield of PBMPBs is due to the presence of high char forming maleimidophenyl groups in PBMPBs which implies the good thermal stability and flame resistance.

Keywords: Cyclohexane, Sulfone, Maleimide, Curing, Char yield, Thermal Stability and Flame resistance.

PP 38

PHOSPHORUS AND SILICON CONTAINING POLYBENZOXAZINE HYBRID MATRICES: THERMAL AND MORPHOLOGICAL PROPERTIES

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Abstract

The Phosphorous (BHPPB and BHPPOB) and Silicon diol (BHDPSB and BHDMSB) benzoxazines were synthesized and their hybrid polymer matrices were developed via in-situ polymerization. Thermal properties such as glass transition temperature, curing behavior, thermal stability were analyzed using DSC and TGA. The char yield and flame

resistance of the hybrid matrices were studied by LOI. The effect and influence of Phosphorous and Silicon diol chemical structures in the thermal properties of the hybrid polymer matrices have been studied. The phosphorus (PBHPPB and PBHPPOB) containing polybenzoxazine matrix systems exhibit higher values of T_g and curing temperatures than those of silicon (PBHDPSB and PBHDMSB) containing polybenzoxazines. The silicon (PBHDPSB and PBHDMSB) containing polybenzoxazine matrix systems retard the degradation temperatures. The incorporation of phosphine oxide and silicon groups in the benzoxazine moiety enhances the char yield and flame retardant behaviour significantly. The homogeneous structure of the hybrid polybenzoxazine matrices was determined by SEM and visual observations.

Key words: Phosphorous diol, Silicon diol, Matrices, Char yield, Thermal Stability, Flame retardance and Morphology.

PP 39

GREEN SYNTHESIS OF IRON OXIDE NANOPARTICLES USING *AVICENNIA MARINA* LEAF EXTRACT

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Abstract

The field of nanoscience is evergreen technology it playing enduring responsibility in the environmental concern. The misconception is the significant part of nano technology. By the way people are preferring bio and greener synthesis and technology for our goods. As we synthesised Iron oxide nanoparticles by mangroves leaves and in recent years researchers approaches the eco friendly, simple, sustainable and cost effective green chemistry methods for synthesizing materials rather than toxic chemical methodology. This research work accounts a safe synthesis of iron oxide using leaf extract of *Avicennia marina*. The UV – Visible absorption spectrum of iron oxide nano particles solution displayed peak at 295 and 301 nm. As identified by FTIR spectroscopy, the stretching vibrations at 3354 cm^{-1} , 610 cm^{-1} . The morphological study was explored by atomic force microscopy. The average size of NPs was determined by FESEM and the range of size is 30 to 100nm. The grain size was

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studied by XRD. The highlight of the articles thinks likely the dye degradation, environment pollution control, Industrial application, tissue curing, sensors, catalysts, electronics, etc...

Keywords: Green synthesis, Avicennia marina, UV, FTIR, AFM, XRD, FESEM.

PP 40

FABRICATION OF SILICA PARTICLES CONNECTED ONTO THE CELLULOSE NANOFIBRE/POLYLACTIC ACID NANOCOMPOSITE FOR BETTER THERMAL AND MECHANICAL PROPERTIES

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Abstract

In the present study, silica nanoparticles connected onto the cellulose nanofibre/polylactic acid (silica-CNF/PLA) nanocomposites were fabricated by using melt mixture method. The respective functional groups and crystalline behaviors of nanocomposites were characterized and confirmed by Fourier transform infrared spectroscopy (FT-IR) and X-ray diffraction (XRD) analysis. The morphological nanostructures of cellulose nanofibre and silica nanoparticles are well dispersion onto the PLA matrix were evidenced by Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). The melting and cooling effects of nanocomposites were analyzed by Differential Scanning Colorimetry (DSC). The influence of silica particles connected onto the cellulose nanofibre/PLA nanocomposites were higher thermal stability and mechanical behavior compared to CNF/PLA and PLA. Thus, the nanocomposites are due to the increased interfacial interactions between Silica-CNF and PLA matrix through the hydrogen bonding formation.

PP 41

FABRICATION OF CUPRIC OXIDE DECORATED B-CYCLODEXTRIN NANOCOMPOSITE IMMOBILIZED NAFION AS A HIGH PERFORMANCE ELECTROCHEMICAL SENSOR FOR L-TYROSINE DETECTION

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Abstract

In the present work, a novel cupric oxide decorated on β -cyclodextrin (CuO/ β -CD) nanocomposite was synthesized by sonochemical method. The CuO/ β -CD nanocomposites were characterized by UV-vis, Raman, FT-IR, FE-SEM, mapping analysis, XRD techniques. Fascinatingly, the CuO/ β -CD nanocomposite Nafion (Nf) immobilized modified glassy carbon electrode (CuO/ β -CD/Nf/GCE) has exhibited a superior electrocatalytic activity towards the L-tyrosine, when compared to the modified β -CD, CuO, and bare GCE electrodes. Besides, the electrochemical sensing performance was revealed as an excellent amperometric *i-t* current response for the L-tyrosine determination with a wide linear range from 0.01 to 100 μ M, high sensitivity 442 μ A μ M⁻¹cm² and low detection limit (LOD) 0.0082 μ M. Furthermore, it manifested a good selectivity, repeatability, stability, and reproducibility. In addition, the CuO/ β -CD/Nf modified GCE electrode shows good sensibleness for the L-tyrosine detection of blood serum, food samples, and urine samples.

Keywords: Electrochemical sensor; L-tyrosine; glassy carbon electrode; low detection limit; sensitivity.



**JACOBSEN CATALYST DRIVEN FRIEDEL-CRAFTS INTRAMOLECULAR
CYCLIZATION OF INERT TERMINAL ALKENES: SYNTHESIS OF 1H-INDENE
DERIVATIVES FROM BAYLIS-HILLMAN ADDUCTS**

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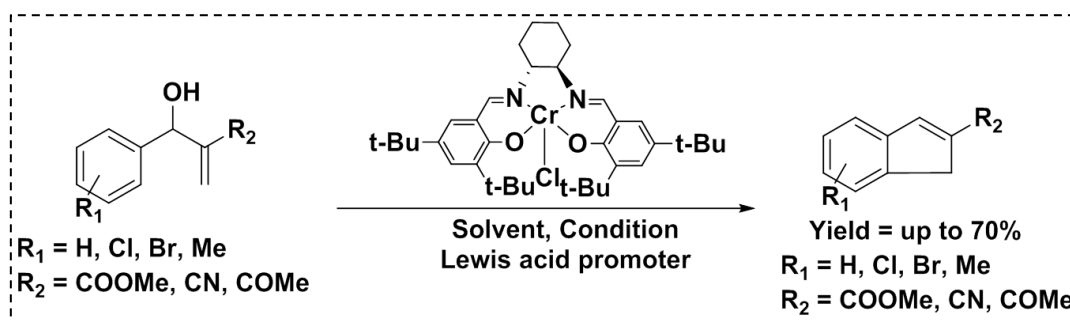
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Abstract

The core structure of indene is an important building block for variety of medicinal drugs and natural products.¹⁻² Therefore search for new synthetic methodologies with atom economy and efficiency are of great interest among synthetic chemists. Interestingly the Baylis-Hillman adducts are powerful synthons due to their diverse and attractive functional groups.³ Though few research groups have utilized BH adducts as synthons for synthesis of indene, conversely their structural restrictions on adducts limits their usage.⁴⁻⁵ Therefore we report a generalized methodology for synthesis of indene from Baylis-Hillman adducts catalysed by Jacobsen chromium catalyst in presence of a promoter.



Scheme 1: Jacobsen chromium catalyzed synthesis of 1H-indene derivatives from BH adducts

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**MOLYBDENUM DISULFIDE NANOSHEETS - CHITOSAN HYBRID
COMPOSITES HIGH PERFORMANCE FOR ANTIBACTERIAL AND
ANTICANCER ACTIVITY**

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Abstract

Cancer is an abnormal growth of tissue or cells. It causes significant morbidity and mortality and is a major health problem worldwide, increasing demands for anticancer therapy. So, conventional methods require the combination of controlled released technology and targeted drug delivery which is more effective and less harmful. Nanomaterials are expected hopefully to revolutionize cancer diagnosis and therapy. Thus developing novel anticancer materials is an urgent need. Herein, chitosan-MoS₂ (CS-MoS₂) nanocomposite was synthesized chemical modification and simple hydrothermal method to achieve more efficient antibacterial and anticancer activity. XRD shows that the strong four intense peaks indicate crystalline nature of composites. Morphology of hybrid composites analyzed by TEM shows that they are mostly nanosheets in shape with size ranging from 6 to 13 nm, the elemental mapping the presence of Mo, S, and C in the synthesized composites. FTIR and Raman reveal the active functional groups in the culture supernatant interaction with MoS₂ composites. CS-MoS₂ exhibited synergistic remarkable capability against Gram-positive *Staphylococcus aureus* (*S. aureus*) and Gram-negative *Escherichia coli* (*E. coli*), where bacterial inhibitions were significantly increased. As a result synthesized stable (CS-MoS₂) show more significant anticancer activity against (MCF-7) cells at 100 µg/ml concentrations of composites. A mechanism study revealed that the positively charged CS-MoS₂ could interact with cell membrane, and then cause damage to the membrane and cellular constituents by generation of reactive oxygen species (ROS). Finally inhibit cancer growth. The CS-MoS₂ could be an attractive antibacterial and anticancer agent with improved efficiency and provide more strategies for application of MoS₂.

Keywords: Chitosan, MoS₂, Nanosheets, Antibacterial, Anticancer

PP 44

PHYSICAL AND ELECTROCHEMICAL CHARACTERIZATION OF PULSE CURRENT ELECTRODEPOSITED Ni-TiN NANOCOMPOSITE COATINGS

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Abstract

The expansion of current machinery requires metallic materials with better surface properties. Acetate-based baths are environmental friendly compared to other baths [1, 2]. In the present investigation, TiN reinforced nickel composite coatings were deposited on a mild steel substrate using pulse current electrodeposition process employing a nickel acetate bath. Surface morphology, microstructure and crystal orientation of the Ni and Ni – TiN nanocomposites were investigated by SEM and X-ray diffraction analysis respectively. Smooth composite deposits containing uniformly distributed Titanium nitride particles were obtained. The crystal grains on the surface of Ni– TiN composite coating are compact. The preferred growth process of the nickel matrix in crystallographic directions <111>, <200> and <220> is strongly influenced at a concentration of 9 g/l. The structure of electrodeposited nickel and nickel nanocomposite coatings were fcc. It was confirmed from ICDD- JCPDS standards [87-0712]. The effect of incorporation is maximum at a current density of 8 A/dm². The microhardness values of the Ni- TiN nanocomposite coatings (840HV) were higher than that of pure nickel (310HV) due to dispersion-strengthening; matrix grain refining and increased with the increase of incorporated TiN particles content [3]. The corrosion potential (E_{corr}) in the case of Ni- TiN nanocomposite coatings had shown a negative shift, confirming the cathodic protective nature of the coatings [4]. The corrosion rates of Ni- TiN nanocomposite coatings (1.45milliinch/yr) were lower than that of electrodeposited pure nickel coating (67.69milliinch/yr) in 3.5% NaCl solution. The charge transfer resistance (R_{ct}) values for Ni- TiN nanocomposite coatings were increased with increased TiN content in the composite coatings due to the distribution of relaxation times.

Keywords: Electrodeposition, Nanocomposite coating, XRD, SEM, Micro hardness.

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PP 45

SYNTHESIS AND CHARACTERIZATION OF TITANIUM DOPED ZINC SULPHIDE NANOPARTICLES FOR CORROSIVE RESISTANT APPLICATION

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Abstract

Ti doped ZnS nanoparticles have been synthesised by chemical co-precipitation method. It is a simple and low cost method to prepared nanoparticles. The prepared samples were characterised by using UV-Vis, FTIR spectroscopy, Scanning Electron Microscope (SEM) with EDAX spectroscopy. Synthesised nanoparticles also characterized by Photoluminescence and electrochemical studies. The peak at 605.61 cm^{-1} is assigned to the ZnS band. The band at 491.81 cm^{-1} is assigned to the metal-metal (Zn-Ti) bond. FTIR spectrum is applicable to confirm the presence of constituents qualitatively or quantitatively. The SEM images exhibit the crystalline size of ZnS nanoparticles, Titanium doped Zinc Sulphide nanoparticles also in nanometer range. The elemental constitution of Zinc Sulphide nanoparticles are found to have atomic percentage 82 of Zn and 16 of S which confirms the formation of ZnS nanoparticles. Excitation wavelength of 348nm and 340nm gave maximum intensity for ZnS and Ti doped ZnS nanoparticle. This has important implications in corrosive applications and other photonic devices. The percentage of inhibition increase for the doped ZnS nanoparticles compared to the undoped ZnS nano particles. This is clearly confirms the anti corrosive activity of synthesized doped nanoparticles.

Keywords: Nanoparticles, Titanium, Zinc sulphide, SEM

PP 46

**EFFECT OF SOIL COPPER ON ROOT OF *RHIZOPHORA ANNAMALAYANA*
UNDER WASTEWATER TREATMENT**

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Abstract

Seedlings of *Rhizophora annamalayana* were raised in the soil, incorporated with copper at the doses of 50, 100, 200 mg. kg⁻¹ soil, irrigated with normal wastewater. Control seedlings were maintained only with wastewater without any incorporation of Cu in the soil. After 60 days of experiment, the roots were analysed for the plant growth parameters, root anatomy, porosity and radical oxygen loss. Heavy metal toxicity in *Rhizophora annamalayana* to copper at higher doses of Cu reduced the plant growth. Higher doses of Cu reduced radical oxygen loss and porosity in roots. Higher doses of Cu increased lignifications of root cells. This lignifications of root cells, with reduced permeability and loss of radical oxygen led to the tolerance of the mangrove species to Cu toxicity. The root of the mangrove seedlings plays an important role in resistance of heavy metal toxicity. Future research is needed to understand how ROL from the roots of mangrove plants regulate the dynamic of Cu in the rhizosphere soil.

PP 47

**“CLICKABLE” BLOCK COPOLYMER SURFACTANTS FOR THE SYNTHESIS
OF COLOR RESILIENT LATEX**

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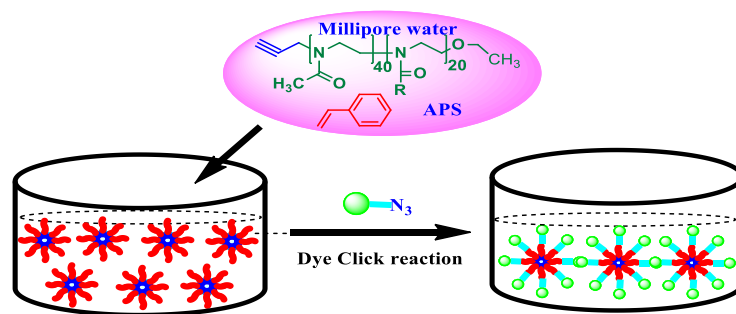
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Abstract

Two different poly(2-oxazolines) block copolymers with methyl, propyl and butyl pendants were synthesized by living Cationic Ring Opening Polymerization (CROP) method.¹ The hydrophobic and hydrophilic segments in copolymer was designed to match the HLB.² So that it can

self-assemble in aqueous solution into micelle. Block copolymers were characterized using FT-IR and NMR. The critical micelle concentration (CMC) of the prepared block copolymer was estimated by using UV-Visible spectroscopy with iodine as non-intrusive probe.³ The block copolymers that showed clear breakpoint in CMC measurements are used as nonionic surfactant in the emulsion polymerization.⁴ A series of polystyrene latexes were synthesized by using different block copolymer surfactant and while maintaining the styrene content. The prepared latex were stable, which are subsequently dried in oven. Azide-alkyne “click” reaction was carried out with the dried white powder with azide dye and subsequently the coloured powder latex was redispersed in water. The size of as prepared latex and coloured latex particles were determined by (DLS) dynamic light scattering. The particles sizes are in the range of 500 nm and redispersed coloured latexes are also of comparable size as that of the original latex.



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PP 48

MESO-SUBSTITUTED PORPHYRINS FOR BOTTOM-GATED OFETs BY SOLUTION PROCESSING TECHNIQUE

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Abstract

Over the last decade, tremendous progress has been achieved in the design and fabrication of OFET devices for applications such as sensors, displays, radiofrequency identification tags (RFIDs) etc. In Organic electronics porphyrins are one of the most important π -conjugated planar molecules. Porphyrins can be employed as active layers in OFETs and OSCs due to their versatile structural and photophysical properties. In the present investigation, a series of *meso*-substituted free base and zinc porphyrins were designed and synthesized to explore their electronic properties. All the synthesized molecules possess high decomposition temperature which ensures the life time and durability of devices. From the absorption onset values, optical band gaps were calculated. Free base porphyrin molecules gave strong absorption λ_{max} values at around 405 nm (ϵ : $361 \times 10^3 \text{ M}^{-1} \text{ cm}^{-1}$) with Stoke's shift value of 240 nm whereas, the zinc porphyrins exhibited red shift. These molecules possess low barrier to charge carrier injection with a high HOMO value of -5.304 eV. The band gap 2.5 eV certifies the potential application of these porphyrins in various electronic applications. OFET devices with bottom gate top contact architecture will be fabricated by spin coating method. The surface morphology will be characterized by XRD, SEM, and AFM. The results ensure that these molecules can be efficient hole transporting materials.

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PP 49

SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL STUDIES OF Ov(IV) & Bi(III) METAL COMPLEXES

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Abstract

V(L1), V(L2), Bi(L1), Bi(L2) Schiff base vanadium and bismuth metal complexes are prepared by using the synthesized ligands as L1-[N,N'-bis(2-hydroxynaphthalidene)benzidine] and L2-[N,N'-bis(O-vanillin)benzidine]. These compounds were characterized using FT-IR, UV-Visible, H-NMR and Mass Spectroscopy. Emission Spectral studies show Bi(L2) complex has the highest emission intensity. Antimicrobial activities give the maximum inhibition zone level in *P. aeruginosa*, *S. aureus*, *E. coli* and *B. subtilis* bacterial culture medium for V(L1) complex. All prepared compounds show maximum inhibition zone in the range in *C. albicans* fungal culture medium. Antioxidant activity of the metal complexes with the decreasing order of Bi(L2) > V(L2) > V(L1) > Bi(L1). Among the four metal complexes V(L2) give the highest anti-diabetic inhibition % value.

Keywords: Schiff's base, Antimicrobial study, Anti-diabetic study.

PP 50

SYNTHESIS, CHARACTERIZATION, DNA-BINDING AND BIOLOGICAL STUDIES OF SURFACTANT COBALT(III)-IP-DODECYLAMINE COMPLEXES

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Abstract

The mixed ligand surfactant cobalt(III)-IP complexes of the type *cis*-[Co(IP)₂(DA)Cl](ClO₄)₂, *cis*-[Co(IP)₂(DA)₂](ClO₄)₃ (IP = imidaso[4,5-f][1,10]phenanthroline, DA = Dodecylamine) were synthesized and characterized by elemental analysis, IR and NMR studies. The critical micelle concentration (CMC) values of these complexes in aqueous solution were obtained from conductance measurements. The specific conductivity data (at 303, 308 and 313 K) served for the evaluation of the temperature dependent CMC and the thermodynamics of micellization (ΔG^0_{mic} , ΔH^0_{mic} , ΔS^0_{mic}). The interaction between

metallo surfactant cobalt(III)-IP complexes and calf thymus DNA in aqueous solution was investigated by spectroscopic methods and viscosity measurements. Results suggest that the complexes bind to DNA via intercalation binding. The cytotoxicity of the metallo surfactant Cobalt(III)-IP complexes has been evaluated by MTT assay. Metallo surfactant Cobalt(III)-IP complexes were tested for antibacterial and antifungal activities having good activities.

PP 51

SYNTHESIS OF 10-HYDROXY-11H-BENZO[B]FLUORENE-11-ONES AND 6-HYDROXY-7H-BENZO[DE] ANTHRACENES-7-ONES VIA DOMINO FRIES-SCHOLL REACTION

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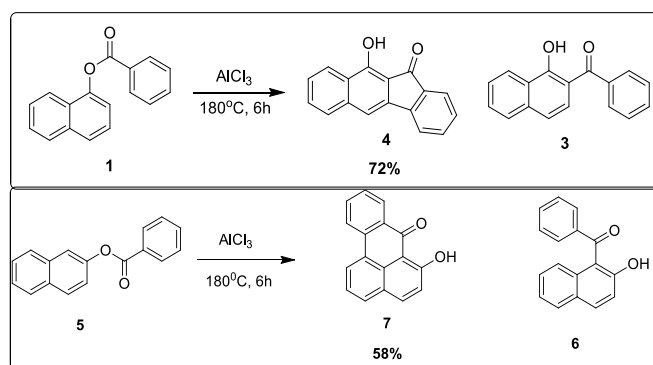
Abstract

The intramolecular cyclisation reaction of arene-tethered nucleophiles reported by Bunnet¹ and Huisgen was successfully employed for the synthesis of benzo-fused heterocycles such as indoline, indole, phenothiazine, benzoxazoles xanthenes and benzothiazoles by using tethered nitrogen, oxygen, sulfur nucleophiles². The typical oxidative aromatic coupling of electron rich aromatic compounds such as phenols and aryl-aryl ethers leads to the formation of one or more carbon-carbon single bonds³. Studies on such C-C bond forming reactions, mediated by both a strong Lewis acid at higher temperature and mild oxidant, has received attention in recent years. Fries rearrangement of 1-naphthyl benzoate **1** in neat condition, using AlCl₃ at 120 °C yielded the 2-benzoyl-1-naphthol **2** in 47% yield along with 4-benzoyl-1-naphthol **3** isomer in 1:1 ratio. Our study began with the screening of the reaction conditions for a domino transformation of 1-naphthylbenzoates to 10-hydroxy-11H-benzo[b]-fluorene-11ones via a Fries rearrangement followed by a Scholl cyclisation in one pot, using Lewis acid (AlCl₃, FeCl₃, TFA and Triflic acid). It was observed that when the AlCl₃ catalyzed Fries rearrangement of 1-naphthyl benzoate, was performed at a higher temperature viz., 180 °C, the major product formed in 72% yield turned out to be the desired Fries-Scholl domino transformation product, viz., 10-hydroxy-11H-benzo[b]-fluorene-11-one **4**. The product of Fries rearrangement, viz., 2-benzoyl-1-naphthol **2** was

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formed only in minor amount (15%). We did not isolate any 4-benzoyl-1-naphthol **3** in this domino reaction. This domino Fries-Scholl transformation was generalized in a few other 1-naphthylbenzoates. Domino Fries-Scholl cyclisation of 2-naphthyl benzoate **5** led to the formation of expected 6-hydroxy-7H-benzo[c]fluoren-7-one **7** from in 58% presumably through the intermediacy of Fries product, viz., 1-benzoyl-2-naphthol **6**. The details of synthesis and characterization of hydroxyl benzofluorenones and its derivatives will be discussed.

Domino Fries-Scholl cyclisation



Reference

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PP 52

MICROWAVE ASSISTED SYNTHESIS OF FLUORESCENT NITROGEN DOPED CARBON QUANTUM DOTS FOR A SELECTIVE SENSING OF MERCURY(II) IONS

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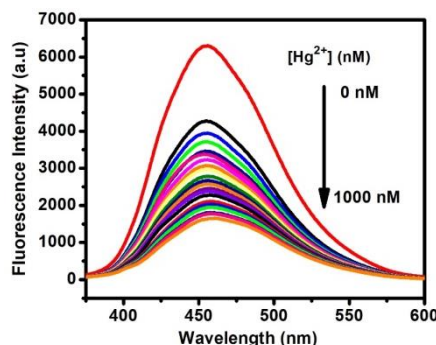
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Abstract

A facile and microwave method was developed for the preparation of highly fluorescent nitrogen-doped carbon dots (N-CQDs). Compared with previous methods, the proposed method is performed at comparatively lower temperature and result in a 20-30 nm

size [1]. The prepared materials were characterized by XRD, FT-IR, UV-Visible spectroscopy, TEM, and Fluorescence spectroscopy. As obtained N-CQDs show a strong emission 455 nm with an optimum excitation at 365 nm, and exhibit high photostability. Because of the Hg^{2+} induced fluorescence quenching of carbon dots (N-CQDs), such N-CQDs can be used as an effective fluorescent probe for highly selective and sensitive detection of Hg^{2+} in aqueous solution. The N-CQDs showed highly selectivity and sensitivity for Hg^{2+} ion rather than other competitive metal ions such as (Al^{3+} , Ba^{2+} , Ca^{2+} , Cd^{2+} , Cr^{2+} , Cu^{2+} , Fe^{2+} , Fe^{3+} , Hg^{2+} , K^+ , Li^+ , Mg^{2+} , Mn^{2+} , Na^+ , Ni^{2+} , Pb^{2+} and Zn^{2+}). During the fluorometric titration the fluorescence emission at 455 nm gradually decreases [2]. Thus the fluorescence studies of the N-CQDs in the presence of Hg^{2+} revealed that the mechanism of quenching involves complexation and the dynamic quenching dominates over static quenching [3].



FL emission intensity of N-CQDs- Hg^{2+} system at 455 nm as a function of Hg^{2+} ion concentration

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PP 53

IONIC LIDUID MEDIATED SYNTHESIS AND CHARACTERIZATION OF ZnO NPs BY LEUCAS ASPERA LEAVES EXTRACT WITH ENHANCED PHOTOCATALYTIC AND BIOMEDICAL APPLICATIONS

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Abstract

Green synthetic approach has a prominent role as it sounds eco-friendly, cost-effective and safe. Various biological means present in the plant extract act as reducing and stabilizing agents and are used for the synthesis of metal nanoparticles. The *Leucas aspera* leaves extract used for synthesis of ZnO NPs assisted with ionic liquid by hydrothermal method. The synthesized nanoparticles was characterized by different characteristic techniques such as XRD, UV-Visible, FT - IR spectroscopy, SEM with EDX and TEM. Scanning electron microscopy has been used to study the morphology and size distribution of the synthesized particles. XRD results revealed the formation of hexagonal wurtzite structure, chemical bond formations of zinc oxide NPs were confirmed by FT-IR analyses, and SEM analyses showed spherical shape with the average size range of minimum (12 -32) nm for the synthesized nanoparticles by zinc acetate and zinc nitrate respectively. EDX analyses confirmed the presence of primarily zinc and oxygen. The synthesized ZnO NPs were found to be potential remedies in various fields of studies for its photo catalytic and biomedical applications etc.

PP 54

ADSORPTION AND ELECTROCHEMICAL STUDIES OF P-TOLYLSULFOXIDE FOR OIL PIPELINE IN 1.0 N HCl

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Abstract

The inhibitive effect of p-Tolylsulfoxide extract on oil pipeline corrosion in 1.0N HCl solution was studied using gravimetric method and electro chemical techniques. Observed result indicates that the corrosion inhibition efficiency was increased with increase of inhibitor concentration and decreased gradually with rise in temperature. The highest inhibition efficiency of 97.13% was observed with 1000ppm of plant extract in acidic
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medium in 303K. The corrosion current (I_{corr}) decreased with increase of inhibitor concentration (from 180.5 to 14.95 mA/cm²) studied by potentiodynamic polarisation. By using impedance spectroscopy the charge transfer Resistance (R_{ct}) value increased from 24.96 to 171 Ω cm². This results very good agreement with the previous result. Thermodynamic parameters (viz; E_a , Q_{ads} , ΔH_{ads} , ΔG_{ads} , ΔS_{ads}) were evaluated for corrosion process, which is also suggested that the adsorption is exothermic, spontaneous and Physisorptions. The inhibitor follows Langmuir adsorption isotherm.

Keywords: Acid, p-Tolylsulfoxide, oil pipeline, Weight loss, Polarization, Impedance spectra.

PP 55

DESIGN AND SYNTHESIS OF PIPERAZINE-PIPERIDONE H37Rv INHIBITORS WITH IMPROVED PHARMACOKINETIC PROFILES

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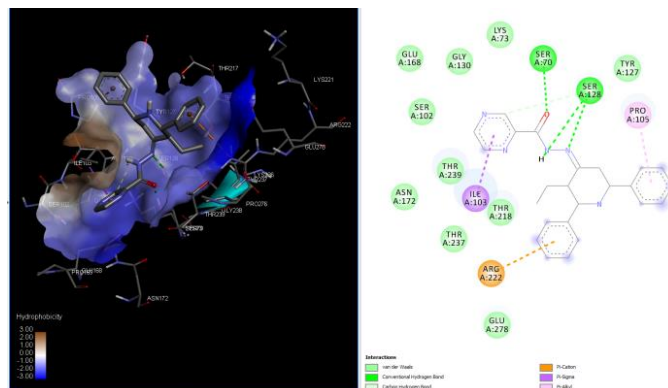
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Abstract

New series of 2,6-diarylpiperidone incorporating piperazine scaffolds in a single molecular framework has been reported. The structures of the synthesized derivatives were assigned by IR and NMR spectral techniques. The hybrid compounds were evaluated for their antitubercular activity. Most of the synthesized compounds showed significant activity against Mycobacterium tuberculosis H37Rv strain in comparison to isoniazide. . In addition, molecular docking study was utilized to explore the binding mode of the synthesized compounds to the target enzyme InhA. The results showed reasonable binding interactions of synthesized molecules and good dock score. Molecular dynamics studies were performed in order to support the docking results. The compound-InhA complex was found to be more stable and exhibited more interaction when compared to Triclosan. The compounds followed Lipinski rule of five and displayed acceptable pharmacokinetic properties depicted via in silico studies.

Keywords: Docking, Conformation, Anti-TB, Hydrazone, Piperidin-4-ones, pharmacokinetic



PP 56

**SYNTHESIS, SPECTROSCOPIC INVESTIGATION AND DFT STUDY OF
4-((4-FLUOROPHENYL)DIAZENYL)-2-FORMYLPHENYL METHYL
CARBONATE**

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Abstract

4-((4-fluorophenyl)diazenyl)-2-formylphenyl methyl carbonate (FFPMC) has been synthesized from 5-((4-fluorophenyl)diazenyl)-2-hydroxybenzaldehyde (FPDB) and methyl chloroformate. Theoretical studies such as polarizability, first order hyperpolarizability, zero-point vibrational energy and natural bonding orbital (NBO) analysis were carried out for the title compound using Hartree-Fock (HF) and Density Functional Theory (DFT) methods with 6-31+G(d,p) basis set. Also, the molecular structure, vibrational frequencies, dipole moment and molecular electrostatic potential energies have been calculated. The comparison in between the experimental and the theoretical values of FT-IR, FT-Raman vibrational spectra and NMR (¹H and ¹³C) have also been discussed.

Keywords: Methyl carbonate, Hyperpolarizability, DFT, HOMO-LUMO, NBO.

PP 57

**MN(II) COMPLEX CONTAINING 1,3 β-DIKETONE AND/OR ANCILLARY
PYRAZOLYL LIGAND**

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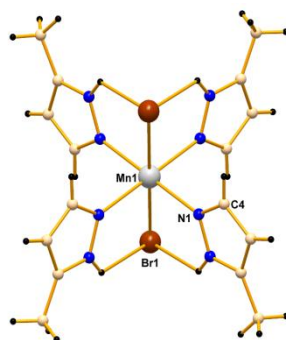
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Abstract

Like NO and H₂S, CO is an important signalling molecule in mammals, especially in the cardiovascular system. Since CO is a virulent gas at normal temperature, it is not easy to control its dose in clinical application. Carbon monoxide releasing molecules (CORMs) is a potential substitute for CO gas, antihypertensive, anti-inflammatory and cell-protective effects.¹ Controlled delivery of CO is best achieved using ‘CORMs’, molecules which release known amounts of carbon monoxide (concentration range up to 300 ppm) in response to a stimulus.² Mn based CORMs are low toxicity and water soluble than other CORMs. [Mn Br₂(3MePz)₄] Complex have been synthesized from the reaction of [MnBr(CO)₅] and the Monodentate ligand as a 3 Methyl 1H Pyrazole (3-MePz).^{3,4} The resultant complex were characterized by single-crystal X-ray diffraction, IR Spectroscopy were region of CO stretching, ESI-Mass Spectroscopy, UV-Spectroscopy.

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PP 58

**MORPHOLOGY DIRECTED SYNTHESIS OF CADMIUM OXIDE
NANOMATERIALSBASED ON MODIFIED KIRKENDALL EFFECT**

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Abstract

Nanotechnology is the most emerging technology. It is the manipulation of matter on atomic and molecular scale. Cadmium oxide nanomaterials have different application based on their size, surface, optical properties, on their size, surface properties, optical and magnetic traits as doping materials in semiconductors, chemical sensors, magnetic storage media, gas sensors, superconducting materials, thermoelectric materials, sensing materials, antimicrobial agents, antifungal spectrum, wound healing activity etc. Thus a project was carried out to synthesize cadmium oxide nanomaterial (Nanotubes, Nanorods, Nanoparticles) by chemical precipitation method. The synthesized nanomaterials were characterized using XRD, UV-Vis spectroscopy and Emission spectroscopy.

Keywords: Nanomaterials, cadmium oxide, nanotubes, nanorods, nanoparticles characterization.

PP 59

**EFFECT OF SUBSTITUENTS ON THE ¹H - NMR CHEMICAL SHIFTS OF 6-(4'-
SUBSTITUTEDPHENYL)-4-METHYL-2-OXO-1, 2, 3, 6-
TETRAHYDROPYRIMIDINE-5-(N-PHENYL)CARBOXAMIDES**

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Abstract

6-4-(substituted-phenyl)-4-methyl-2-oxo-1,2,3,6-tetrahydropyrimidine-5-(N-phenyl) carboxamides have been prepared and characterized by ¹H NMR spectral analysis.

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Investigation of substituent's effect and mode of transmission of electronic effects have been carried out by ^1H NMR chemical shifts measurement and correlated it with LFER parameters in 6-(4-substituted-phenyl)-4-methyl-2-oxo-1,2,3,6-tetrahydropyrimidine-5-(N-phenyl) carboxamides

Keywords: ^1H NMR, 6-4-(substituted-phenyl)-4-methyl-2-oxo-1,2,3,6-tetrahydropyrimidine-5-(N-phenyl) carboxamides, substituent effects.

PP 60

ELECTROCHEMICAL DEGRADATION OF MORDANT BLUE 9 USING FLOW REACTOR

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Abstract

Electrochemical degradation of mordant blue-9 using flow recirculation reactor was investigated. The degradation process was operated at pH 7 and the different current density was applied to investigate the electrochemical degradation of mordant blue-9 in the presence of NaCl supporting electrolyte. The anode and the cathode potentials were studied at regular interval. Electrode potentials were found to be increased with increase of current density. The potentials observed were plotted with time and were found to be almost constant throughout the electrolysis time. Higher anode potential values showed the dye adsorption on the anodic surface. Absence of further increase in anodic potential showed the regeneration of anodic surface after dye degradation. The electro oxidations of dyes with different functional groups have been studied well using UV-Visible spectrometry.

Keywords: Textile Dye, Electro-degradation, Mordant blue 9

PP 61

**SYNTHESIS, GROWTH, STRUCTURE, SUPRAMOLECULAR ARCHITECTURE
AND HIRSHFELD SURFACE ANALYSIS OF CROWN ETHER
POLYOXOMOLYBDATE COMPLEX: NLO APPLICATIONS**

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Abstract

A novel supramolecular crown ether polyoxomolybdate complex, C₄₀H₈₀Mo₈N₄O₄₇ (TAM) was grown and crystallized by slow evaporation solution growth method at room temperature. Crystals of TAM are monoclinic, space group C2/c. The various functional groups present in the molecule were confirmed by FT-IR analysis. The crystalline nature and phase purity of the synthesized material was confirmed by powder XRD. Linear and nonlinear transmission characteristics of TAM were analyzed. Hirshfeld surfaces derived from X-ray diffraction analysis reveal a summary of molecular interactions and their relative contributions. Constructed supramolecular assembly by crown ether complex is described.

PP 62

**DEVELOPMENT OF ABUNDANT AND ACTIVE CATALYST HOST FOR
OXYGEN EVOLUTION REACTION IN ALKALINE MEDIUM**

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Abstract

Electrochemical/Photochemical water splitting (ECWS/PCWS) offers a way of storing of renewable energy as a chemical fuel (H₂) and easy generation of industrially important H₂ in higher pure form in pollution free manner. In the electrochemical water splitting process, 4e⁻ transfer oxygen evolution reaction (OER; 4OH⁻ → 2H₂O + O₂ + 4e⁻) on anode is energy intensive than compared to 2e⁻ transfer hydrogen evolution reaction (HER;

$2\text{H}_2\text{O} + 2\text{e}^- \rightarrow \text{H}_2$) on the cathode. Hence, ECWS process requires excessive overpotential (η) from the theoretical potential. An appropriate anodic and cathodic electrocatalysts was to minimise η and increase the efficiency of water splitting process such as IrO_2 , RuO_2 and Pt/C in acidic medium. Higher cost and lower in availability of precious metal catalysts minimize the wider commercialization of ECWS process. Development of low cost, active and efficient catalysts is crucial for the progressive commercialization of ECWS process. In the study, we have designed and developed abundant Fe based catalyst substrate and host for the OER by electrochemical treatment. Designed, developed catalyst and other counters physic-chemical and electrochemical characteristic were analysed systematically. The developed catalyst showed a lower η of 267 mV at 10 mA cm^{-2} with a Tafel slope of 66 mV dec^{-1} , and good stability in alkaline medium. The results suggest that reason beside catalytic characteristics of designed catalyst and counters, a possible way to utilize the proposed Fe based catalyst substrate as catalyst and as a host for OER.

PP 63

TERTIARY COMPOSITE MATERIAL USED FOR NANOFIBEROUS FORMATION IN BIOMEDICAL APPLICATION

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Abstract

In this most currently power full technique on synthesis of nanofibrous materials by electrospinning method. This work focused on the tertiary component based synthesis of nanofiber formation. Silk fibroin extracted from *Bombyx mori* silk cocoon are natural polymer materials as well as it consist of two protein (fibroin, sericin).The silk fibroin (SF) have been different amino acids (Gly-Aly-Ser). The tertiary composite materials are silk fibroin/metal oxide/ionic liquid used for nanofiber formation. Nanofiber (NF) is unique character because of high porosity, stability, large surface area to volume ratio and mechanical flexibility. In synthesis of nanofiber material for analyzed the several

characterizations of XRD, RAMAN, FTIR and XPS. The most observed fiber morphological shapes identify using FE-SEM with EDX and TEM analysis. The synthesized nanofiber material may be used for biomedical and electrochemical application.

Keywords: Nanofiber, Electrospinning, Silk fibroin, Metal oxide, Ionic liquid, Biomedical.

PP 64

**LYOTROPIC LIQUID CRYSTAL DIRECTED SYNTHESIS OF
ANISOTROPIC COPPER MICROPARTICLES AND THEIR APPLICATION
IN CATALYSIS**

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Abstract

A simple, room-temperature approach for the synthesis of stable microparticles of copper in a lyotropic liquid crystal (LLC) template is described. The LLC phase having a hexagonal ordering is prepared using a mixture of non-ionic surfactant triton-X 100 and water in the ratio of 40:60 wt%. A controlled growth of copper particles is achieved in this medium by reducing cupric chloride using hydrazine hydrate under basic condition without the aid of any external stabilizing agent. Monodisperse, platelet-like copper microparticles (size ~0.25 μm) are formed in this synthesis, which are well-dispersed in the lyotropic phase without aggregation. Besides, the copper particles are found to be stable for several months in the liquid crystalline medium. The LLC medium directed the growth of anisotropic microparticles and also acted as a stabilising agent. These micro platelets of copper are found to exhibit significant catalytic and electrocatalytic activity for the sodium borohydride mediated conversion of 4-nitrophenol to 4-aminophenol and for the reduction of hydrogen peroxide respectively.

Keywords: Lyotropic liquid crystal Hexagonal Copper microparticles Catalytic Electrochemical

PP 65

**ELECTROCHEMICAL PERFORMANCES OF SURFACE MODIFIED CePO₄-
COATED LiMn₂O₄ CATHODE MATERIALS FOR RECHARGEABLE LITHIUM
ION BATTERIES**

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Abstract

Improved electrochemical performances of Spinel LiMn₂O₄ cathode was prepared by a sol-gel coating of CePO₄ to the surface of the LiMn₂O₄ powder and subsequent heat treatment at 600 °C for 8 h in air. The surface modified LiMn₂O₄ cathode materials were characterized by using TG/DTA, X-ray diffraction, Scanning electron microscope, X-ray photoelectron spectroscope, cyclic voltammetry techniques and charge/discharge studies. XRD and SEM results show that no significant bulk structural differences are observed between the coated and pristine LiMn₂O₄. XPS data illustrated that, the CePO₄ was completely coated over the surface of the LiMn₂O₄ core materials. Galvanostatic charge/discharge studies of the uncoated and CePO₄-coated LiMn₂O₄ cathode materials were carried out in the voltage range between 3.0 and 4.5 V at elevated temperature. The composition of CePO₄ coating was increased from 0.0 to 3.0 Wt.%, the initial capacity of the samples decreased slightly. But the cycling stability was increased remarkably between 3-4.5 V. 2.0 Wt.% CePO₄-coated LiMn₂O₄ cathode has satisfied the structural stability, high reversible capacity and excellent electrochemical performances. This result indicates that, the surface treatment should be an effective way to improve the comprehensive properties of the cathode materials for lithium ion batteries.

Keywords: CePO₄-coated LiMn₂O₄, XRD, XPS, Charge/discharge

PP 66

SYNTHESIS OF PHOTO-RESPONSIVE POLYSILOXANE-BASED AZOBENZENE LIQUID CRYSTALLINE ELASTOMERS PREPARED BY HYDROSILATION REACTION

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Abstract

In this present work, a polysiloxane-based azobenzene containing liquid crystalline elastomers (LCEs) has been designed and synthesized via a hydrosilation reaction by grafting azobenzene based monomer and two different crosslinker onto polymethylhydrosiloxane (PMHS) backbone. The synthesized compound was characterized by fourier transformer infrared spectroscopy (FT - IR), nuclear magnetic resonance spectroscopy (NMR), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), polarizing optical microscopy (POM), X-ray diffraction (XRD), and UV-visible spectroscopy (UV - vis). The photoisomerization effect of monomer and LCEs is reported, they revealed the photoisomerization effect in solution. In solution, the trans – cis and cis – trans isomerization occurred around 240-250sec and 730-750sec respectively. Interestingly the variation in back relaxation is due to nature of the spacers involved in the system. Moreover as we increase the aromatic ring on spacer, there is increase in mesophase range also observed in these LCEs. The synthesized LCEs are expected to be more useful in optical devices.

PP 67

GREEN APPROACH FOR SYNTHESIS OF Yb₂O₃ NANOPARTICLES BY COUROUPITA GUIANENSIS ABUL LEAVES EXTRACT AND BIOMEDICAL APPLICATIONS

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Abstract

Green approach with 1- Butyl 3- Methyl imidazolium hexafluorophosphate Ionic liquid assisted rare earth Ytterbium oxide (Yb_2O_3) nanoparticles using *Couroupita guianensis abul* (*C.guianensis abul*) leaves extract by hydrothermal method. The crystallinity, particle size and morphology of the IL assisted Yb_2O_3 NPs were studied by various properties such as structural, spectral, optical and biological studies. From the powder X-ray diffraction studies confirmed that the Yb_2O_3 NPs belongs to cubic crystal system and the high intensity peaks were indexed. The chemical elements and states on the synthesized Yb_2O_3 NPs were identified by X-ray photoelectron spectroscopy and energy dispersive X-ray spectroscopy. The various functional groups such as Yb - O and COO^- were identified by FTIR spectroscopy. The agglomerated particles of hexagonal, spherical and parallelogram shape were observed in the TEM images. The optical behaviors of the Yb_2O_3 NPs were characterized by UV-Vis and photoluminescence studies. The Yb_2O_3 NPs for good biological activities were discussed by antibacterial and anti oxidant studies.

Keywords: Green synthesis, Ionic liquid, Morphology, Antibacterial and Anti oxidant.

PP 68

SYNTHESIS AND APPLICATIONS OF GOLD NANOPARTICLES USING FENUGREEK SEED EXTRACT WITH THEIR ANTIBACTERIAL, UV PROTECTION AND ANTICANCER

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Abstract

Gold nanoparticles (AuNPs) have been synthesized by greener method using chloroauric acid as precursor and fenugreek seed extract (*Trigonella-foenum graecum*) as bio-reducing agent. A narrow surface plasmon resonance (SPR) band of high intensity peak was observed at 543 nm in UV-Visible spectral analysis revealed the formation of mono-dispersed AuNPs from higher (0.01M) concentration of chloroauric acid (precursor of Au^{3+}).

XRD and FT-IR spectral analysis were performed for characterization. SEM images show granular spherical in shape with higher distribution and HR-TEM images reveal nano size of AuNPs. The AuNPs was coated on cotton fabric and characterized by SEM with EDAX technique to recognize the deposition of AuNPs on the surface of cotton fabric. AuNPs coated cotton fabric was tested for antibacterial activity against *Staphylococcus epidermidis* (*S.epidermidis*) and *Escherichia coli* (*E.coli*) bacterial strains. The AuNPs coated cotton fabric has shown significant improvement on antibacterial function against *S. epidermidis* bacteria. UV-DRS analysis performed on AuNPs coated cotton fabric showed improved UV-protection efficacy. In addition to this, AuNPs showed anticancer activity against HepG2 cell line. Therefore, this study is strongly point out a greener approach to synthesize noble gold nanoparticles and its applications in medical technology.

Keywords: AuNPs, cotton, coating, antibacterial, UV protection, anticancer.

PP 69

FABRICATION OF BROMELAIN DECORATED ON POLYVINYL ALCOHOL/HYDROXY ETHYL CELLULOSE NANOFIBERS AND THEIR APPLICATIONS AS WOUND DRESSINGS

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Abstract

Bromelain is a group of sulfhydryl-containing proteolytic enzyme and exhibited antibacterial, antioxidant and anti-inflammatory activities. First, bromelain was assembled into the Polyvinyl alcohol/Hydroxy ethyl cellulose matrix by electrospinning approach. In this study, the fabricated nanofibrous mats were characterized by FTIR, SEM, AFM and TGA/DSC analysis. The surface modification of the bromelain with PVA/HEC polymer matrix has highly hydrophobic property and inherent hydrophilic nature. The important properties of the nanofibrous mats such as porosity and swelling properties also enhanced due to the formation of fibrous structure. The *in vitro* release profile illustrated the sustained release of bioactive bromelain. Furthermore, the nanofibrous mat showed significant inhibition against the growth of *Escherichia coli* and *Staphylococcus aureus* owing to the

antibacterial activity of bromelain. The *in vitro* antioxidant assays shows the free radical scavenging ability of the fabricated nanofibrous mats. These results suggested that the improved antibacterial and antioxidant properties of bromelain-PVA/HEC nanofibrous mat have great potential for the application in infection-resistant wound dressings.

Keywords: Electrospinning, Nanofibrous mat, Bromelain, Antibacterial activity, Antioxidant activity.

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PP 70

CHEMICAL SYNTHESIS AND CHARACTERIZATION NANO SIZE POLY (ANILINE-CO-ETHYL 4-AMINO BENZOATE) COPOLYMERS AND ITS SPECTROELECTROCHEMICAL STUDIES

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Abstract

Aniline was copolymerized chemically in presence of five different concentrations of ethyl 4-aminobenzoate using potassium persulphate as an oxidant. The copolymer exhibited good solubility in many organic solvents. Copolymers were characterized by UV-Vis, FTIR, XRD, SEM, TEM and AFM studies. The TG/DTA studies suggested to good thermal stability of the copolymer. The formation of copolymer was confirmed by FTIR spectral data. The spectroscopic studies confirmed incorporation of ethyl 4-aminobenzoate units in the copolymers and hence the presence of C=O group in the copolymer chains. The X-ray diffraction studies revealed the formation of nano sized crystalline copolymer. When more ethyl 4-aminobenzoate was incorporated in the copolymer the crystalline nature changed from less to more. The grain size of the copolymer calculated from Scherrer's formula was

found nanometer scale. The nano size copolymer formation was also confirmed through surface morphology (100 nm) studies. The electrical property of the copolymer was studied by four-probe conductivity meter. The voltammetric and spectroelectrochemical results were also presented.

Keywords: Electrochromics, Copolymerization, Chemical synthesis, Ethyl 4-aminobenzoate, Aniline.

PP 71

ELECTRIC FIELD INDUCED EXCITON BINDING ENERGY IN A NARROW BAND GAP NANOMATERIALS

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Abstract

The effect of electric field on the binding energy, interband emission energy and the non-linear optical properties of exciton as a function of dot radius in an InSb/InGa_xSb_{1-x} quantum dot are investigated. Numerical calculations are carried out using single band effective mass approximation variationally to compute the exciton binding energy and optical properties are obtained using the compact density matrix approach. The dependence of the nonlinear optical processes on the dot sizes is investigated for various electric field. The linear, third order non-linear optical absorption coefficients, susceptibility values and the refractive index changes of electric field induced exciton as a function of photon energy are obtained. It is found that electric field and the geometrical confinement have great influence on the optical properties of dots.

Keywords: Exciton Binding Energy, Electronic states; Optical absorption; Quantum dot

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PP 72

**A STUDY ON EXTRACTION, ISOLATION AND PHYTOCHEMICAL
EVALUATION OF *TARENNA ASIATICA* LEAVES**

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Abstract

Evaluation of natural products and their extracts are gaining importance to the various applications it finds in the areas medicinal to cosmetics. But isolation of phytochemicals and achieving the purity of the same remains a constant challenge to the chemists. Hence the present work attempts to extract the active ingredients present in a medicinal plant leaves and envisages the phytochemical evaluation of the same. The preliminary results have shown the presence of important flavonoids and steroids. Characterization techniques such as FTIR and chromatographic tools have been used and the results have substantiated the above findings.

Keywords: Phytochemistry, chromatography, TLC, flavonoids, steroids.

PP 73

**FACILE GREEN SYNTHESIS OF CeO₂ AND AG DOPED CeO₂ NANOPARTICLES
USING IONIC LIQUID MEDIUM AND THEIR ANTIBACTERIAL ACTIVITY**

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Abstract

CeO₂ and Ag/CeO₂ (NPs) were synthesized by using *Justicia adhatoda* leaves extract in ionic liquid medium. The ionic liquid of 1-butyl-3-methyl imidazolium hexafluorophosphate can be important role play in the synthesized nanomaterials such as it can be improved surface morphology of the Ag doped CeO₂ NPs. The synthesized nanoparticles were characterized by various techniques, including XRD, FT-IR, UV-DRS, RAMAN, SEM with EDX and HR-TEM analyses. X-ray diffraction studies displayed that the undoped and doped CeO₂ nanoparticles are cubic structure. FTIR spectrum is useful method to identify the functional group of *Justicia adhatoda* leaves extract and synthesized nanoparticles. SEM analysis confirmed the Ag- doped CeO₂ (NPs) are nanorod in structure. The band gap energy of Ag/CeO₂ nanoparticles estimated at 3.27 eV in UV-DRS spectrum. EDX spectrum is useful method to confirm the presence of Ce, Ag and O in the synthesized nanomaterials. The Ag doped CeO₂NPs exhibited good antibacterial activity against a Gram positive (*S.aureus*) and Gram negative (*E.coli*) bacterial strains. The Ag/CeO₂NPs has highest antibacterial activity compared with CeO₂. Hence the Ag doped CeO₂ NPs could to be used as biomedical applications.

Keywords: *Justicia adhatoda*, Ionic liquid, Ag/CeO₂NPs, imidazolium, Antibacterial activity.

PP 74

DEVELOPMENT OF FUNCTIONAL ANTIBACTERIAL PAPERS USING CHITOSAN/AGAR-SILVER NANOPARTICLES (Cht:Agar-AgNPs)

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Abstract

In this study, the synthesis of Chitosan:Agar-silver nanoparticle (Cht:Agar-AgNPs) coated cellulose papers are being reported for antibacterial packaging applications. Agar was used as a reducing and capping agent for the synthesis of AgNPs. Synthesized Agar assisted AgNPs were examined through UV-visible, FT-IR, XRD, SEM with EDX analyses. The synthesized Agar-AgNPs are structured as face-centered cubic. Chitosan was mixed into the synthesized Agar-AgNPs. Chitosan was mixed into the synthesized Agar-AgNPs solution with different ratios of 5:5, 7:3, 8:2 and 9:1 by weight. Further, the influence of different ratios of Cht:Agar-AgNPs on the various paper investigated by AFM and SEM analysis, and coated papers revealed a smooth surface morphology and good dispersion of AgNPs. It was observed that the properties of the coated papers were strongly dependent on the composition of Cht:Agar-AgNPs. Coated papers were investigated against Gram positive and Gram-negative bacterial strains. Different ratios of Cht:Agar-AgNPs coated papers were showed excellent water sorption, burst strength and antibacterial activity. The findings in this study are significant for developing functional antibacterial papers, which can be potentially applicable in agricultural food packaging and antibacterial coating for air conditioning, filters, and cleaning components.

Keywords: Agar, silver nanoparticles, water sorption, antibacterial activity

PP 75

NOVEL FeVO₄ ASSISTED PHOTOCATALYTIC DEGRADATION OF AQUEOUS METHYL VIOLET SOLUTION UNDER SUNLIGHT IRRADIATION

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Abstract

FeVO₄ was synthesised and characterized by XRD, FT-IR, FE-SEM, EDX, Colour mapping and UV-DRS. The enhanced photodegradation was attributed to the high production of hydroxyl radicals via two-way heterogeneous Fenton like mechanism of FeVO₄. Moreover the nanocatalyst can perform effectively multiple runs without change in efficiency.

Furthermore COD reduction values reflect the complete mineralization of MV under solar light.

Keywords: Photocatalytic degradation; Methyl Violet dye; FeVO₄; Hetero-Fenton; Wastewater treatment.

PP 76

Ni-CNT NANOCOMPOSITES BASED ELECTROCHEMICAL SENSOR FOR SIMULTANEOUS DETERMINATION OF EPINEPHRINE AND DOPAMINE

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Abstract

A promising electrochemical sensor based nickel-carbon nanotube (Ni-CNT) modified on glassy carbon (GC) electrode had been developed and the properties of the modified electrode were characterized by multispectroscopic analysis. The fabricated sensor (GC/Ni-CNT) electrode was utilized to determine the catecholamines such as epinephrine and dopamine simultaneously. Differential pulse voltammetry and amperometry were used to verify the electrochemical behavior of the studied compounds. The GC/Ni-CNT based amperometric sensor showed a wide linear range and low detection limit with high analytical sensitivity of 8.31 and 6.61 $\mu\text{A } \mu\text{M}^{-1}$ for EP and DA, respectively which demonstrates better characteristics compared to other electrodes reported in the literature. Further, no significant change in amperometric current response was observed in presence of biological interference species such as glucose, cysteine, citric acid, uric acid and ascorbic acid in the detection of EP and DA. The utility of this GC/Ni-CNT electrode was well established for the determination of EP and DA in human urine samples.

Keywords: Ni-CNT nanocomposites, electrochemical sensor, epinephrine, dopamine, differential pulse voltammetry, amperometry.

PP 77

**CYCLIC VOLTAMMETRIC STUDIES ON NEW ACETYLNAPHTHONE
CHALCONES**

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Abstract

The chemistry of chalcones has generated intensive scientific studies throughout the world. Especially interest has been focused on the synthesis and antimicrobial activities of chalcones. At the present study, A facile synthesis of 2-acetylnaphthone chalcones were synthesized by the aldol condensation reaction of 2-acetylnaphthoe with various aromatic aldehydes in the presence of sodium hydroxide in ethanol. The structures of 2-acetylnaphthone chalcones were confirmed by UV, IR, ¹H-NMR and ¹³C-NMR Spectral Studies. All the synthesized 2-acetylnaphthone chalcones were studied using cyclic voltammetry in an aqueous medium has been performed. The effects on the first reduction potential (*E*) were analyzed with the help of Hammett Equation and the ρ values were evaluated for various substituents.

Key Words: 2-acetylnaphthonechalcones, Cyclic voltammetry, Hammet Equation

PP 78

**CHARACTERIZATION OF POLYMER ELECTROLYTE MEMBRANE BASED ON
BLEND POLYMER (PVP+PPA) WITH MAGNESIUM SULPHATE**

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Abstract

A solid polymer electrolyte system based on the blend polymer Poly vinyl pyrrolidone (PVP) and poly p- amino benzoic acid complexed with different concentration magnesium sulphate has been prepared by solvent casting method. The conductivity measurements are
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carried out on these films as a function of frequency at room temperature. FT- IR analysis proved that the proton accepting carbonyl group in the PVP involves the complex formation to magnesium salt, which was confirmed by the bands at 1649 cm⁻¹ is attributed to cyclic amide group C=O stretching of pure PVP is shifted to lower wave number side or higher wave number side in the PVP +PPA – MgSO₄ polymer electrolyte system. Also the shifting of all the bands in the pure PVP +PPA – MgSO₄ isomers has also been proved the complex formation. The complex impedance spectroscopy results reveal that the high-frequency depressed semicircle is due to the bulk effect of the material. The conductivity is enhanced to the order of S/cm upon increase in salt concentration at room temperature. The AlS1 (2.07X10⁻⁷ S/cm) enhances the conductivity of PVP by donating its magnesium ion very effectively. A dielectric spectroscopy study has been carried out on the polymer electrolytes to identify the optimized salt composition, which is having high ionic conductivity. The dielectric behaviours of the samples have been analyzed using dielectric permittivity and electric modulus. The dielectric spectra show the low frequency dispersion, which implies the space charge effects arising from the electrode-electrolyte interface. The high dielectric loss (ε'') values at lower frequencies are due to the free charges build up at the interface between the material and the electrodes.

PP.79

SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL STUDIES ON INDOLE DERIVATIVES

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Abstract:

A new series of specifically substituted pyrazole, isoxazole and pyrimidine derivatives containing cyclohepta[*b*]indole moiety, has been synthesized. Structures of all synthesized compounds were supported by spectral and elemental analyses. Their molecular docking with protein kinase CK2 and *in-vitro* cytotoxic activity against cervical cancer cell line (*HeLa*) was studied. Among the sixteen molecules docked, compound 6c was the one with the best glide and E model score of -7.61 and -58.27 respectively and compound 3a

exhibited the least glide and E model score of -6.19 and -36.01 respectively. Among all the molecules studied, compounds 5c, 6d and 6c exhibited better IC₅₀ value when compared to the other molecules. All the IC₅₀ values were compared with the standard drug *Ellipticine*. The antibacterial study was carried out by agar dilution method, and their minimum inhibition concentration was calculated using *Sparfloxacin* and *Norfloxacin* as standards. The pyrazole derivatives exhibited better MIC values against Gram-positive bacteria and Gram-negative bacteria when compared with isoxazole and pyrimidine derivatives. Structure activity relationship (SAR) analyses confirmed that the compounds are potential lead compounds for future drug discovery studies.

Key words: Cyclohepta[b]indoles, molecular docking, antibacterial, anticancer, Structure activity relationship.

PP 80

**COMPARATIVE STUDY ON NANOENCAPSULATED SYNTHETIC AND
AYURVEDIC MATTERS; IN VITRO EVALUATION OF NEUROPROTECTIVE
AND ANTIMICROBIAL EFFICACIES**

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Abstract

Starch is a natural, renewable biopolymer widely used in pharmaceutical industry for the controlled release of drugs and hormones. Methyl Gallate (MG) is a gallic acid's methyl ester and Triphala churna (TC) a tridoshic rasayana, both compounds are rich in polyphenols and vitamin C possess balancing and rejuvenating effect on three constitutional elements that govern the human life. To enhance the solubility and efficiency of the hydrophobic drugs TC and MG, attempts were made to encapsulate the TC& MG into starch biopolymers. Starch encapsulated triphala churna (SETC) and Starch encapsulated Methyl Gallate (SEMG) were characterized by spectroscopic and microscopic analyses. UV-visible spectrum of SETC and SEMG showed a sharp absorption peaks at 686nm and 275 nm specific for Polyherbal formulation and Polyphenolic content respectively. XRD analysis illustrated that SETC and

Department of Industrial Chemistry, Alagappa University, Karaikudi.

SEMG were amorphous in nature. Zeta potential and dynamic light scattering analysis illustrated that the SETC and SEMG were highly stable at -12 mV. DLS shows the average size of 282.9 nm for SETC and 468.7 nm for SEMG. High drug encapsulation efficiency and fast drug release at physiological pH 7.4 was observed for both SETC and SEMG. Evaluation of neuroprotective effect illustrated that SETC & SEMG showed excellent free radical scavenging activity, reducing power and acetylcholinesterase inhibitory activity. SETC and SEMG also showed potent antibacterial activity against *Salmonella typhi* and *Shigella dysenteriae* and antibiofilm activity against ATCC MRSA 33591 and clinical strain N7. Results conclude that SETC retained its excellent antimicrobial, antibiofilm and neuroprotective activities when compared to the SEMG. However, this approaches illustrating the starch as suitable drug delivery system.

PP 81

SYNTHESIS AND THROMBOLYTIC ACTIVITY OF NITROGEN CONTAINING HETERO CYCLIC COMPOUNDS

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Abstract

The aim of this study was to synthesize and thrombolytic activity of acetohydrazide derivatives. Check the purity of all the synthesized compounds using thin layer chromatography. The synthesized compound was subjected to thrombolytic activity. The thrombolytic activity was observed in 2 different concentrations of synthesized compounds. The result from the study showed that the synthesized compounds have excellent thrombolytic activity that was comparable to the activity of Streptokinase. As from the research findings of the under taken in vitro clotlysis study, we demonstrated that the compounds showed mainly moderate thrombolytic activity. Our findings support the reported therapeutic use of these compounds as clotlysis or thrombolytic agent in the Indian system of medicine.

Keywords: Thrombolytic activity, streptokinase, clotlysis.

PP 82

ANTIMICROBIAL STUDIES OF SCHIFF BASED NOVEL LIGAND AND ITS COMPLEXES

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Abstract

The novel Schiff based ligand is expected to exhibit variety of characteristics such as biological and catalytic properties. Schiff bases are studied widely due to their synthetic flexibility, selectivity and sensitivity towards the central metal atom; structural similarities with natural biological compounds and also due to presence of azomethine group (-N=CH-) which imports in elucidating the mechanism of transformation and racemization reaction biologically. The imine group present in such compounds has been shown to be critical to their biological activities. This review concentrates on the synthesis and microbial properties of Schiff bases and their complexes. The main aim of the present work is to synthesise a novel ligand derived from hydroxypyrimidine and its complexes due to their wide range of application as antimicrobial agents. The Schiff base and metal complexes displayed good activity against the Gram-positive bacteria and Gram-negative bacteria. The antimicrobial results also indicated that the metal complexes displayed better antimicrobial activity. The synthesized ligand was characterized by various physical and chemical methods of analysis such as UV-Vis, FTIR, NMR, fluorescence, CV, TGA and elemental analysis.

Keywords: Antimicrobial Study, Schiff base, pyrimidine derivative.

PP 83

NOVEL & SMART SENSING OF ACETATE & HYPOCHLORITE IONS WITH FLUORESCENCE TURN-ON: APPLICATION IN REAL SAMPLE ANALYSIS

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Abstract

Designing and development of cation and anion sensors have many interesting applications in the field of biological, clinical and environmental chemistry. Due to the toxic nature of these ions, there is a need to develop an effective system for their detection. Previously, these analytes were detected by highly expensive instruments and other chemical method. However, they were very costly; require difficult sample preparation, To reach this goal, colorimetric chemosensor field has been implemented due to the advantage of facile, visual output, and high response. These problems made us the driving force to design novel and simple sensor molecules for the detection of anions. The extreme toxicity of acetate ions in physiological systems causes eye irritation, headache, and unconsciousness. High concentrations of acetate ion can cause CNS depression and congestion of the kidney^[1]. However, until now, selective detection of chromogenic and fluorescent sensors for AcO^- ions is somewhat limited. In addition excess amount of hypochlorite can cause some diseases like arthritis, atherosclerosis, and cancers^[2]. To overcome this drawback, we have designed the receptor for the selective detection of acetate and hypochlorite ions.

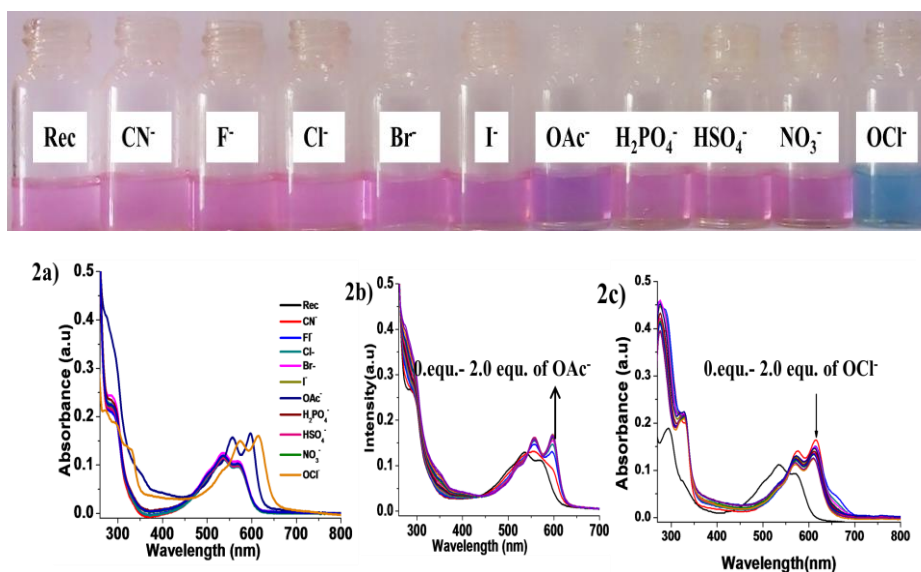


Fig.1. Naked and (2a-c) spectral change of the receptor with all anions

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PP 84

**SYNTHESIS, CHARACTERIZATION OF FERRITE NANOPARTICLES AND ITS
SUNLIGHT PHOTOCATALYTIC ACTIVITY**

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Abstract

Hydrazine precursor for ferrite nanoparticles were prepared by co-precipitation technique. Infrared (IR) and Thermogravimetric and Differential Thermogravimetric Analysis (TG-DTA) of the precursor were indicated the bridging bidentate nature of hydrazine and multi step thermal decomposition. Ferrite nanoparticles prepared from the hydrazine precursors were characterized by IR, Energy Dispersive Spectroscopy (EDS), Powder X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Vibrating Sample Magnetometry (VSM) and UV- Diffuse Reflection Spectroscopy (UV-DRS) which proposed the phase structure, morphology, magnetic and optical properties. An effective photocatalytic activity of ferrite nanoparticles were studied on Congo Red (CR), Malachite Green (MG), Methylene Blue (MB), Methyl Red (MR), Rose Bengal (RB) and Rhodamine B (RhB) under sunlight. Ferrite nanoparticles showed good recycling ability using an external magnet.

Keywords: Hydrazine, ferrite, bidentate, photocatalytic, recycling.

PP 85

**A NOVEL ELECTROCHEMICAL DOPAMINE SENSOR BASED ON
HIERARCHICAL MoS₂ WRAPPED CuMn₂O₄ NANOCOMPOSITE MODIFIED
GOLD ELECTRODE**

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Abstract

Molybdenum disulfide/ CuMn₂O₄ nanocomposite were synthesized through one-pot solvothermal facile method for the first time and modified on Au electrode for constructing a highly sensitive and selective electrochemical sensor for dopamine (DA). The prepared MoS₂/CuMn₂O₄ nanocomposite was characterized by XRD, FT-IR and SEM studies. The electrochemical characteristics were evaluated by cyclic voltammetry (CV) and impedance spectroscopy techniques. The MoS₂/CuMn₂O₄/Au electrode exhibited more enhanced electron transport property, higher surface area and more efficient electrocatalytic activity towards DA than the single compound modified electrode. The outstanding electro catalytic performance of MoS₂/CuMn₂O₄/Au is attributed to the synergistic effect, definite size and unique morphology, which provides good micro-environment for convenient conjugation of biomolecules and improved charge transfer between the electrode surface and biomolecules for effective oxidation. The proposed electrochemical sensor showed relatively low detection limit of 2 nM. Additionally, practical utility of the proposed sensor was evaluated for the determination DA in commercial DA injection and human urine by standard addition method, showed satisfactory recoveries. It is expected that MoS₂/CuMn₂O₄/Au is a good candidate for low cost and highly sensitive biosensor for the detection of dopamine.

PP 86

SYNTHESIS AND CHARACTERIZATION OF A TITANIUM BASED METAL ORGANIC FRAMEWORK

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Abstract

Metal-Organic frameworks as a class of organic-inorganic hybrid materials has attracted considerable research interest in the past two decades because of their intrinsically porous structures and unlimited tunability. MOFs are usually constructed by connecting inorganic nodes and organic linkers through coordination bonds. Titanium based Metal-Organic Frameworks synthesized by solvothermal method, which is simple and environment friendly method. As prepared Ti-MOF using precursor of 1,4-benzene dicarboxylic acid and

Titanium(IV)Isopropoxide. The synthesized Ti-MOF was characterized by several technique, such as FT-IR, UV-DRS, PXRD, RAMAN and HR-SEM analysis. The molecular interaction and structural conformation were studied by FT-IR and Raman spectroscopy. The Raman analysis shows the asymmetric stretching vibration of (-COO) in Ti-MOF was attributed at 1631 and 1442 cm^{-1} . The vibration of 1124 and 827 cm^{-1} assigned –CH- in plane and out-plane bending aromatic ring (MOF), The vibration of 260, 348 cm^{-1} are assigned to O-Ti-O stretching of Ti (IV) coordinated to BDC ligand. The scanning electron microscopy shows agglomerate the various size of tetragon plate and porous structure of Ti-MOF. The powder XRD showed the crystallinity of the Ti-MOF sample. The diffraction peaks at $2\theta=15, 20$ and 22.5° are proof of crystalline nature of Ti-MOF. The spectrum of Ti-MOF shows absorption band at 350 nm. The band gap energy 3.3 eV was calculated by UV-DR spectroscopy. All the characterization was proved by Ti-MOF, which is applicable for energy conversion fields.

KEYWORDS: Metal-Organic Frameworks, Titanium (IV) Isopropoxide, Solvothermal method-MOF, Ti-MOFs.

PP 87

**JUSTICIA LEAF ASSISTED REDUCED GRAPHENE OXIDE /ZINC OXIDE
NANOCOMPOSITE FOR ANTIBACTERIAL APPLICATIONS**

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Abstract

The leaf extract of *Justicia gendarussa* consists many phytoconstituents, it is used in the treatment of diseases like jaundice, and rheumatic pain etc., in the present scenario necessity of emergence of new antimicrobial substance to treat pathogenic organisms is inevitable. Reduced graphene oxide along with the *Justicia* leaf extract has proven the remedy for antibacterial and anti inflammation studies. Different concentration of leaf extract of *Justicia gendarussa* is used to reduce the metal oxide (Zinc oxide) and dopped it on RGO sheet. This synthesized nanocomposite was evaluated against gram positive bacteria *Bacillus*

subtilius and *Staphylococcus aureus*. The prepared materials were characterized by X-ray diffraction (XRD), Fourier Transformer-infrared spectroscopy (FTIR), UV-visible spectroscopy (UV-Vis), Transmission electron microscopy (TEM), Scanning electron microscopy (SEM) and energy dispersive X-Ray spectrometry (EDX), which confirmed the simultaneous formation of nanocomposite. The antibacterial study was evaluated by Agar well diffusion method, anti inflammatory activity, membrane stability was also evaluated against the drug di-chlofenac. The examined results confirmed that leaf extract assisted metal oxide/reduced graphene oxide showed significant biological applications than the standard drug.

Keywords: Nanocomposites, hydrothermal process, antibacterial activity, Agar well diffusion method.

PP 88

POLY PARAPHENYLENE DIAMINE/TITANIUM DIOXIDE/EXFOLIATED GRAPHITE NANOCOMPOSITES: SYNTHESIS, CHARACTERIZATION AND APPLICATION

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Abstract

Polymer nanocomposites based on carbon nanotubes or graphene have been used to enhance a wide range of properties, giving rise to functional materials for a wide range of high added value applications in fields such as energy conversion and storage, sensing and biomedical tissue engineering. Composite materials made with polymers and metal nanoparticles like titanium dioxide can be made electrically or thermally conductive with the addition of small amounts of Exfoliated graphite. These nanoparticles can change the fundamental properties of polymers, enabling them to perform more like metals with metallic properties. These new nanoparticles also improve barrier properties, modulus, and surface toughness when used in composites. . PPPD has a variety of applications in the field of electrochromism, sensors, rechargeable batteries and corrosion protection.

In the present study, polymerization of PPD leads to formation of PPPD. Composites are prepared by mixing of TiO₂, exfoliated graphite and the polymer by magnetic stirring.

These nanocomposites are characterized by using analytical techniques such as UV-Vis, IR, FE-SEM, analysis and cyclic voltammetry. Absorption maximum is seen to be at 309 nm due to π - π^* transitions in the benzenoid and quinonoid rings of the polymer and 453 nm due to π - π^* of phenazine ring. IR spectra shows bands at 3368cm^{-1} due to N-H stretching, 1514cm^{-1} due to C=N stretching, 1571cm^{-1} due to C=C stretching and 501cm^{-1} due to Ti-O stretching. FE-SEM shows agglomerated structures in nanometer range. Capacitance deduced from CV curves are significant, showing their eligibility for capacitors.

Keywords: Nano composites, para phenylene diamine, titanium dioxide, Exfoliated graphite.

PP 89

ELECTROCHEMICAL, THERMODYNAMIC AND ADSORPTION STUDIES FOR THE CORROSION INHIBITION OF MILD STEEL BY HENNA EXTRACT IN ACID MEDIUM

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Abstract

Corrosion inhibition of mild steel in the presence of different concentrations (100-400 ppm) of aqueous extract from henna leaves in 1M HCl solution has been studied using the weight loss, polarization techniques and electrochemical impedance spectroscopy (EIS) measurements. The effect of temperature on the corrosion behavior of mild steel was studied in the temperature range 303–333 K. The inhibition efficiency increases with increasing of inhibitor concentration but decreases with increasing with temperature. Maximum inhibition efficiency (85.64%) was obtained at 1M HCl in 400 ppm concentration. The activation and free energies for the inhibition reactions support the mechanism of physical adsorption. The adsorption of henna extract on mild steel surface is endothermic, spontaneous and consistent with the Langmuir adsorption isotherm. The polarization and EIS measurements indicate that henna extract acts as a mixed type inhibitor. The results obtained

from the different methods are in good agreement. A protective film analysis has been carried out using Fourier transforms infrared (FT-IR) spectroscopy analysis. Therefore the henna extract functioned as good corrosion inhibitor in 1 M HCl.

Keywords: Mild steel, Corrosion inhibition, Henna extract, Thermodynamic parameters.

PP 90

**THIN FILM FORMATION OF PHYLA NODIFLORA LINN LEAVES EXTRACT
ON MILD STEEL IN ACID ENVIRONMENT BY ADSORPTION STUDIES**

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Abstract

Thin film formation of Phyla Nodiflora Linn leaves extract on mild steel in Acid Environment was studied by mass loss measurements with various periods of contact and temperature. Inhibition Efficiency increased with inhibitor concentration. Maximum of Inhibition efficiency attained 93.13%. By temperature studies, the Inhibition efficiency gradually decreased from 93.57% to 85.18% suggests that the adsorption is Physisorption and also Inhibitor was found to attempt by various adsorption isotherms viz., Langmuir adsorption, Temkin adsorption, Florry-Huggins adsorption, Frumkin adsorption, Freundlich adsorption and El-Awady adsorption isotherm at different concentration and temperature investigated, but it obeyed only Temkin adsorption isotherm.

Keywords: Mild steel, Phyla Nodiflora Linn leaves, Mass Loss, Adsorption.

PP 91

**CRYSTAL GROWTH, STRUCTURE, CHARACTERIZATION AND
THEORETICAL STUDIES OF D-VALINIUM PICRATE**

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Abstract

Amino acids D-valine, L-valine and DL-valine are employed to form picrates with picric acid by slow evaporation of an equimolar mixture. Comparison of cell parameters
Department of Industrial Chemistry, Alagappa University, Karaikudi. 154

reveals that picrates are formed. The structure of D- valinium picrate (DVP), as determined by single crystal XRD diffraction analysis reveals that it belongs to the monoclinic system with space group $P2_1$ and the cell parameter values are, $a=9.9269(2)\text{\AA}$; $b=6.2841(2)\text{\AA}$; $c=12.6051(3)\text{\AA}$; $\beta=110.46(2)^\circ$; $V=736.70(3)\text{\AA}^3$; $Z=2$. The characteristic functional groups in the DVP is confirmed by FT-IR vibrational patterns and the good crystallinity indicated by powder X-ray diffraction method. The relative second harmonic generation (SHG) efficiency measurements reveal that the DVP has a superior activity than that of the reference material potassium dihydrogen phosphate. The optical transparency has been studied using UV-vis spectrophotometer and the crystal shows minimum absorption in the visible region. The first order molecular hyperpolarizability (β) estimated by Hartree – Fock calculations at the level 6-31G(d,p) is ~13 times that of urea.

Keywords: Crystal growth, Crystal structure, Grown from solution, Characterization methods, Optical materials.

PP 92

SYNTHESIS OF SILVER DOPED NANO ZINC OXIDE AND EVALUATION OF INTERACTION BETWEEN NPS AND CALF THYMUS DNA

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Abstract

The effect of the surface chemistry of biomaterials on the protein adsorption process has been a topic of great interest for many years. Protein adsorption to various materials has been widely studied and it has been found that factors such as electrostatic interactions, hydrophobic interactions, and specific chemical interactions between the protein and the adsorbent play important roles. These interactions with the surface can easily disrupt the native conformation and therefore, the protein function. On the other hand, the conjugation of protein with nanoparticles not only allows stabilization of the system, but more importantly, it also introduces biocompatible functionalities onto these nanoparticles for further biological interactions or coupling. Nanoparticles rapidly interact with the proteins present in various biological systems. However, to date, few studies have been conducted focusing on the

nanoparticles that are commonly exposed to the general public, such as the metal/metal oxides. Therefore, understanding how and why proteins are adsorbed to these particles are important for understanding their biological response.

In our present investigation, we conducted an in-depth study on the synthesis and characterization of Ag doped ZnO nanoparticles and their application on biological system. The *in vitro* anticancer activity and cell cytotoxicity potential of Ag doped ZnO nanoparticles against on human cervical cancer cell line HeLa. The interaction between Ct-DNA protein and Ag doped ZnO nanoparticle was monitored. The structural change of the protein upon interaction with NP was monitored using UV-visible, Viscosity measurements and Effects of ionic strength.

Keywords: CT-DNA, Nano particles, Ag doped nano ZnO, DNA bindings

PP 93

ELECTROCHEMICAL DEGRADATION OF MALACHITE GREEN DYE USING DSAIN A BATCH REACTOR

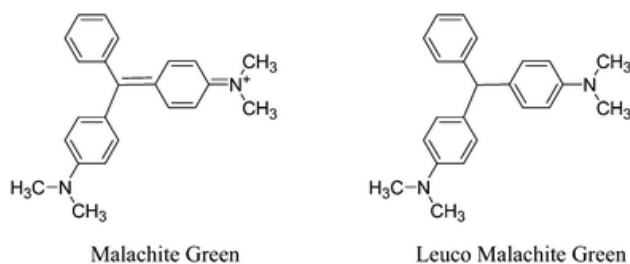
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Abstract

Since the availability of clean water for various human needs in the next decades seem to become a challenge to take up, the effects of many water pollutants on the environment have been investigated and discussed in different scientific areas. Remediation of water contaminated with toxic organic compounds such as dyes, detergents and many other highly toxic compounds has been the subject of many investigations [1]. The present work deals with the degradation of wastewater containing Malachite green (MG) dye using DSA (Dimensionally Stable Anode) and Stainless Steel electrodes as a Cathode. And Sodium Chloride (2g/l) was also used as the supporting electrolyte solution for this oxidation process. The colour removal efficiency, decrease in absorbance, COD removal efficiency has studied in the electrochemical oxidation process. The effect of pH, Current Density, Time for degradation of dye solution has also been evaluated. The COD removal percentage of the dye increased with increase of the applied current density and maximum COD removal Percentage (99%) was observed for 0.45 A/cm². Absorbance values also measured at λ_{\max} 618 nm and are found to be decreases with increase of current density. For lowest current

density value for the complete color removal was observed. Change in pH of the solution increases/decreases the H^+ or OH^- ions concentration. In acidic pH range, $-N^+(CH_3)_2$ and H^+ interaction gets enhanced, while in the alkaline pH range, OH^- ions interact with cationic ring and convert it into stable colourless leuco form [2,3].



Chromatographic analyses

High performance liquid chromatographical analyses were done for untreated and treated samples and were mixture of acids. We assume prolonged oxidation (for 2 more hours) finally leads to the formation of CO_2 , H_2O and salts.

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PP 94

PHYSICO CHEMICAL ANALYSIS OF DIFFERENT SOIL SAMPLES IN AND AROUND THIRUVARUR DISTRICT, TAMILNADU-INDIA

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Abstract

Soil is a component of the terrestrial ecosystem fulfils many functions including that are essential for sustaining plant growth. The change in physico chemical properties of soil leads to infertile or barren soil that does not support normal growth of vegetation for years. The climate and other factor largely affect the soil formation. In the present study analysis of soil was carried out for the studies of various parameters like total Organic Carbon (OC), Nitrogen (N), Phosphorus (P) Potassium (K), Zinc (Zn), Iron (Fe), Boron (B), pH, conductivity. This study leads us to the conclusion of the nutrients quantity of soil of Thiruvarur District-Tamilnadu. Results show that on an average all the villages of Thiruvarur have medium or high minerals content. This information will help farmers to solve the problems related to soil nutrients amount of which fertilizers to be added to soil to increase the yield of crops.

PP 95

GREEN ROUTE SYNTHESIS OF NOVEL NANO COMPOSITE MATERIAL BASED ON NICKEL OXIDE/*OCIMUM AMERICANUM* LEAVES EXTRACT DERIVED CARBON FOR SUPERIOR SUPERCAPACITOR APPLICATIONS

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Abstract

In the present study, we report the green route biosynthesis of nickel oxide/carbon nano composites were prepared by novel green synthesis method using aqueous and alcoholic extract of *Ocimum americanum* Leaves and this method is eco-friendly and cost effective. A nickel oxide/carbon composite was prepared by chemically precipitating Nickel nitrate on an active carbon and heating the hydroxide at 600° C for 2 hrs in the inert gas atmosphere. The properties of nickel oxide/carbon nano composites as the electrode materials for supercapacitors are discussed. Phase compositions of the products were characterized using X-ray diffractometry (XRD). The morphology of the composites was observed by FESEM. The electrochemical performances of electrode used in electrochemical capacitors were studied in addition to the properties of electrode consisting of separate active carbon and nickel oxide only. The electrochemical measurements were carried out using cyclic voltammetry, galvanostatic charge/discharge, and impedance spectroscopy. The composites were tested in 6M KOH aqueous electrolyte using two (2032 coin cell) and three-electrode

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Swagelok systems. It is the confirmation of the fact that such an amount of nickel oxide is optimal to take advantage of both components of the composite, which additionally can be a good solution as a negative electrode in asymmetric configuration of electrode materials in an electrochemical capacitor.

Keywords: Asymmetric Supercapacitor, NiO nano material, Aqueous electrolyte, Bio-synthesis

PP 96

**IONIC LIQUID MEDIATED SYNTHESIS AND CHARACTERIZATION OF
TITANIUM DI OXIDE NANOPARTICLES BY *TABERNAMENTANA DIVARICATA*
LEAVES EXTRACT WITH ENHANCED BIOMEDICAL APPLICATIONS**

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Abstract

Green synthesis of TiO₂ nanoparticles using *Tabernaemontana divaricate* (*T.divaricata*) leaves extract by precipitation method. The crystallinity, particle size and morphology of the IL assisted TiO₂ NPs were studied by various properties such as structural, spectral, optical and biological studies. From the powder X-ray diffraction studies confirmed that the TiO₂ NPs belongs to cubic crystal system and the high intensity peaks were indexed. The various functional groups such as Ti - O and COO⁻ were identified by FT - IR spectroscopy. The surface morphology and elemental analysis were examined by SEM images and energy dispersive X-ray spectroscopy. The optical behaviors of the TiO₂ NPs were characterized by UV-Vis studies. The chemical elements, particle size and shape are prepared in the TiO₂ NPs were identified by TEM images. The TiO₂ NPs for good biological activities were discussed by antibacterial and anti oxidant studies.

PP 97

SYNTHESIS AND CHARACTERIZATION OF PVP-ZnO COMPOSITE FOR ENHANCED ANTIBACTERIAL ACTIVITY

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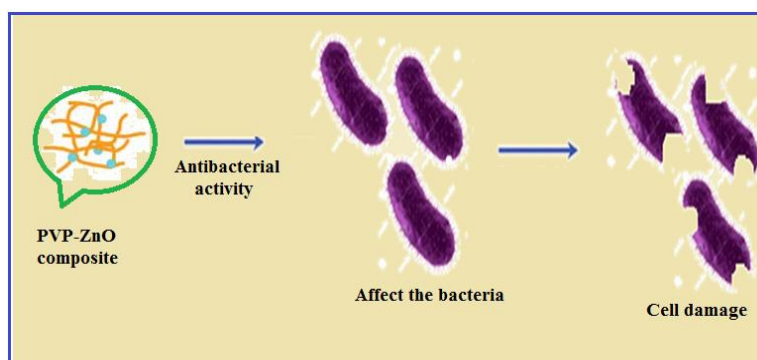
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Abstract

In this work, the PVP-ZnO Composites was prepared by simple co-precipitation method. The composites were prepared by using PVP as stabilizing agent, zinc nitrate as a source material and NaOH as a precipitating agent. The chemical bonding and crystalline behaviors of zinc oxide and PVP were confirmed by FT-IR and XRD analysis. The optical properties of composite are studied by UV-Vis DRS spectroscopy. Higher Resolution Scanning Electron Microscope (HR-SEM) and Transmission Electron Microscope (TEM) for morphological studies. The synthetic polymer connected ZnO particles was rice and rod like structure appeared in nanometer range confirmed by HR-SEM and TEM analysis. The surface topography image of PVP-ZnO nanocomposite was obtained in the average thickness of 12 nm was confirmed by AFM analysis. The PVP-ZnO composite tested against gram positive (*S.aureus*) as well as gram negative (*E.coli*) microorganisms. The PVP-ZnO composite material showed enhanced antibacterial activity. The enhancement of mechanical and antibacterial properties of PVP-ZnO composites would be a suitable candidate for implant application in biomedical field.

Key words: PVP, ZnO, Composite, Antibacterial activity.

Graphical Abstract



ALL SOLID-STATE HIGH-PERFORMANCE ELECTRIC DOUBLE LAYER CAPACITOR FABRICATED USING ENVIRONMENT BENIGN BIOMASS-DERIVED STARCH AS THE SOURCE FOR BOTH DEGRADABLE BIO-ELECTRODE AND BIO-POLYMER ELECTROLYTE

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Abstract

The demand for high energy and power density from electric double layer capacitors (EDLC's) urges the electrochemical energy storage community to develop the high surface area, hierarchically porous and low-cost materials. The challenges are intensive in developing supercapacitor materials with high performance, yet, there are limited numbers of works regarding the synthesis and electroactive components of EDLC, made with ecological awareness. Herein, we establish a naive one step chemical activation technique to convert *Artocarpus Heterophyllus seed* "starch" into bio-electrode for EDLC application. Chemical activation performed on AHS starch with $ZnCl_2$ resulted with a turbostratically structured, a specific surface area of $1841 \text{ m}^2/\text{g}$, inbuilt with an unexpectedly high concentration of nitrogen functionalities (2.1 at.wt %) and relatively porous, with interconnected micro and meso-porous network and high wettability. Adjacently, solution casting method was used to develop a highly flexible bio-electrolytic film from *Manihot esculenta* starch powder. The as-prepared bio-electrode and bio-electrolyte materials produced a volumetric capacitance of 240 Fg^{-1} at 0.5 mA, when employed as an all solid-state supercapacitor. Moreover, the device delivered a good specific energy (17 Wh kg^{-1}) and specific power (3823 W kg^{-1}), a high coulombic efficiency of 97% compared to other starch-based bio-polymeric electrolyte constructed so far. Also, the as-synthesized flexible, thermally stable, cheap bio-polymer electrolyte film degrades easily when buried under soil without hazarding the environment. Therefore, this approach is to expose the electrochemical energy storage efficiency of bio-degradable materials derived from biomasses in context with the EDLC application.

**SUBSTANTIAL INVESTIGATION TOWARDS CORROSIVE INHIBITION
PROPERTIES OF *STACHYTARPHETA JAMAICENSIS* LEAF EXTRACT ON MILD
STEEL IN 1.0 N HCl MEDIUM**

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Abstract

Corrosion control of mild is of technical, economical, environmental, and aesthetical importance. The use of inhibitors is one of the best options of protecting mild against corrosion. The environmental toxicity of organic corrosion inhibitors has prompted the search for green corrosion inhibitors as they are biodegradable, do not contain heavy metals or other toxic compounds. As in addition to being environmentally friendly and ecologically acceptable, plant products are inexpensive, readily available and renewable.

This paper reports the corrosion inhibition performance of *Stachytarpheta jamaicensis* leaf extract on Mild steel in 1.0N HCl was evaluated by both Potentiodynamic polarisation and Electrochemical Impedance spectroscopy (EIS). The experimental results show that the investigated inhibitor effectively retard the corrosion process that occurs on mild steel with a hydrochloric acid solution by providing a protective coating for the mild steel. From Electrochemical Polarisation studies corrosion current (I_{corr}) decreases with the increase of inhibitor concentration. Corrosion Potential (E_{corr}) value shifted to high negative value from -0.515mV to -0.432mV . This observed result indicates that the ligand is act as mixed type of inhibitor and attained the maximum of 90.70% IE. Charge Transfer Resistance (R_{ct}) value increased and also decrease of Double layer capacitance (C_{dl}) value by EIS studies. The maximum percentage of IE observed value 82.80% at 1000ppm inhibitor concentration. The inhibitor behaved as mixed-type. Surface Analysis (SEM/EDX) was also carried out to establish the corrosion-inhibitive properties of the samples.

Keywords: 1.0NHCl *Stachytarpheta jamaicensis* leaf, Mild steel, electrochemical studies, SEM/EDX.

PP 100

BIOLOGICAL SYNTHESIS AND CHARACTERIZATION OF SILVER NANOPARTICLES FROM SEEDS OF LAWSONIA INERMIS AND THEIR ANTIBACTERIAL ACTIVITY

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Abstract

Among the different methods employed for synthesis of nanoparticles, the biological method is most favorable and well established. In this study biological synthesis of silver nanoparticles from seeds of *lawsonia inermis* was carried out. Nanoparticle was produced due to reduction of silver ions from silver nitrate, the formation of which was monitored by uv-visible spectrophotometry. x-ray different (XRD) data illustrated the crystalline nature of silver nanoparticles, further these bio synthesized silver nanoparticles were found to be highly toxic against clinical pathogens such as klebsiella, salmonella, proteus s.aureus was analyzed by 20ml of inhibitor.

Keywords: Silver nanoparticles, Antibacterial activity, Biosynthesis, Clinical pathogens.

PP 101

STUDY OF INIBITON POTENTIAL OF SYNTHESIS GREEN INHIBITOR ON MILD STEEL IN ACID MEDIUM

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Abstract

Development of corrosion inhibitor based on organic compounds has much scope in industrial environments. In the recent years, Scientific interest has focused on Nitrogen – contain heterocyclic because of abundant data showing effective corrosion inhibitors for mild steel in acid medium. They particular components commonly distributed concerning plant source of the Rutaceae family. These are furano, pyrano, indoloquinoline, acridine and some of the naphthyridine alkaloids. The structural core of 3-indolylquinoline has been synthesized

by various conventional name reaction such as Michal additions, aldol condensations, Diels–Alder reactions, rearrangement of epoxides, Wittig reaction of the phosphorene these classical synthesis methods are well known and are frequently used for the preparation of pharmaceutical agents. Here our objective is focused on synthesis of a indolylquinoline alkaloids derivative of 3-(3-hydroxy-2,4-dioxo-1,2,3,4-tetrahydroquinolin-3-yl)indoline-2-carboxylic acid from available starting material by microwave assistant Eco-Friendly methodologies. which have more active ingredients and can reduce metal dissolution from the acid medium significantly.

PP 102

**SYNTHESIS OF CARBON DOPED WO₃ NANOMATERIALS FOR
PHOTOCATALYTIC APPLICATIONS**

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Abstract

Water has been polluted by industrial and agricultural sectors and it affects the environment. The organic dyes are mostly used in textiles, pulp and paper and food industries. The organic pollutants are the primary sources for contamination of the water due to their toxicity and non-biodegradability. Various methods have been proposed to remove the organic pollutants but it produces some secondary waste. Thus, another technique i.e the photocatalytic degradation process has been suggested as a good technique for the degradation of organic pollutants. Hence, it is necessary to develop highly effective, visible light active photocatalyst to solve the water pollution problems in the environment. Recent years, numerous active semiconductor metal oxides such as TiO₂, ZnO, SnO₂ and Fe₂O₃ have been synthesized and used for the treatment of organic pollutants in wastewater. Among the semiconductor metal oxides, WO₃ is one of the possible metal oxides for photodegradation process. WO₃ is one of the n-type and visible light active materials. The photocatalytic activity of WO₃ is limited due to the fast recombination of charge carriers. So, to suppress the recombination charge carriers by doping carbon into WO₃ and improving the photocatalytic activity of WO₃ nanomaterial. C doped WO₃ has been synthesized by various methods. Microwave irradiation method is one of alternative and attractive eco-friendly method to

prepare C doped WO₃ nanomaterial. In this work, we successfully synthesized C doped WO₃ nanomaterials by microwave irradiation method and subsequently structural characterization was carried out. The photocatalytic activity of the newly synthesized C doped WO₃ nanomaterial was also investigated and it will be discussed.

Keywords: Microwave irradiation; Metal oxide; Photocatalysis

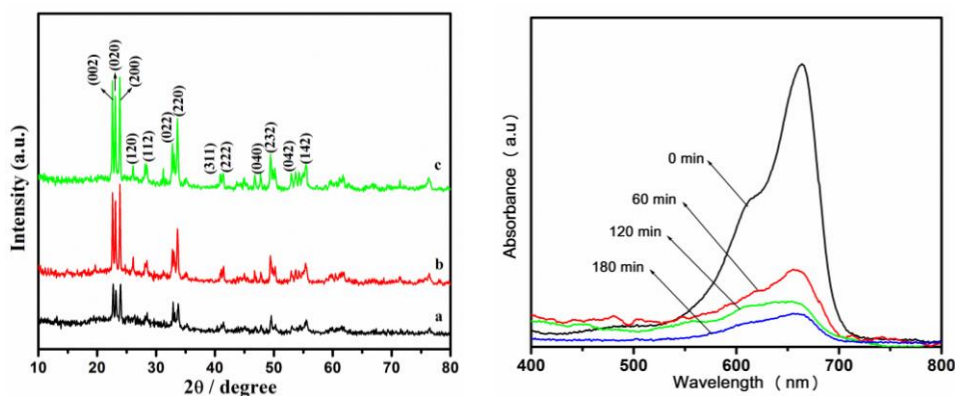


Fig. 1 & Fig. 2. UV-visible spectra of methylene blue in the presence of C-WO₃ XRD patterns of C-WO₃ nanomaterials prepared by microwave irradiation of 160 W for 10 min and varying starch 0.2g (a) 0.4g (b) and 0.6g (c)

PP 103

SENSING PERFORMANCE OF B₁₂N₁₂ NANOCAGE TOWARDS TOXIC AZIDES DETECTION: A COMPUTATIONAL STUDY

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Abstract

Nowadays Gas sensors are inevitable which detect the toxic and flammable gases that highly pollute our environment. Human beings are the major victim for the so called toxic gases in the modern era. BN nanostructures such as nanosheet, nanotubes, nanocapsules, nanocone and nanocage have received much attention towards gas sensor applications due to their excellent chemical stability, thermal conductivity and dipolar nature. Some organic and covalent azides are highly toxic and explosive in nature. Exposure to small amount of Sodium azide (NaN₃) resulted in dizziness, vomiting, rapid heart rate etc. So far varieties of materials (Carbon Nanotubes, Graphene sheet and Metal oxide Nanoparticles) are utilized to detect toxic azides, but none of them are better sensor materials. The present work

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deals with Detection of Toxic Azides such as hydrogen azide, Sodium salt of hydrogen azide and lithium salt of Hydrogen azide using $B_{12}N_{12}$ cage using Density Functional Theory (DFT) implemented in Gaussian 16 software package. The structural optimizations were performed at B3LYP/6-31+G* basis set. The Binding energy (E_B) is higher for NaN_3 (-36.96kcal/mol) compared to Lithium azide (-32.63kcal/mol) and Hydrogen azide (-3.42kcal/mol) adsorbed $B_{12}N_{12}$ cage. The negative sign indicates the existence of strong interaction between sodium azide and the considered $B_{12}N_{12}$ cage. The interaction distances were found to be 2.13 Å (N-H), 1.58 Å (B-N) and 1.59 Å (B-N) respectively for Hydrogen azide, Sodium azide and Lithium azide. The presence of covalent bond ensures more interaction and in turn more binding energy in the case of Sodium azide and Lithium azide complexes. Moreover, the Density of states (DOS) indicates that there is a drastic change in the band gap value of sodium azide adsorbed $B_{12}N_{12}$ cage. Hence it is believed that the $B_{12}N_{12}$ cage may serve as a better sensing material for toxic gas detector applications in the near future.

Keywords: $B_{12}N_{12}$ cage, Organic/Inorganic Azides, Density Functional Theory and Toxic gas Sensor

PP 104

ANTIBACTERIAL AND PHOTOCATALYTIC APPLICATION OF Ag DOPED ZnO NANOPARTICLES ASSISTED BY *VITIS VINIFERA*

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Abstract

Green synthesis of nanoparticles is gaining importance and has been suggested as possible alternatives to chemical and physical methods. The present work reports low- cost, green synthesis of Zinc oxide (ZnO) and Ag doped ZnO nanoparticles using *Vitisvinifera* extract. The biosynthesized nanoparticles were characterized by SEM, EDX, UV–Vis, and FT-IR. ZnO nanoparticle and Ag doped ZnO nanoparticle have been used for antibacterial and photocatalytic applications. The antibacterial activity of characterized samples was determined against Gram-positive and Gram-negative

bacteria. The obtained results revealed that the bacterial growth decreases with increase in concentration of biosynthesized ZnO nanoparticles. In addition, Gram-positive bacteria seemed to be more sensitive to ZnO & Ag doped ZnO nanoparticles than Gram-negative bacteria. The biosynthesized ZnO nanoparticles showed photocatalytic activity under the UV light enhancing the degradation rate of methyleneblue (MB), which is one of the main water- pollutants from textile industries.

Keywords: Green synthesis, *Vitis vinifera*, ZnO, SEM.

PP 105

SOIL MICROBIAL FUEL CELL ASSISTED SAFE DISPOSAL OF HEXAVALENT CHROMIUM ADSORBED CHALCAS KOENIGII LEAVES BIOCHAR

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Abstract

Soil-microbial fuel cell (SMFC) is an eco-friendly power production technology that generates electricity with bioremediation of heavy metal present in water or soil. The current study aims to generate potential using SMFC with simultaneous degradation of Chalcas Koenigii biochar adsorbed hexavalent chromium ions from aqueous solution. The biochar said was prepared by slow pyrolysis process at 450°C with yield percentage of 42. The prepared biochar was used to adsorb various concentrations of Cr (VI) ions such as 100, 200, 300, 400, 500, 600 and 700 ppm from aqueous solution by individual experiments. The chromium (VI) concentration before and after adsorption was determined by semicarbazide method. The amount of substrate adsorbed is then calculated and the obtained data obeyed nicely with Freundlich and Langmuir's model. The studied biochar possessing Cr(VI) ions adsorbed from 700 ppm chromium concentration was employed for further study in soil microbial fuel cell. Four soil microbial fuel cell (SMFC) were constructed in 150 mL glass beakers and graphite sheets of proper geometric dimensions were employed as electrodes. The soil near the anode varied in a such way that soil without amendment act as control, soil exposed to 700 ppm of Cr(VI), soil exposed to biochar and adsorption soil

Department of Industrial Chemistry, Alagappa University, Karaikudi. 167

exposed to 700ppm Cr(VI) absorbed biochar as experimental sets. The reduction process was effected in float cathode. The investigation showed that soil microbial fuel cell (SMFC) worked remarkably in presence of chromium absorbed biochar for 61 days. The obtained results were supported by FT-IR, SEM, and XRD studies. The study thus concluded that chromium contaminant adsorbed chalcaskoenigii leaves biochar were safely disposed in soil microbial fuel cell with subsequent power generation.

PP 106

**SYNTHESIS AND CHARACTERIZATION OF CHITOSAN-GOLD
NANOPARTICLES WITH PDMA HYBRID COMPOSITE**

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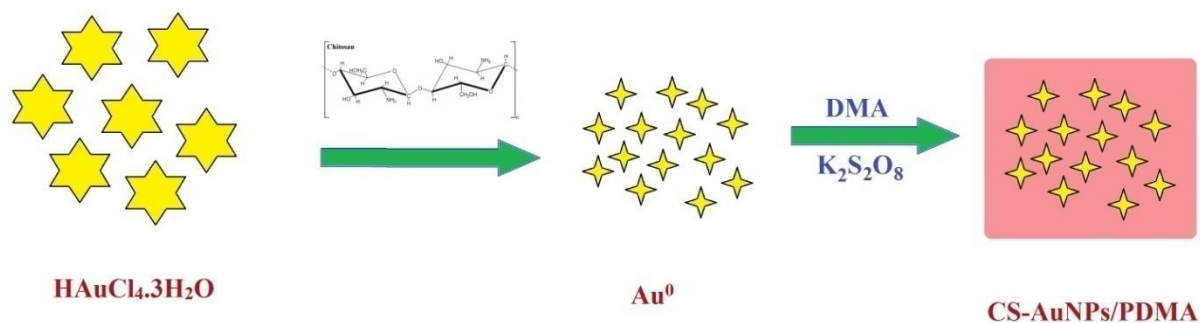
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Abstract

In this study, we report the catalytic bio-nanocomposite based on chitosan containing Gold nanoparticles AuNPs synthesis in situ is reported. The AuNPs were synthesised using green method without using any harmful chemicals. This method involves the use of chitosan biopolymer and a gold salt precursor. Unlike other methods the addition of external reducing and stabilizing agents to generate AuNPs, is not needed because these roles are played by chitosan. Additionally, the described this method added DMA and the gold nanoparticles contained in the bio-nanocomposite and then characterised by Fourier transform-infrared spectroscopic (FT-IR) analysis, X-ray diffraction (XRD), UV-Visible spectroscopy and Scanning electron microscopy energy dispersive spectroscopy (SEM-EDS). The particles size for the green synthesised AuNPs from chitosan was approximately 22 nm.

Keywords: Gold nanoparticles, Chitosan, Hybrid composite, XRD, SEM



Scheme 1. The diagram of the preparation route for CS-AuNPs/PDMA composite.

PP 107

MALEONITRILE SCHIFF BASE DERIVATIVE AS A CHEMOSENSOR FOR THE DETECTION OF Cr^{2+} AND HSO_4^- IONS AND ITS BIO-IMAGING APPLICATION IN LIVING CELLS

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Abstract

The novel 2,3-bis(2-hydroxy-5-nitrobenzylideneamino)maleonitrile Schiff base derivative was synthesized and characterized by ^1H & ^{13}C NMR, ESI-Mass and FTIR spectral studies. Both the colorimetric as well as fluorescent titration studies were performed with different cations and anions. The results suggested that the probe L was very selective and sensitive towards Cr^{2+} and HSO_4^- ions with significant spectral and color changes. The probe L exhibited $6.25 \times 10^5 \text{ M}^{-1}$ and $5.42 \times 10^6 \text{ M}^{-1}$ binding constant values for Cr^{2+} and HSO_4^- ions respectively. The detection limit of the probe towards Cr^{2+} and HSO_4^- was found to be 0.18 and 0.02 μM . The fluorescence turn-on recognition process for detection of Cr^{2+} and HSO_4^- is attributed to the restricted imine isomerization and blocking of intramolecular charge transfer (ICT) quenching process in the analyte-bound sensor. The selectivity of L for Cr^{2+} and HSO_4^- are based on the chelation - enhanced fluorescence effect (CHEF) mechanism. The time-resolved single-photon counting (TCSPC) studies were determined and the average lifetime value for the probe L and L+ Cr^{2+} and L+ HSO_4^- ions are 1.02 with 1.03 and 1.42 ns, respectively. The theoretical DFT studies well supported the experimental outcomes. The practical application of the probe in visualizing intracellular L+ Cr^{2+} and L+ HSO_4^- ions

distribution in live *Artemia saline* proved the low cytotoxicity and cell membrane permeability of the probe, which makes it capable of sensing Cr^{2+} and HSO_4^- ions in Breast cancer cells. Thus, the probe L could act as a selective recognition of chromium ions and hydrogen sulphate ions in living cell imaging.

Keywords: Maleonitrile Schiff base derivative, Chemosensor, DFT calculation, Bio-imaging sensor application.

PP 108

ADSORPTION OF NICKEL (II) FROM AQUEOUS SOLUTION ONTO ZnCl_2 ACTIVATED CARBON PREPARED FROM STEMS OF LEUCAS ASPERA

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Abstract

Adsorption of nickel (II) from aqueous solution using activated carbon prepared from stems of *Leucas aspera*. 850 W power of microwave radiation, 12 minutes of radiation time, 60 % of ZnCl_2 solution and 24 hours of impregnation time are the optimal parameters to prepare efficient carbon effective activated carbon. It was designated as MWLAC (Microwave assisted zinc chloride activated *Leucas aspera* carbon). Various adsorption characteristics such as dose of the adsorbent, agitation time, initial nickel (II) concentration, pH of the solution and temperature on adsorption were studied for removal of nickel (II) from aqueous solution by batch mode. Batch mode adsorption experiments were conducted. The characteristics of the MWLAC were determined by SEM, XRD, FTIR, BET analysis. The maximum removal efficiency of nickel (II) was 79% at pH 5. Under the chosen conditions, experimental data obtained were fitted with linearised forms of Lagergren and kinetic models. The sum of error squares percentage (SSE %) for first order and second order kinetics were 23.25 & 1.03 respectively. Thus this adsorption followed pseudo second order kinetics. The equilibrium adsorption data were analyzed with four isotherm models. Order of best fitting isotherm models were found to be Freundlich > Tempkin > Langmuir > Dubinin Raduskevich. The results in this study indicated that MWLAC could be employed as an adsorbent for the removal of crystal nickel (II) from an aqueous solution.

Key words: Adsorption, Nickel (II), Microwave assisted Zinc Chloride Leucas Aspera Activated Carbon (MWLAC), Isotherms, Kinetics.

PP 109

STUDIES ON EFFECT OF AQUEOUS SOLUBILITY, *IN-VITRO* DISSOLUTION RATE, ANTIMICROBIAL, ANTIBIOFILM ACTIVITY OF TORSEMIDE: B-CYCLODEXTRIN INCLUSION COMPLEX

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Abstract

The supramolecular structure of the inclusion complex of β -cyclodextrin (β -CD) with Torsemide drug (TRS) has been investigated. The 1:1 stoichiometry of complexation was achieved by phase solubility study, and the solid inclusion complex with 1:1 molar ratio was prepared by physical mixture, kneading and solvent evaporation methods. FT-IR, ¹H NMR, XRD, DSC and SEM analysis confirmed that the inclusion complex was formed. These results suggested that Torsemide could form inclusion complex with β -CD and was deeply included in the cavity of β -CD. Additionally, the dissolution rate and antimicrobial activity of the inclusion complex were greatly improved compared with that of Torsemide. These results strongly showed that the use of β -CD could be a promising approach to improve the physicochemical characteristics of Torsemide.

Key words: β -Cyclodextrin, Torsemide, Dissolution, Antimicrobial activity.

PP 110

GREEN CORROSION INHIBITOR FOR CARBON STEEL BY *ABUTILON INDICUM* POWDER/EXTRACT IN 1 M HCL USING WEIGHT LOSS METHOD

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Abstract

The corrosion inhibition of carbon steel in 1M HCl by *Abutilon Indicum* Powder/Extract has been studied by weight loss method. The results showed that increase in concentration of *Abutilon Indicum* Powder/Extract decreases the rate of carbon steel dissolution which indicates the inhibitive behaviour of *Abutilon Indicum* in acid medium. Inhibition efficiency of the plant extracts increased with increase in concentrations of extract suggesting physisorption mechanism. The significance of this area of research is primarily due to the fact that natural products are environmentally friendly and ecologically acceptable. Nevertheless, the known hazardous effects of most synthetic organic inhibitors and the need to develop cheap, non-toxic, and environmentally benign processes have now made researchers focus on the use of natural products. Maximum inhibition was attained 96% (1/2 h)/ 92% (1/2 h) at the concentration of 1g for *Abutilon Indicum* Powder/Extract.

Keywords: Plant corrosion inhibitor, Carbon steel, *Abutilon Indicum*, 1M HCl and Weight loss method

PP 111

DENSITY FUNCTIONAL STUDY OF THE ELECTRONIC AND STRUCTURAL PROPERTIES OF SEVERAL POLYMORPHS OF MgH₂

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Abstract

Hydrogen energy is considered to be the most promising candidate for renewable energy storage and magnesium hydride is an attractive system for hydrogen storage. This paper focuses primarily on the study of the electronic and structural properties of the six considered polymorphs of magnesium hydride (α - rutile TiO₂, P42/mnm, β - cubic modified CaF₂, Pa3, γ - orthorhombic PbO₂, Pbcn, δ' - orthorhombic, Pbcn and cubic - Fm3 m). The total energy calculations are performed in the framework of the density functional theory using the generalized gradient approximation (GGA-PBE). Furthermore, the energy band structure, the density of states (DOS), bulk modulus and its derivative are calculated for all the six possible structures.

The Wyckoff positions of Mg, H atoms for α -MgH₂ (P42/mnm) are 2a,4f and their fractional coordinates are x(0.0000,0.3043), y(0.0000,0.3043), z(0.0000,0.0000) respectively. The parameters E_0 and V_0 obtained by fitting the EOS and those corresponding to the equilibrium structures are in very good agreement with the previously reported results, which indicates the validity of the EOS for the investigated systems. In the band structures for all the systems investigated, the magnesium atoms become positively charged with about 0.6 |e-| by transferring about 0.5 |e-| from the 3s orbital to the orbital 1s of each nearest-neighbor hydrogen atoms and about one electron to its own 3p states. The total and partial DOS of the studied polymorphs of MgH₂ shows stronger hybridization between H and Mg atoms near the Fermi level, which indicates the strong interaction between H and Mg atoms. From these studies it can be seen that the tetragonal MgH₂(α -MgH₂) is the most stable structure and the bonding in α -MgH₂ must be a combination of the covalent and the ionic characters.

PP 112

CYCLOPENTADIENYL RUTHENIUM COMPLEXES OF FERROCENYL LIGANDS: SYNTHESIS, SPECTRAL CHARACTERIZATION AND THEIR BIOLOGICAL EVALUATION

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Abstract

Four new hetero binuclear Ru(III)/Fe(II) complexes were prepared from acetylferrocene-4(*N*)-substituted thiosemicarbazone ligands and characterized by various spectral techniques like IR, UV-Vis, EPR and ESI-MS. The ligands coordinated to ruthenium metal by utilizing their azomethine nitrogen and thiolate sulphur atoms. The binding affinity of the ligands and complexes with nucleic acid (Calf Thymus DNA) and bovine serum albumin were examined by means of absorption and emission methods. The complexes exhibited better binding ability than the ligands. Three dimensional fluorescence studies with bovine serum albumin indicated changes in molecular micro-environment of protein.

PP 113

**EVALUATION OF GROUNDWATER QUALITY IN THE COASTAL STRETCH OF
CUDDALORE DISTRICT, TAMILNADU, INDIA**

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Abstract

The hydro-geochemical study was carried out to the coastal region of Cuddalore district, which lies on the southeast coast of India in Tamilnadu. The rapid urbanization, extensive agriculture and industrial activity have deteriorated the quality of ground water. In order to assess the groundwater quality, 18 groundwater samples had been collected in year 2018 pre-monsoon, which has been analyzed for pH, electrical conductivity (EC), total dissolved solids (TDS), total hardness (TH), major cations like sodium, potassium, calcium, magnesium, anions such as bicarbonate(HCO_3), chloride, sulphate. This parameters suitability for domestic purpose by comparing with WHO and Indian standards. TDS, Sodium Adsorption Ratio (SAR), and permeability index were used for suitability irrigation. However, the most of the parameters exceeding the permissible limit recommended by the World Health Organization (WHO 2005). Analysis of various water quality parameters indicated the contamination of groundwater in the selected sites.

Keywords: Water quality, Ground water, Hydro-geochemical, Cuddalore district.

PP 114

**HOST-GUEST COMPLEX OF 4-HYDROXYBENZOPHENONE: β -
CYCLODEXTRIN AND ITS APPLICATION FOR ENHANCING THE UV
PROTECTIVE ABILITY OF COTTON FABRIC**

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Abstract:

The inclusion complexation behavior, of 4-hydroxybenzophenone (HBP) with beta-cyclodextrin (β -CD) and its ultraviolet rays protection ability on cotton fabric were investigated. Absorbance intensities of DHBP were enhanced due to the formation of a 1:1 inclusion complex with β -CD. The inclusion complex formation was characterized using FTIR and NMR spectral analysis. Ultraviolet protection factor estimation for the cotton fabric treated with HBP: β -CD inclusion complex showed enhanced ultraviolet rays protection behavior.

PP 115

SUPRAMOLECULAR COCRYSTALS OF 18-CROWN-6 WITH 5-NITROISOPHTHALIC ACID: SOLVENT EFFECT AND OPTICAL NONLINEARITIES

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Abstract

Novel cocrystals of 18-crown-6 (18C6) with 5-nitroisophthalic acid (5NIPA) have been prepared by reaction in a solution of $\text{CH}_3\text{OH} - \text{H}_2\text{O}$ (2:3, v/v) and $\text{C}_2\text{H}_5\text{OH} - \text{H}_2\text{O}$ (2:3, v/v) systems. The cocrystals 18-crown-6.5-nitroisophthalic acid. $\text{CH}_3\text{OH}.2(\text{H}_2\text{O})$ (**I**) and 18-crown-6.5-nitroisophthalic acid. $3(\text{H}_2\text{O})$ (**II**) have been characterized by X-ray diffraction and constructed supramolecular assembly is thoroughly investigated. CH_3OH incorporation inducing centrosymmetric crystallization and acentric crystal packed supramolecular construction in presence of ethanol are the highlights of the study. Intermolecular interactions are quantified by Hirshfeld surface analysis. First-order molecular hyperpolarizability estimated by theoretical calculations indicate a significant microlevel nonlinearity in both cases and Z-scan studies suggest a promising third-order nonlinear optical behaviour. Supramolecular assembly afford multiple strong $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds creating a facile atmosphere for optical nonlinearity and mainly $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds stabilize the structure.

PP 116

FUNDAMENTALS OF SUPERCAPACITORS: BASED ON NANOMATERIALS FOR ENERGY STORAGE

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Abstract

With the rapid growing market of hybrid-electric vehicles and electronic devices, there has been an ever urgent demand for electric energy storage devices with extremely high energy/power densities and good cycle life time. Super capacitors are emerging as one of the most promising energy storage device for the future energy technology. Transition metal oxides are one of the suitable materials for pseudo capacitors because of their existence in different oxidation states which obviously increases the extent of the faradaic reactions. Nickel oxide (NiO) is one of the emerging and promising electrode materials for the energy storage application due to its high thermal stability, high chemical stability, high theoretical specific capacity, abundant in nature, environment friendly at affordable cost. In this report, we focused on the pure nickel oxide nanoparticles which has been synthesised by sol- gel method in which nickel nitrate hexahydrate acts as a precursor and citric acid serves as a surfactant. The synthesised NiO has been characterized by Raman spectroscopy. Further, the supercapacitive performance of the NiO nanoparticles were examined by means of cyclic voltammetry (CV) at a scan rate of 5, 10, 20, 30, 50, 100mVs⁻¹ in the potential range of 0-0.5, Galvanostatic charge discharge test 0-0.45V potential windows in 1M KOH and electrochemical impedance spectroscopy (EIS). The nanoparticles exhibited a high specific capacitance of 166.66 Fg⁻¹.

Keywords: Faradaic reactions, Nickel oxide Nanoparticles (NiO), nickel nitrate hexahydrate, Super capacitor application.

**BENT-CORE LIQUID CRYSTAL ALIGNMENT OVER A FUNCTIONALISED
FLEXIBLE SUBSTRATE**

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Abstract

A cellulose acetate containing flexible polymer film is chemically functionalized with a bent-core liquid crystal (BCLC) compound for the effective alignment of the nematic phase exhibited by bulk BCLC samples at the substrate-LC interface. The polymer substrate is surface functionalized with dimethylchlorosilane-terminated BCLC molecules that provided necessary structure and shape compatibility for the bulk LC sample to be aligned. The surface attachment was achieved *via* a simple procedure which involved the pre-treatment of the cellulose acetate containing over-head projector polymer film using piranha solution followed by chemically attaching the BCLC compound through silane condensation reaction. Surface characterization of this BC modified flexible film was carried out through X-ray photoelectron spectroscopy (XPS), attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy, contact angle (CA) and atomic force microscopy (AFM) techniques. Utility of the BC modified flexible substrates for the alignment of bulk LC sample is assessed for a nematic phase (N) displayed by both BC and rod-like LC samples. Remarkably, the chemically modified polymer substrates are highly efficient in vertically aligning both the BC and rod-like LC samples at the substrate-LC interface, in comparison to their unmodified and octadecyltrimethoxysilane modified counterparts. The described method is simple, reproducible, surface modified substrates are highly stable and more importantly reusable. The demonstrated method for the alignment of BCLCs advances a step forward towards the realization of applications proposed for these fascinating compounds.

Keywords: Liquid crystal, Bent-core, Monolayer, Flexible polymer substrate, Nematic, Homeotropic alignment.

PP 118

HYDROTHERMAL SYNTHESIS OF NiMn₂S₄ NANOSHEET ARRAYS FOR HIGH-PERFORMANCE OF SUPERCAPACITOR APPLICATIONS

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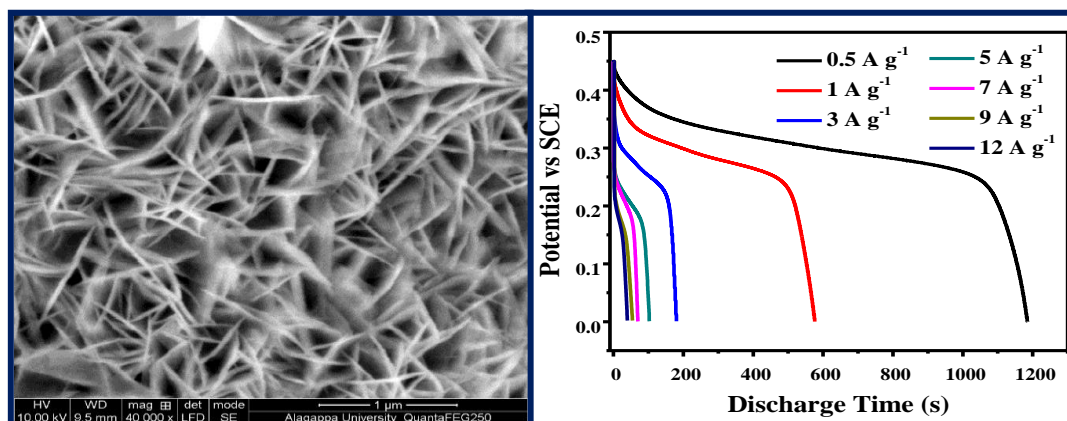
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Abstract

Here, we report a facile synthesis of binder free NiMn₂S₄ nanosheet arrays by a simple hydrothermal route. We demonstrate that morphologies of various three-dimensional NiMn₂S₄ nanosheet arrays manipulated by tuning the reaction additive amount alone in the reaction. The nickel foam grown on the surface of NiMn₂S₄ nanosheet arrays shows a large electro active surface area and superior electrochemical properties. The structure and morphology were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR) and scanning electron microscopy (SEM). The electrochemical characterization of cyclic voltammetry, galvanostatic charge-discharge and impedance analysis. The electrode made of NiMn₂S₄ nanosheet arrays shows greatly improved electrochemical performances with an ultrahigh specific capacitance of 1305 Fg⁻¹ at a current density of 0.5 A g⁻¹. The electrode also exhibits an excellent cycling stability by retaining 83.2 % of its original state after 2700 cycles, rendering the NiMn₂S₄ nanosheet arrays potential electrode material for high performance super capacitors.

Keywords: NiMn₂S₄ nanosheet arrays, Hydrothermal method, Specific capacitance, Supercapacitor, Cyclic stability.



THE EFFECT OF ZrO₂ FILLER PARTICLE CONCENTRATION ON THE IONIC CONDUCTIVITY VARIATION OF PVC/PEO BASED GEL POLYMER ELECTROLYTE

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Abstract

In this work an attempt has been made to study the variation of ionic conductivity and structural changes on the gel polymer electrolyte comprising of PEO (70wt%) / PVC (30wt%) / DEC (12wt%) / LiClO₄ (8wt%). With the changes in the ZrO₂ concentration in weight percentages.. Out of the three samples prepared with ZrO₂ (4wt%), ZrO₂ (8wt%) and ZrO₂ (12wt%), the film with ZrO₂ (8wt%) exhibited maximum ionic conductivity (1.45×10^{-3} S/cm). The XRD pattern of this combination also showed a higher degree of amorphousity which is the consequence of better ionic conductivity. The best kind of complex formation for this sample has also been observed from the appearance of new peaks, shifting and disappearance of existing peaks in the FTIR analysis of the prepared samples sample. The photoluminescence studies were carried out for all the films at an excitation wavelength of 280 nm and the corresponding emission spectra was obtained around 380 nm. The film with PEO (70wt%)/ PVC(30wt%) / DEC (12wt%) / LiClO₄ (8wt%) / ZrO₂ (8wt%) showed minimum fluorescence emission intensity. It has been reported that the fluorescence intensity is inversely proportional to the local free volume and which in turn is directly proportional to the local viscosity of the electrolyte medium. The optical band gap value of this film calculated from the UV-Visible spectra was also found to be minimum. Hence this kind of composite polymer electrolyte is suitable for Li ion battery applications.

PP 120

**SYNTHESIS, CHARACTERIZATION OF SrO/ β -CD NANOCOMPLEX
FOR BIOLOGICAL APPLICATION**

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Abstract

We have reported the metal nanoparticle (NPs) doped on beta cyclodextrin (β -CD) for complex formation. The nanoparticle synthesis in chemical approached by hydrothermal method. This work is complex formation on inorganic salt of metal oxide SrO react with organic salt of glucose containing the polymer of β -CD complex have formed 1:1 ratio are prepared by sol - gel method. The beta cyclodextrin one of the cluster compound so, It has been simply complex formed in metal oxide nanoparticle. The study in crystalline structure, functional groups, absorption, various morphology and elemental analysis for identify the characterization of XRD, FI-TR, UV-DRS, and FE-SEM with EDX analysis. The SrO/ β -cyclodextrin complex formed present in identify the range crystalline structure of nanoparticle size 45.85 nm. In finally moreover, the biosynthesized SrO NPs and composite formed in SrO/ β CD complex are showed significant antibacterial activity against Gram-negative bacteria such as E.coli and S.aureus of Gram-positive bacteria.

Keywords: Metal oxide, Beta-cyclodextrin, Complex formation and biological activity.

PP 121

**GREEN SYNTHESIS AND CHARACTERISATION OF IRON NANOPARTICLE
FROM GREEN TEA LEAF EXTRACT AND THEIR WASTE WATER
TREATMENT**

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Abstract

The interest in synthesizing nanoparticles in an easy and environmental friendly way has been increasing in the recent years. Physical and chemical methods are conventionally used for synthesis of nanoparticles, however due to limitations of these methods, the focus of research has been recently shifted towards the development of clean and eco-friendly synthesis protocols. The green synthesis of iron nanoparticles has been achieved using environmental acceptable plant extract. It was observed that the aim of this study is to synthesize iron nanoparticles using green tea leaf extract in an environmental and sustainable way. The synthesized iron nanoparticles were characterized using UV and XRD spectroscopy. This study shows that the iron nanoparticles can be synthesized using green tea leaf extract and their waste water treatment.

Keywords: Iron nanoparticles, green tea leaf extract, characterization, waste water treatment.

PP 122

EXPLORING THE RHIZOBIUM LEGUMINOSARUM- LEGUME ROOT NODULE ASSOCIATED BACTERIA RL(LRNAB) AS POTENTIAL CORROSION INHIBITOR ON MILD STEEL IN ACIDIC MEDIUM

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Abstract

The *Rhizobiumleguminosarum* is isolated from legume root nodule of *Vignamungo* and screened for exopolysaccharide production along with biofilm forming ability by bacterial attachment assay. The selected bacterial isolate is used for the corrosion inhibition on mild steel in 0.5M H₂SO₄ using gravimetric analysis at different temperatures between 293 and 313K. Adsorption isotherm models, electrochemical impedance spectroscopy, potentiodynamic polarization measurements. UV-Visible spectroscopy, FT-IR spectroscopy, SEM- EDAX, AFM and XRD confirmed the adherence of biofilm and inhibition of corrosion on mild steel surface. Temperature studies revealed that the inhibition efficiency is observed to be maximum at 303 K and increase with increasing the concentration of bacterial inoculum. Impedance diagram revealed that an increase of biofilm forming bacterial isolate concentration increased the charge transfer resistance and decreased double layer

capacitance. Polarization curves indicate that biofilm forming bacterial isolate is a mixed type inhibitor.

Keywords: Corrosion inhibition, bacteria, *Rhizobiumleguminosarum*.

PP 123

MANAGEMENT OF CASSAVA CROP RESIDUES USING TERMITES

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Abstract

The roots of Cassava plants are a rich source of carbohydrates and the shoot is considerably a remainder after the harvest. These residues of the plants are used in different ways such as ethanol production but in a certain point of time, the residues are forced to be burnt in order to process the agriculture field. If left, the cassava residues is slowly degraded by the microorganisms but it is somehow difficult because of the presence of lignin in the plant. Termigradation is a concept developed at the Centre for Pollution Control and Environmental Engineering to process bio-waste rich in lignin and cellulose.

The main aim of this work is to degrade cassava residues by placing the cassava residue (1 kg dry weight basis) in a chamber providing optimum environment for the termites to survive. The termite species *Hypotermesobscuriceps* was used in this study to process the substrate. The chamber and the reactor were designed in the manner that the termite attains the maximum performance. Initially the reactor showed 50.6 to 52.3 % efficiency in processing the substrate at 30th day and at the end of the 180th day the consumption of the substrate increased up to 81%. Thus the study shows that cassava residue can be utilized in a beneficial way which otherwise is generally burnt causing air pollution. In addition, the termite processed soil can be used as a manure/ soil conditioner.

PP 124

**PREPARATION AND CHARACTERIZATION OF PVP-ZnO-CuO COMPOSITE
FOR ENHANCED ANTIBACTERIAL ACTIVITY**

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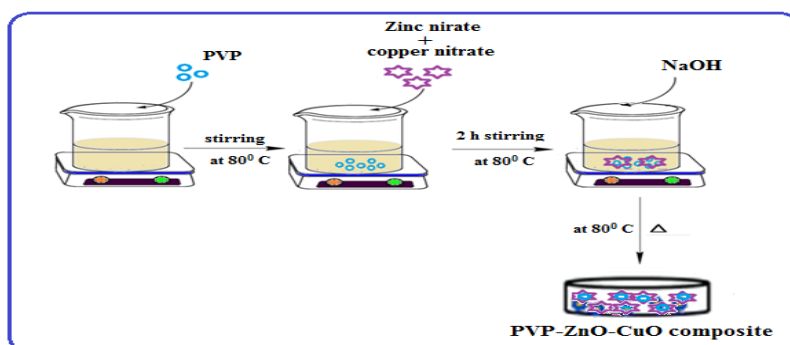
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Abstract

The polymer based nanocomposite has been recognized as the most attractive field in several research areas due to its dynamic properties. The mixing of polymers and inorganic metal oxide has become an active field of research and received much attention owing to the significant electrical, thermal, mechanical, magnetic properties. In the present investigation, synthesis of ZnO- CuO nanoparticles is achieved by employing Zinc nitrate and copper (II) nitrate as the initial agents and NaOH as a precipitating agent. Poly vinyl pyrrolidone (PVP) is used to stabilize the aggregation of metal atoms. It is the most commonly used polymer in the preparation of metal oxide because of its distinct shape and it consists of repeating chains of polar groups, which helps to dissolve metal salts and facilitate transport. The ZnO-CuO/PVP nanocomposite was synthesized via the co- precipitation method and characterized by UV-Vis, FT-IR and XRD analysis and the morphological features of the composite were investigated by HR-SEM analysis. The prepared nanocomposite is then used as an antibacterial agents tested against the Gram positive (*S.aureus*) and Gram negative (*E. coli*) bacterial pathogens.

Keywords: Composite, ZnO-CuO, PVP, Antibacterial activity.

Graphical Abstract



PP 125

MIXED METAL OXIDE NANOCOMPOSITES OF Ce/Ti/Mo – SYNTHESIS AND CHARACTERIZATION FOR SUPERCAPACITOR APPLICATION

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Abstract

Literature shows that transition metal oxide nanoparticles can enhance surface electrochemical reactivity and increase the capacity retention capability for higher number of cycles. The high redox potential of these metal oxide nanocomposites is expected to provide a higher potential window as well as increase the specific capacity and energy density of the system.

The present study describes fabrication and electrochemical analysis of Ce/Ti/Mo mixed metal oxide nano composites for supercapacitor application. The nanocomposites were synthesized from their precursors using hydrothermal route. The samples were characterized using UV-Vis, IR, X-ray diffraction (XRD), Field emission scanning electron microscope (FESEM) and Transmission electron microscope (TEM). UV-Vis studies show absorption at 380nm due to charge-transfer transitions from oxygen 2p to cerium 4f which overturns the well-known f-f spin orbit splitting of the Ce 4f state. IR spectrum shows the presence of all three metal-oxide stretching vibrations. XRD shows presence of sharp peaks which may be due to crystalline nature of the composite. EIS is used for measuring the electrochemical performance of the mixed metal oxide nanocomposites. The capacitance values are in the range of 400 F/g showing that Ce/Ti/Mo mixed metal oxide nanocomposites are an appropriate electrode material for supercapacitor device fabrication.

Keywords: supercapacitor, hydrothermal, FESEM.

PP 126

IODINE–CATALYZED RING CONTRACTION REARRANGEMENT OF TETRAARYLPIPERIDIN-4-ONES TO 5-ARYL-2-METHOXY-2,4-DIPHENYL-1H-PYRROLE-3-ONES

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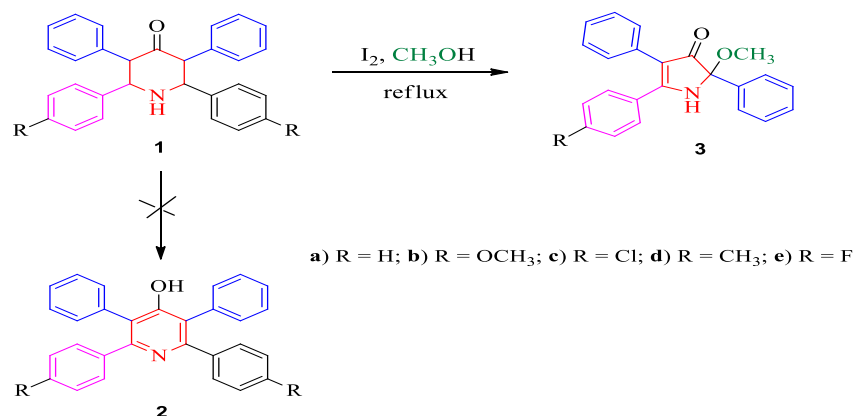
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Abstract

Iodine in methanol has been found to be effective in the aromatization of carbo and heterocyclic six membered compounds. In an attempt to dehydrogenate tetra aryl substituted piperidin-4-one to pyridine-4-ol (**2**), the oxidative aromatization of 2,3,5,6-tetraarylpiperidin-4-one (**1**) was aimed employing iodine and methanol. It was anticipated that the presence of four aryl groups could drive the piperidone ring to complete aromatization providing conjugation delocalizing the pyridyl ring electrons. The product obtained has been shown to be 2,4,5-triaryl-2-methoxy-1H-pyrrol-3-one (**3**) (*vide infra*) instead of the expected 3,5-diphenyl-2,6-diaryl pyridin-4-ol (**2**). The unambiguous structural proof for **3** has been provided by the NMR data and the single crystal X-ray analysis of one of the compounds **3e**.



Scheme 1. Synthesis of 5-aryl-2-methoxy-2,4-diphenyl-1H-pyrrol-3-ones

PP 127

POROUS ORGANIC POLYMER DERIVED METAL-FREE CARBON COMPOSITE AS A TRIFUNCTIONAL ELECTROCATALYST FOR CO₂ REDUCTION AND WATER SPLITTING

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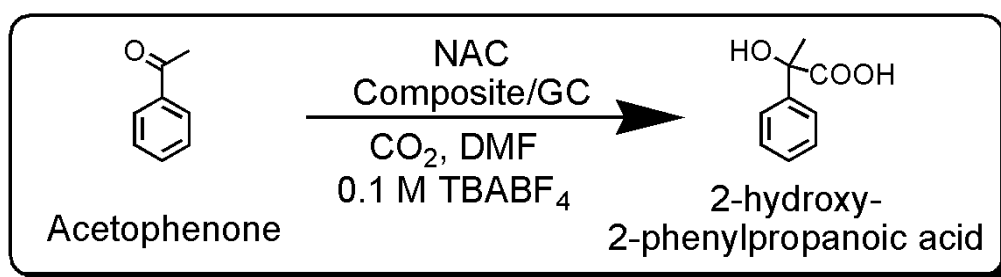
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Abstract

A hybrid porous organic polymer comprising of phenylenediamine, phloroglucinol and triazine was synthesized, carbonized at different temperatures and characterized.¹ Solid state ¹³C and ¹⁵N CP-MAS NMR spectra showed evidences for the presence of the three moieties in varying composition. Raman analysis of the carbonized samples exhibited varying degrees of graphitization and XRD analysis showed patterns corresponding to N-doped amorphous carbon. Surface morphological characteristics obtained from SEM and TEM analysis confirm different morphologies with slight variations in the particle size and porosity formed by inter-linking of irregular shapes with a wide range of size distribution of several micrometres. Further, the prepared metal-free catalysts were evaluated for their electrocatalytic activity by performing electrocarboxylation, hydrogen and oxygen evolution reaction (OER) under standard conditions. Sample carbonized at 700 °C (PPT-700) showed excellent catalytic activity towards electrocarboxylation of 4-bromoacetophenone in 0.1 M TBABF₄/DMF² medium and OER in 1 M KOH as indicated by their onset potential and current density, whereas the sample calcined at 900 °C (PPT-900) exhibited excellent HER activity in 1 M H₂SO₄. The results were further supported by XPS analysis. XPS analysis of PPT-500 showed the presence of pyrrolic, oxidized and molecular nitrogen's, PPT-700 showed the existence of pyridinic, pyrrolic and quaternary nitrogen and PPT-900 exclusively had pyridinic and pyrrolic nitrogen's. The catalytic activity of PPT-700 towards electrocarboxylation and OER activity is ascribed to the presence of pyridinic, pyrrolic and quaternary nitrogen's, whereas the presence of pyridinic and pyrrolic nitrogen's are responsible for the enhanced HER activity of PPT-900 sample. Overall, the results clearly indicate that these materials have promising and attractive electrochemical applications by further fine tuning of their structural properties.



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PP 128

**FACILE SYNTHESIS AND *IN VITRO* MICROBIAL EXPLORATION OF FURYL
BASED 2-CYANOIMINODIHYDROPYRIMIDINES**

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Abstract

The target pharmacophore, 2-Cyanoimino-4-Aryl-6-(5-Methyl-fur-2-yl)-3,4-dihydro-1H-pyrimidines were synthesized in a simple and hazardous free route : the furyl substituted styryl ketones obtained from Claisen- Schmidt condensation of aromatic aldehydes with 2-acetyl-5-methylfuran in a basic alcoholic medium and the formed styryl ketones on further treatment with cyanoguanidine in the presence of base affords the titled compounds. The synthesized eight pyrimidine derivatives are characterized with the help of IR, NMR, MASS and Quantum Mechanical calculations. The *in vitro* antimicrobial screening proves the potency of synthesized compounds against tested microbes.

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PP 129

INVESTIGATION ON THE BINDING INTERACTION BETWEEN 2,4-DINITROANILINE AND γ -CYCLODEXTRIN USING SPECTROSCOPIC TECHNIQUES

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Abstract

Effect of solvents, buffer solutions of different pH and γ -cyclodextrin(γ -CD) on the absorption and fluorescence spectra of 2,4-Dinitroaniline(2,4-DNA) have been investigated. The inclusion complex of γ -CD with 2,4-DNA is investigated by UV-vis, fluorometry, UV-DRS, FTIR and XRD methods. The Stokes shifts of 2,4-DNA correlated with various solvent polarity scales, suggest that the 2,4-DNA molecule is more polar and the change in dipole moment is large in the S_1 state. The pKa value of 2,4-DNA is lower than aniline (pKa~18.46) which indicates that 2,4-DNA molecule more acidic than aniline. The pKa value for the equilibriums is determined by spectrophotometrically and the stoichiometric ratio of the inclusion complex was found to be 1:1 and the binding constant of the inclusion complex at 303 K were calculated using Benesi-Hildebrand plot and the inclusion interaction was examined and the thermodynamic parameter (ΔG) of inclusion process is also determined. UV-DRS, FT-IR and XRD results suggest 2,4-DNA formed a solid inclusion complex with gamma-CD and the 2,4-DNA play a significant role in gamma-CD aqueous medium.

Keywords: 2,4-Dinitroaniline(DNA), Solvent effects, pH effects, γ -Cyclodextrin, Inclusion complex.

PP 130

ANTIBACTERIAL ACTIVITY, STRUCTURAL, OPTICAL AND MORPHOLOGICAL PROPERTIES OF AI DOPED ZnO NANOPARTICLES SYNTHESIZED BY SOL-GEL METHOD

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Abstract

ZnO nanoparticles were synthesized by sol-gel method. The synthesized particles were characterized by XRD, SEM, EDAX, UV, FTIR and antibacterial studies. The X-ray diffraction studies reveals that the synthesized ZnO nanoparticles have wurtzite structure and the particle size varies from 10 to 26 nm. A change in morphology after doped with aluminum has been observed. The Energy Dispersive X-Ray Diffraction Spectroscopy (EDAX) reveals that the elemental composition of prepared samples and the incorporation of the Al ions into the ZnO lattice. The antibacterial activities of Al doped ZnO nanoparticles were examined using the disc diffusion method against four pathogenic bacteria (*Escherichia coli*, *Staphylococcus aureus*, *Aspergillus flavus* *Aspergillus niger*) were observed.

Keywords: Zinc Oxide, Nanoparticles, Antibacterial, XRD, UV, FTIR, SEM

PP 131

SPECTRAL STUDY OF EXCITED-STATE PROTON TRANSFER PROCESS OF 2-NAPHTHOL: α -CYCLODEXTRIN IN INCLUSION COMPLEX AND CETYL TRIMETHYL AMMONIUM BROMIDE

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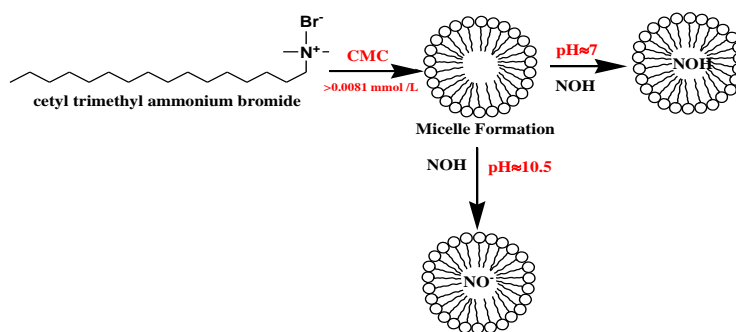
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Abstract

In the present study, inclusion complex formation between 2-Naphthol (NOH)/ α -Cyclodextrin (α -CD) and Cetyl trimethyl ammonium bromide (CTAB)/NOH have been presented. The excited state proton transfer reaction of the NOH is in the neutral form to an anionic form were observed in the aqueous, α -CD and CTAB mediums. Here, the emission intensity of the anionic form is enhanced for both CTAB and α -CD mediums, compared to the neutral form. The mechanism behind that is the cationic surfactant induced the CMC (Critical Micelle Concentration) by forming the inclusion complexes with micelles on the surface of both neutral and anionic form of NOH. The absorption spectroscopy is used to enhance the ability to detect CMC changes in the neutral form of NOH to the anionic form of NOH. Moreover, the binding constant of the inclusion complexes was calculated by the

Benesi-Hildebrand equation and the stoichiometric ratio 1:1 is proposed by this method. The binding constant is higher for CTAB than α -CD medium because, the micelles are strongly bound to the surface of NOH. The overall results demonstrated that the interaction of cationic surfactant (CTAB) with an anionic form of NOH exhibited higher binding constant and critical micelle concentration.

Keywords: 2-Naphthol, α -Cyclodextrin, Cetyl trimethyl ammonium bromide, Excited state proton transfer.



OP 67

EFFECT OF MOISTURE, TEMPERATURE AND HUMIDITY ON THE MANUFACTURE OF FIREWORK COMPOSITION

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Abstract

Pyrotechnic mixtures are at risk to explosive decompositions. The effect of moisture, humidity and temperature are studied on the manufacture of firework composition like White powder (Aluminium, Sulphur and potassium nitrate) and Inner core of the colour pellets during the mixing and filling of above composition. This mixtures are studied with different particle size (grade) of Aluminium, varying the composition of Aluminium, sulphur and potassium nitrate, different size of inner core colour pellets are exposed to different conditions like varying the temperature and different percentage of relative humidity. The moisture content, thermal characteristics, stability of composition, purity and any other physical changes of above composition of pure sample and moisture loaded samples were

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studied by Hot air oven method, Differential Scanning Calorimeter (DSC), Thermo gravimetric differential thermal analyzer (TG-DTA), Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) and Fourier Transform Infrared Spectroscopy (FT-IR) respectively.

Keywords: Pyrotechnic mixtures, White powder, thermal characteristics, firework composition.

PP 132

BIOSYNTHESIS OF IRON OXIDE NANOPARTICLES BY USING *ACORUS CALAMUS* EXTRACT AND THEIR DNA INTERACTION STUDIES

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Abstract

Biosynthesis is that the usage of natural plants has offered a reliable, simple, nontoxic and eco-friendly method. In this work, it was used a convenient and biosynthetic method for the synthesis of iron oxide (Fe_3O_4) nanoparticles with the size of 5 nm by reducing the ferric ions with the leaf extract of *Acorus Calamus* Linn. The UV-Visible spectra, XRD, TEM and AFM techniques confirmed the structure, composition, average particles size, and surface morphology of iron oxide nanoparticles. The phyto constituents and their functional groups were authenticated by FT-IR analysis. Polyphenol, reducing sugar etc. present in the plant extract reduced ferric ions to iron oxide nanoparticles. The nanoparticles were further stabilized by polyethylene glycol which was used not only to stabilize but also reduced the size of the nanoparticles. Iron oxide nanoparticles with copper ions could able to bind with herring sperm DNA. These interactions were supported by AFM studies.

AUTHOR

INDEX

AUTHOR INDEX

- Abinaya V 77
Abraham John S 38
Aiswarya R 77
Aiswarya V 78
Akilan A 79
Alagar M 109
Alphonse Fr.L 80
Ambika S 159
Anancia Grace A 81
Anandakumaran J 82,154
Anisha Shaji 23
Antony rajam J 15
Anusiya V 83
Aparna M 16
Archana Devi C 83
Arokia Nepolean Raj A 139
Arokiasamy A 126
Aruldeepa V 84
Arumugam Shanmuga Priya 171
Ashok Kumar Mishra 3
AsmathaBeham B 179
Azhagumeenal N 85
Balaji M 17,78,88,99,114,123,131,134,178
Balakrishnan B 63
Balakrishnan C 66
Balalakshmi C 141
Balambiga B 86
Balasubramanian K. K 121
Balu P 18
Bama K 99
Banukarathi G 104
Banupriya G 178
Baranipriya Sampathkumar 94
Baskaralingam Vaseeharan 172
Bharathi E 88
Bharathi K 89
Bhuvanalogini G 18
Bhuvaneshwari D.S 181
Bhuvaneshwari G 89
Bhuvaneshwari V 160
Boomi P 136
Brindha V.G 19
Cathrine L 26
Chandramohan A 109, 110
Chinnappa Arumugam 90
Chinnasamy K 92
Chitra S 20
Collins Arun Prakash V
Cristina Delerue-Matos 74
Dallemer F 98
David Velayutham 107, 185
Deeparani P 155. 163
Devibala P 21
Dharani S 22
Dharsini Devia N 164
Dheepika R 21, 23, 87, 119
Dhilip Kumar C 34
Dhineshkumar S 94, 130
Diana Sangeetha R.S 144
Dinola A 167
Divakar Kumaravel 95
Divya B 96

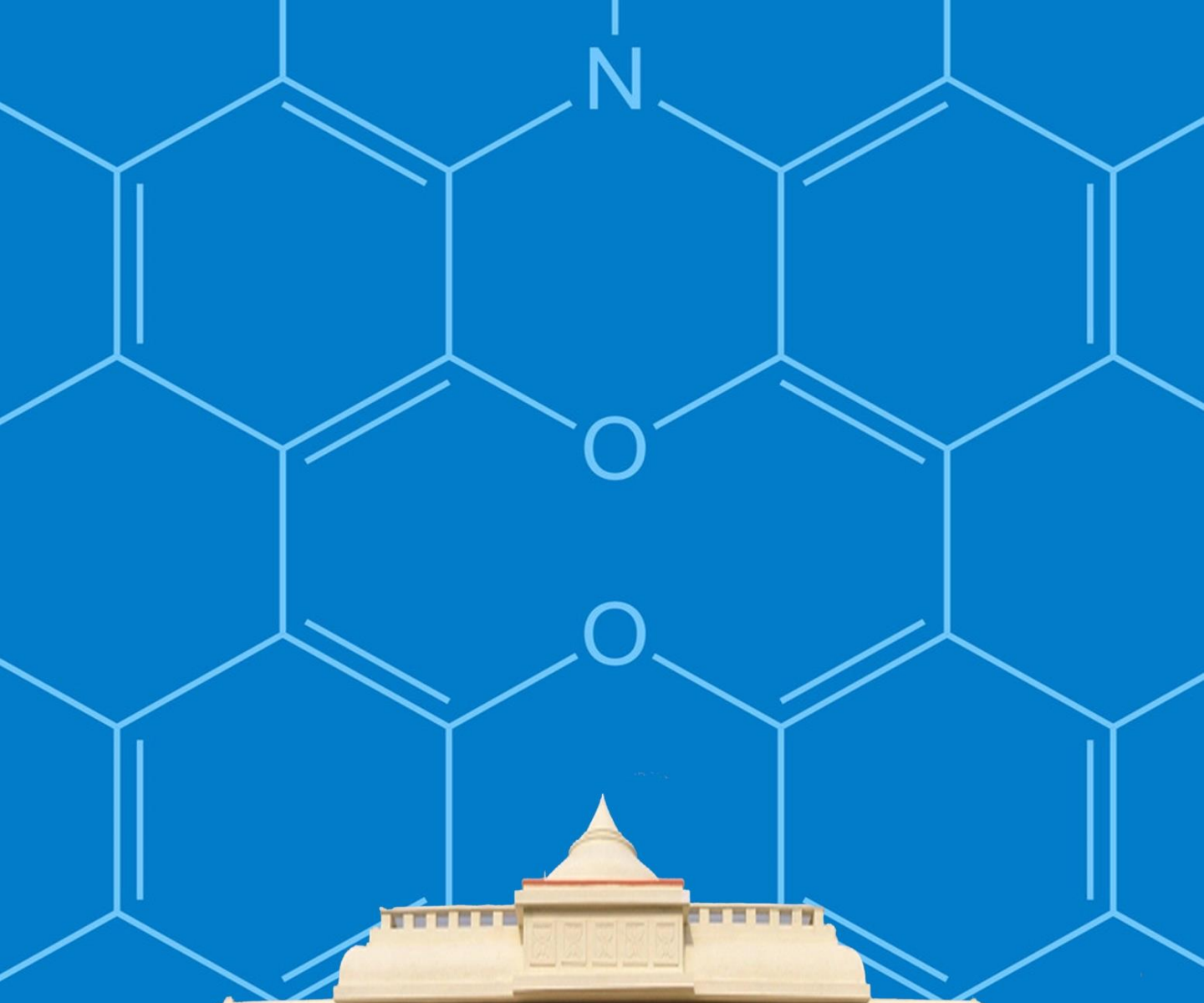
Divya D 97
Divya K 24, 67
Elamathi C 98
Elumalai P 176
Emi Princess Prasanna A 99
Esakkimuthu. S 57, 100
Firthawsha Yasmin L 142
Gajalakshmi S 18, 25, 182
Ganesan Punithakumari 148
Ganesan R.M 136
Ganesan Selvanathan 17
Ganesh V 177
Gaurav Pandey 31
Gayathri V 100
Giftynol Elizabeth 138
Gomathi A 15
Gomuraj S 101
Gopinath K 141
Gopu G 34, 43, 93, 123
Govindaraju R 102
Gowri S 79
Gowsalya Bharathi R 180
Gowthami K 44, 142
Gunaseelan K 25
Gurumallesh Prabu H 36, 78, 135, 152
Gurunathan Karuppasamy 28
Gurupriya S 26
Gurusamy S 103
Habibulla Imran 27
Hajara Banu U
Harini Priya PA 172
Heiner Albaris 28
Helen Ratna Monica J 114
Hemalatha p 16
Indhumathi T 136
Indurani P 180
Ingarsal N 187
Janeeta Priya F 28
Jeevika A 104
Jegatheeswaran S17,29,88,99
Jemini Jose 29
Jenifer J 40
Jeniffa R 30
Jenny R 37
Jessica Fernando 152,183
Jeyachandran Sivakamavalli 171
Jone Celestina J 103
Kalaiarasi G 22
Kalaiarasi S 104
Kalaiselvi K 32
Kalaivanan C 104
Kalaivani P 173
Kaleeswari K 105
Kalirajan K 124,162
Kalpana T 106
Kanagaraj Madasamy 106
Kanagavel D 95
Kang Hyun Park 5
Kanimozhi B 108
Karikal Chozhan C 108,109
Karpagavinayagam P 110
Karpuraranjith Marimuthu 111
Karthick K.A 33
Karthick S 92
Karthik Krishna Kumar 113
Karthika A 112
Karthika P 106
Karthikeyan B 87

Karthikeyan S 113
Karthiyayini S 188
Karunakaran M 114,123,178
Karuppuchamy S 164
Karutha Pandian Divya 81
Karuthapandian S 35
Karvembu R 22
Kasirajan, K 114
Kasturibai S 115
Kathiresan K 106,117,185
Kavitha AL 36
Kavitha G 110
Kavitha M 116
Kavitha N 37,48
Kayalvizhi K 117
Keerthi 45
Keerthika Devi R 43
Keerthika N 117
Kirthika Rani B 38
Komal Kurlekar 118
Komala V 163
Kottaisamy K 19,78,99
Kottaisamy M
Krishnaveni K 120
Krishnaveni R 39
Krishnaveni V 121
Krishnaveni V120
Kulangiappar K 40
Kumaraguru AK 83,120
Kumaraguru N 121
Kumaresan M 121
Lajwen zuleka 119
LeemaRose A 28
Lourdu Robert D 139
Lynch V.M 22
Madankumar A 97
MadiFatiha 81
Maheswari A.R 122
Maheswari J 123
Majur Mading Makur 55
Malar vizhi I 124
Mangaiyarkarasi, R 40
Mangalam M 125
Manikandan G 126
Manikumar A 127
Manimegalai P 143
Manimekalai A 128
Manimekalai S 128
Manisankar P 20,40,168
Manonmani A 129
Manonmani M 66
Marimuthu S 74,111
Mario Leo Joseph 94
Markkandan R 130
Maruthapandian V 130
Mathavan A100.102.119
Mathu Sudhan 162
Mayakrishnan A 17,131,134,139,179
Meenakshisundaram S.P 66
Meyyathal P.R 132
Mohan P 133
Mohana M 134
Mohanapriya S 42
Murugan Veerapandian 31
Murugavel Kathiresan 184
Murugesan A 170,174
Muthu Kaviya M 83
Muthuchamy Nallal 7

Muthuchudarkodi R.R 104,116
Muthukumar P 175
Muthulakshmi M 159
Muthulakshmi V 17,123,131,134,139,,178
Muthumanickam
Shenbagapushpam71,135
MuthuMareeswaran P 60,64
Muthusankar G 43,122
Muthuselvi. P 136
Muthusubramanian S 20,133
Muthuvel I 44,141
Muzakkira Y 139
Nagarajan A 137
Nagarajan Loganathan 127
Nagarajan S 86,118
Nagendran A 24,67
Nalini A 174
Namsheer K 53
Narayanan M 139
Naveenkumar P 44
Nedunchezian G 187
Nehru L C 190
Nishanthi S.T 85
Nithya G 139
Nithya M 45
Nithya P 78,88,99,114.123,131,134,178
Nivethitha S 141
Palanisamy Rupa Kasturi 161
Palanisamy S 93
Pandian K 88
Pandimuthu G 46
Pandiyaraj Kanagavalli 31
Paramasivaganesh K 46,59
Parthiban S 141
Paruthimal Kalaigan G
32,41,44,49,115,133
Pathanjali. G.A 12
Prakashkumar Nallasamy 146
Rajeswari R 151
Rajiv Gandhi R 159
Rajkumar R 153
Raju C.V 67
Raju T 40
Rama V 154
Ramakrishnan Kalai Selvan 65
Ramakritinan CM 83
Ramalakshmi M 99
Ramanjaneyulu Mala 96
Ramanujam K 131
Ramapandian S 102
Ramasamy G 82,154
Ramesh Duraisamy 55
Ramesh M 155
Ramkumar S.G 117
Ramya C 83
Rani C 156,164
Rasith Ali H 157
Revathi M 158
Revathi S 159
Revathi T 56
Rishwandhani A 37
Robin Clara X 106
Roshni A 159
Rukmani A 134
Sakthi velu K 57
Sakunthala A 164
SamayananSelvam 17
Sambandam Anandan 8

Sanay Naha 58
Sangeetha C 162
Sangeetha R 162
Sankar A 46,59
Sankar C 96,125,155
Sankarganesh M 104
Santhi K 156,164
Saranya J 123
Saraswathi M 24
Saraswathy V 130
Saravanadevi K 166
Saravanakumar Shanmuganathan 61
Saravanan C 60
Sarojadevi Muthusamy 89
Sasikumar R 137
Satheeshkumar K 63
Sathiah Thennarasu 96
Sathya C 167
Sathya U 45
Sathyanarayanan Shanmugapriya 65
Sebastian Antony Selvan C 125
Selvakumar Kodirajan 71
Selvaraj S 124,154,162
Sengottuvelan N 37,48,169
Senguttuvan S 79,142
Senthil Kumar S 67
Senthilkumar A.N 167
Senthilkumar Arumugam 89
Senthilkumar P 168
Senthilkumaran M 64
Senthilvelan S 87
Sethupathi M 48,169
Shakkthivel Piraman 149,177
Shankar R 22
Shanmugalingam A 170
Shanmugam M 143
Shanmugam V.M 40
Sheela C.D 84,103,146
Shrigayathiri 171
Shrivalli R 172
Sindhu M 73
Sindhuja D 22
Sivakumar K 66,87,174
Sivakumari G 87
Sivan Velmathi 58,68,130,147
Sivaraman S 130
Sivaranjini B 176
Sockalingam R.M 66
Sornambigai M 67
Soundarya N 175
Sozhaveni S 187
Sreeja P B 29
Sri Abirami Saraswathi M 24,67
Srikumar S.R 19
Srimathi M 83,171
Srinivasan A 133
Srinivasan K 177, 190
Srinivasan Prabhakaran 68
Stalin T 46,57,70,99,136,171,187,188, 190
Subalakshmi M 69
Subbiah A 42
Subbu C 121,178
Subhalakshmi R 178
Subramania A 9,30
Sudha P 157,162
SuganthiA 112
Suganthy Natarajan 146
Suganya Bharathi. B 57,70,99,131

Sumathi Sowrirajan 121
Sundaravadivelu M 183
Sundaresan K 146
Sundrarajan M
17,78,88,99,123,131,134,137,159,178,179
Suresh J 178
Suryanarayanan V 142,184,185
Suthi M 179
Tamil Selvi A 33,105
Tamilselvi B 180
Tewodros Birhanu 85
Thambidurai S 56,77,159,181
Thamizharasan A 181
Tharini K 146
Tharmaraj P 80,84,103,146
Thenmozhi Ramalingam 146
Thennila Muthukumar 71
Thileep Kumar K 158
Thillainatarajan S 141
Thirumalai D 18
Thirumalaikumar M 160
Thirunarayanan G 75
Toemsak Srihirin 11
Umadevi S 40,132,135,176
Umaiya Bharathi V 181
Umamatheshwari S 91,155
Uthayakumar N 88
Uthiraselvi B 182
Vasantha Kumar P 72
Vasu V 19,108,172
Vedhi C 15,95,98, 99,110,
Velayutham D 40,106,184
Vembu Suryanarayanan 142,184
Vengatesh G 183
Venkatachalam Rajagopal 184
Venkataraman Dharuman 27,81
Vidhya S 28
Vignesh C 136
Vignesh M 30,63
Vigneshkumar G 57,187
Vijayalakshmi Ganesan 146
Vijayaraj C 187
Vimalasruthi N 57,188
Vinotha S 73
Vishvatha S 150
Viswanathan S 106,129,150,164
Wilson Bosco Paul Michael 94
Yosuva Suvaikin M 104
Young-Soo Seo 11
Yuanfu Chen 11



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