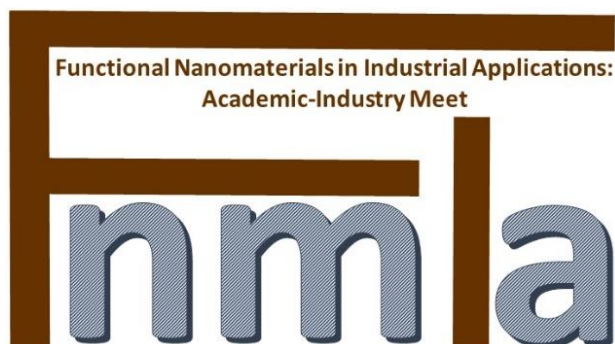


# **Conference Abstract Proceedings**

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**Collated and Edited by Dr. Tapas Sen, University of Central Lancashire, UK**

**2<sup>nd</sup> International  
Symposium**



**Functional nanomaterials in industrial & clinical  
applications:Academia-Industry-Clinicians meet  
14<sup>th</sup> to 16<sup>th</sup> July 2020**

**Organised *via* Virtual Zoom Platform**

**Theme 1: Recent Trend in Nanotechnology  
Theme 2: Nanomedicine (General & Clinical)  
Theme 3: Nano-Energy & Green Technology  
Theme 4: Nano-environment (Water & Land)  
Theme 5: Nano-Catalysis and Green Technology**

**Functional Nanomaterials in Industrial & Clinical Applications: Academic-Industry-  
Clinician Meet (14<sup>th</sup> to 16<sup>th</sup> July 2020), UCLan, Preston, UK**

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**Functional Nanomaterials in Industrial & Clinical Applications: Academic-Industry-Clinician Meet (14<sup>th</sup> to 16<sup>th</sup> July 2020), UCLan, Preston, UK**

**Keynote (KN-1-01): Graphene and Related Materials: From Production to Applications**



**Prof. Andrea Ferrari,**

Professor of Nanotechnology, Director, Cambridge Graphene Centre,  
Cambridge University, UK

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**Functional Nanomaterials in Industrial & Clinical Applications: Academic-Industry-Clinician Meet (14<sup>th</sup> to 16<sup>th</sup> July 2020), UCLan, Preston, UK**

**Keynote (KN-1-01):** Nanocatalysts and the sustainable manufacture of nanomaterials at industrial scale



**Prof. Edward Lester**, Department of Chemistry, University of Nottingham, UK

Continuous hydrothermal synthesis is a relatively new technology that is still proving its value as a sustainable and scalable route to manufacture nanomaterials. The portfolio of materials that can be made using this route is ever increasing and solvothermal processing means that this portfolio is more diverse than ever.

In recent years Promethean Particles has been operating a full scale continuous hydrothermal synthesis plant in the UK which will be capable of producing up to 1000 tons/year (dry weight equivalent) of a range of nanomaterials, from metals, metal oxides, hydroxides, carbonates and sulphides, as well as some more complex materials such as metal organic frameworks. This presentation will discuss the journey from bench scale to pilot scale to full scale. The scaling process introduced a number of new challenges but also new opportunities for cost savings and design innovation.

The talk will show examples of how the choice of precursors and precursor concentration impact cost of production. Specific examples of MOFs, ZnO, LDHs, AgS<sub>2</sub> and TiO<sub>2</sub> will be given to compare the hydrothermal technology with other technologies.

More information:

<https://www.nottingham.ac.uk/engineering/departments/chemenv/people/edward.lester>

Keynote (KN-2-01): Plasmonic and Magnetic NPs for Biomedical Applications



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The development of new chemical methods for the next generation of nanoparticles with very high magnetic moment, fine tuning Au nanorods and novel hybrid and multifunctional nanostructure is presented.

Detailed mechanistic studies of their formation by sophisticated and advanced analysis of the nanostructure allows tuning of the physical properties at the nanoscale; these can subsequently be exploited for diagnosis and treatment of various diseases. The studies are conducted to provide insight for future material design approaches. It will also help to identify the critical process parameters that can be manipulated in order to obtain the suitable physical properties for the intended applications.

In collaboration with chemical engineers in designing the reactors in microfluidic systems, this allowed for the first time to detailed study the physical properties such as X-ray diffraction (XRD), magnetic moment and morphology to unravel the particle formation mechanism during co-precipitation synthesis of iron oxide magnetic nanoparticles, which is very important for their robust, reproducible formation process for cancer treatment.



**Figure 1.** Schematic of the set-up for nanoparticle synthesis showing the syringe pumps used to feed reactants to a T-mixer, pre-heated water bath, and aging bath; and the synchrotron X-ray diffraction set-up showing the solution injected into a quartz capillary for analysis.

More information: <https://www.ucl.ac.uk/physics-astronomy/people/professor-thanh-nguyen>  
<https://ntk-thanh.co.uk/>



**Keynote (KN-2-02): Light-driven molecular nanomachines as targeted photodynamic therapy agents**

**Dr. Robert Pal**, Professor of Nanomaterials

Durham University, UK

More information:

<https://www.dur.ac.uk/research/directory/staff/?mode=staff&id=6011>

**Light-driven molecular nanomachines as targeted photodynamic therapy agents**

Thomas Bradford,<sup>1</sup> Liu Dongdong,<sup>2</sup> Richard S. Gunasekera,<sup>2</sup> Víctor García-López,<sup>2</sup> Lizanne G. Nilewski,<sup>2</sup> James M. Tour<sup>2</sup> and Robert Pal,<sup>1,\*</sup>

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**ABSTRACT**

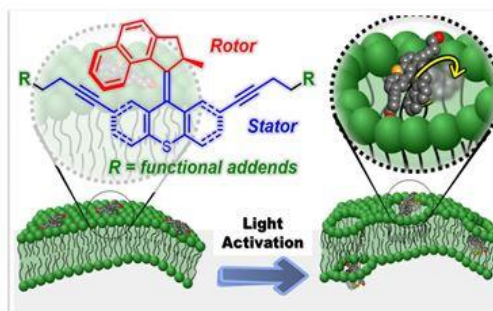
**Keywords:** nanomachines, light activation, multi-photon, PDT, anti-bacterial

An important need for personalised therapeutics is the effective targeted in vivo destruction of selected cells and cell types, that are currently being highlighted by emergence of powerful optogenetic strategies. Using a new generation of light activated uni-directional molecular nanomachines (MNM) we have demonstrated their application to expedite necrotic cell death using single photon excitation in the UV domain. [1,2]

Recently we have embarked to promote our “proof of principle” technology into in vivo biomedical applications using two photon (2PE) activation, as UV light activation in vivo has significant limitations associated with shallow tissue penetration and non-uniform excitation/activation, limiting the 3D precision required for therapeutics.

This direction in activation not only allow deeper tissue penetration to realise in vivo photodynamic therapy (PDT) development, but also remove UV radiation as a confounder of biomedical efficacy. Since with 2PE MNM activation will only occur in a small truly diffraction limited 3D voxel it allows the next phase of targeted photodynamic therapy protocols and methods to be designed, as with careful chemical engineering of the MNMs cell type and target receptor specific binding can be facilitated with experimental therapeutic precision as small as a single cell. We demonstrated that by scanning a safe dose of NIR light in a 3D raster pattern for a predetermined period of time and repetition, only the surface bound MNM bearing cancerous cells are lysed, whereas all ‘healthy’ neighbouring cells remain intact and unaffected.[3]

Once fully developed and validated 2PE activation of cell type and condition specific MNMs could be potentially adopted as a new form of extremely high optical precision, facile and non-invasive Type IV PDT for cancer treatment via selectively induced apoptosis. This alongside their emerging application as ‘mild-UV’ activated antibacterial agents[4] renders light driven molecular nanomachines to be one of the most promising candidates for nano-biomedical applications.



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**Keynote (KN-2-03): Nanobiointerfaces: Implications of Biomolecular Corona**



**Professor Morteza Mahmoudi**

Michigan State University, USA

More

<http://research.rad.msu.edu/People/mahmoudi.html>

information:

This talk summarizes the existing overlooked factors at the nanobiointerfaces which negatively affected the successful clinical translation of nanomedicine. Deep analysis of the current nanomedical literature reveals a history of well-intentioned missteps/errors caused by these overlooked factors. Understanding and consideration of these factors in nanomedicine reports and/or developments may facilitate successful clinical translation of nanotechnologies.



**Keynote (KN-3-01): Colloid-Templated Nanoporous Materials for Commercial Applications**



**Prof. Andreas Stein,**

Department of Chemistry, University of Minnesota, Minneapolis, MN 55455, USA

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Nanoporous materials have a well-established track record in industrial applications, the archetype being zeolites with pore sizes suited for small-molecule catalysis in the petroleum industry. Over the last 25 years, numerous synthetic techniques have been developed to control pore architecture in solids at pore dimensions extending those of zeolites, including surfactant templating of mesoporous solids and colloidal templating for even larger pore sizes. Such nanoporous materials have been explored in numerous potential applications, ranging from energy storage and conversion to catalysis, biomedical applications, and various host-guest interactions. In this presentation, I will highlight two applications of colloid-templated porous materials, in which our laboratory has collaborated intensively with industrial partners: (1) colloid-templated nanoporous carbon as a solid contact for ion-selective electrodes and (2) colloidal-crystal templated 3D-ordered macroporous (3DOM) silica as a durable, non-toxic pigment that relies on a structural color mechanism. Each of these applications are uniquely enabled by the porous solid. As a solid contact, nanoporous carbon is the contributing factor to achieve world-record signal stability in potassium-ion selective electrodes and a low-cost platform for ion-sensing devices on flexible substrates. In the case of 3DOM silica pigments, the periodic pore structure obtained by templating methods is the basis for tunable color from a single composition with the ability to cover an RGB color palette from just three master-batch colors.



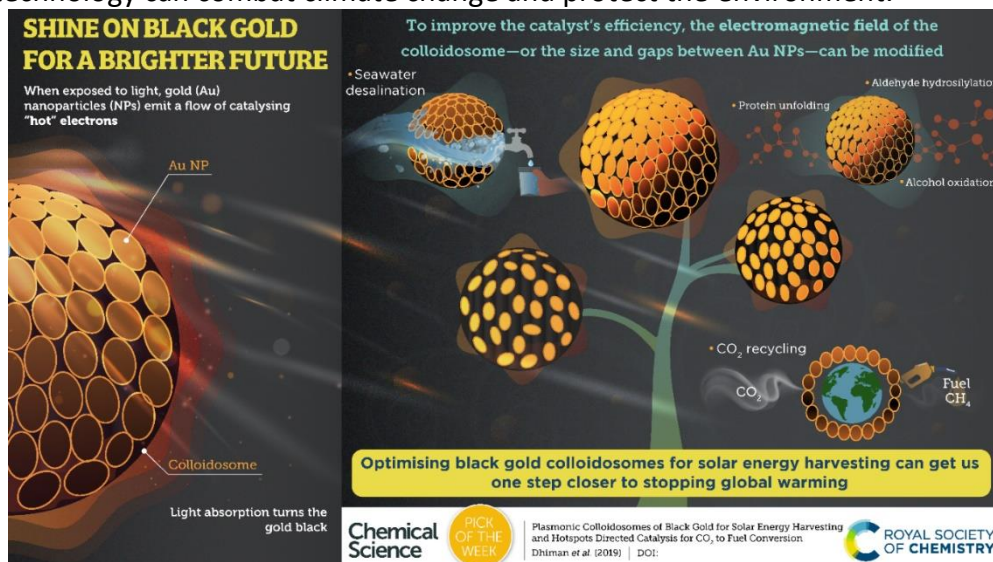
Keynote (KN-3-02): Nanocatalysts for Solar Energy Harvesting and CO<sub>2</sub> to Fuel Conversion



Professor Vivek Polshettiwar  
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Energy and environment are two of our critical societal challenges. Climate change hits a giant weak spot in human history. Disproportionate use (or misuse) of natural resources including fossil fuels, created an extreme imbalance on planet earth and first priority of all of us to take on this challenge. *In this seminar* I will explain some of our work in the Field of Catalysis & Nanotechnology, to Resolve Critical Challenges of Energy and Environment.

We recently reported the synthesis of a new class of dendritic fibrous nano-silica (DFNS).<sup>1-12</sup> More than 150 groups worldwide are now using our patented DFNS for various applications such as catalysis, solar-energy harvesting, energy storage, self-cleaning antireflective coatings, surface plasmon resonance-based ultrasensitive sensors, CO<sub>2</sub> capture, and biomedical applications.<sup>1d</sup> Using our recent results on synthesis and application fibrous nano-silica (including single-atom catalysis, black gold, amorphous zeolites and defected silica) for fine chemical synthesis, solar energy harvesting, CO<sub>2</sub> capture-conversion and waste plastic to chemicals, in this seminar, I will discuss how nanotechnology can combat climate change and protect the environment.



**Keynote (KN-4-01): Clean water using nanotechnology: Current status**



**Prof. T Pradeep**

*Institute Professor*

*Deepak Parekh Institute Chair Professor and Professor of Chemistry*

*DST Unit of Nanoscience and Thematic Unit of Excellence*

*Department of Chemistry, Indian Institute of Technology Madras,  
Chennai 600 036*

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Sustainable nanotechnology has made substantial contributions in providing contaminant-free water to humanity. In this talk, I present the compelling need for providing access to clean water through nanotechnology-enabled solutions and the large disparities in ensuring their implementation. I will discuss the current nanotechnology frontiers in diverse areas of the clean water space with an emphasis on applications in the field and provide suggestions for future research. Extending the vision of sustainable and affordable clean water to environment in general, I note that cities can live and breathe well by adopting such technologies. By understanding the global environmental challenges and exploring remedies from emerging nanotechnologies, sustainability in clean water can be realized. I suggest specific pointers and quantify the impact of such technologies.

\*This lecture will be based on our recent review: A. Nagar and T. Pradeep, *ACS Nano*, 14, 6420-6435. please cite this as: <https://dx.doi.org/10.1021/acsnano.9b01730>

For more details, please visit: [www.dstuns.iitm.ac.in/pradeep-research-group.php](http://www.dstuns.iitm.ac.in/pradeep-research-group.php)

**Functional Nanomaterials in Industrial & Clinical Applications: Academic-Industry-Clinician Meet (14<sup>th</sup> to 16<sup>th</sup> July 2020), UCLan, Preston, UK**

**Keynote (KN-5-01):**



**Dr. Antonio Zanotti-Gerosa**

Johnson Matthey

<https://matthey.com/en>



**Dr. Dan Mortimer**

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**ABSTRACT**

Johnson Matthey catalysts enable a vast number of catalytic processes in the fine chemical industry for the production of pharmaceutical intermediates (API) and other active ingredients (AI). Dr Antonio Zanotti-Gerosa, R&D director of the chiral catalysis team in Cambridge, UK, will focus on the application of transition metal catalysts and biocatalysts, highlighting complementarities and key technical and economical requirements for the processes to become industrially viable. Dr Danny Mortimer, Product Specialist, heterogeneous catalysts in Royston, UK, will describe how understanding and design of supported metal catalysts allow control of the properties of the catalysts, making possible their application on selective transformations of complex substrates.

**Keywords:** catalysis, homogeneous, heterogeneous, biocatalysis

Keynote (KN-5-02): Photo-catalysis



Prof. Anne Davidson, Sorbonne University, Paris, France

More information: <http://www.lrs.upmc.fr/fr/equipe-du-lrs/personnel-permanent/anne-davidson.html>

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<sup>4</sup> Libanese University, Materials, Catalysis, Environment and Analytical Methods, Beyrouth, Liban  
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Our goal is to develop nanotechnologies based on semi-conducting oxides nanoparticles and their use under visible light activation. The term “photocatalysis” describes the activation of a chemical process by a light absorption and most of the published work is devoted to UV excitation [1]. We have selected to use Visible irradiation, to open our work in the Future to Solar activation. We use semiconducting oxides nanoparticles or isolated metallic sites that are excited by visible light to generate electron-hole pairs of excitons, further involved in redox reactions.

Three distinct catalysts, of increasing complexity, will be described by usual characterization technics (XRD, N<sub>2</sub> physisorption, MEB, TEM) with a special attention devoted to their optical characterizations (band-gap measurements, Tauc method [2], as described in details for ZnO [3]). Our work has been performed by Diffuse Reflectance Visible Spectroscopy. We will describe: 1) an anatase commercial support of surface modified by 3 wt% of Zn-dispersed species, 2) particularly small hematite nanoparticles dispersed on SBA-15 silica, 3) Hybrid materials obtained by combination of different carbon-based solids (oxidized graphene GO and partially exfoliated graphite GR) used as supports for mixed catalysts containing two distinct oxides, ZnO and Zn-ferrite.

Examples of activity will be selected between methanol oxidation, the decomposition of large organic molecules (pesticides and antibiotics). Antibacterial activity has also been measured with the most active catalysts.

We have taken into account the costs to the prepared model samples, the availability of the elements and the reproducibility of our catalysts formulation. Future perspectives will be analyzed as the end of the presentation.

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IL-2-01

Title: Magnetic Particle Imaging Applications in Inflammation, Theranostics, and Cell Tracking

Dr Nicolas Carvou

*Magnetic Insight, USA*

<https://www.magneticinsight.com/>

Advances in cancer immunotherapy have fueled a boom in immuno-oncology research. There is an urgent need to track and accurately quantify cells *in vivo*. In addition, researchers need a method to systematically measure the biodistribution of immune cells in solid tumors over time.

**Magnetic Particle Imaging (MPI)** is a novel preclinical imaging technique used to non-invasively track iron-oxide-tagged immune cells *in vivo*.

MPI can be used to track *in vivo* the biodistributions of macrophages, T-cells, stem cells or tumor cells for several days. The data is specific and quantitative. MPI can also be applied to drug delivery monitoring and image-guided theragnostics. Data acquisition from nanoparticles can be combined with MRI or CT. Researchers can generate localized hyperthermia zones, for nanoparticle actuation and tumor immunogenesis as an adjunct to radiation or immune therapies. Results from immune cell tracking, *in vivo* quantitation, drug-delivery monitoring and localized hyperthermia will be discussed.

**IL-3-01**

**Title: Nano Chemistry Solutions for Green and Energy Efficient Tires**

Dr Debabrata Rautaray  
*Tata Chemicals Innovation Centre., Pune, India*

<https://www.tatachemicals.com/About-Us/Innovation>

<https://www.linkedin.com/in/dr-debabrata-rautaray-82190717/?originalSubdomain=in>

The impending introduction of tighter emission norms in the automobile industry is driving the tire industry to accelerate evaluation of options that enhance tire performance and bring green quotient to the all-black tires today. A vehicle engine must overcome rolling friction to propel the vehicle forward — this requires fuel consumption. Low rolling friction/ resistance tires can reduce fuel consumption and emissions.

In this talk, I will present our work on the development of “green tires” by incorporating dispersible nano-silica into tire rubber matrix. This study resulted in reduction of rolling resistance (improved fuel efficiency), also leading to lower greenhouse gas emissions. Furthermore, the nano-silica incorporation into tires has been shown to improve greater wear resistance (for longer tire life) and improved wet / snow grip (a safer tire).



**IL-4-01**

**Microbial challenges in water supply - maintaining safe water in buildings**

Mr. Gary Hogben,  
Technical Manager, Feedwater Ltd., Wirral, United Kingdom  
<https://feedwater.co.uk/>

Infections relating to water can be broadly divided into two categories.

Those caused by organisms that should not be present in drinking water supplies. These organisms are usually derived from faecal contamination, either from direct ingress of sewage or waste but may also gain entry from animal or insect ingress to water systems. Current control measures focus on exclusion of the faecal material and vectors by good engineering. This approach is allied to chemical or physical treatment (usually chlorination and/or filtration) to reduce any remaining contamination. The focus is firmly on the former approach, especially in low tech areas where chemical supply and power is not available. Infections caused by organisms that are usually present in water but may be pathogenic when numbers of organisms increase significantly or where especially vulnerable persons are present. The phenomenon of growth within water systems is known as regrowth.

For these regrowth associated infections, the application of chemical products (biocides) may assist in control, but use of biocides in drinking or domestic water supplies is necessarily limited by toxicity concerns as well as taste and odour problems.

The presentation will consider these infections and the problems associated with control, including discussing serious outbreaks associated with water.

Organisms of concern include:

*Pseudomonas aeruginosa*  
*Legionella* spp (The causative agents of Legionnaires' disease and other Legionelloses)  
*Stenotrophomonas*  
*Burkholderia cepacia* complex  
*Mycobacterium avium* complex

Functional Nano-materials offer significant potential in control of microbial regrowth in water systems. We will consider the necessary and desirable properties of those materials and likely areas of application, together with a consideration of market potential.



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**IL-5-01 (Ref: KN-5-01)**

See: KN-5-01 earlier

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**Clinician talks: CL-01**

**Potential Applications of Nanotechnology for Hepatopancreatobiliary Cancers**

**Dr Asma Sultana MBBS MD, FRCS (England) (General Surgery/HPB), FRCS (Glasgow), MS, DNB**

Consultant Hepatopancreatobiliary/General Surgeon, East Lancashire Teaching Hospitals NHS Trust, UK

Cancers of the liver and pancreas are among the top ten causes of cancer mortality in the UK. There is urgent need for better more targeted treatments, with less toxicity and enhanced efficacy in this area.

Pancreatic cancer is the tenth most common cancer in the UK, and is the fifth leading cause of cancer mortality. Eighty percent of patients present with advanced disease at diagnosis and conventional treatments of chemotherapy, radiotherapy or chemoradiotherapy often fail. Even in the twenty percent who are operable, overall survival remains poor with the development of either local recurrence or distant metastases. Nanomedicine is a novel modality that could surmount this. There are many approaches using nanotechnology tested both in vitro on cell lines and in vivo in animal models, and a few have even made it to early phase clinical trials in humans. However only two have made it to clinical use, human albumin nanoparticles encapsulated with paclitaxel, and liposomal irinotecan.

Liver cancers can either be primary cancers with hepatocellular cancer (HCC) the most frequent, or secondary cancers, with colorectal liver metastases being the leading cause. Early HCC are treated with surgery or liver transplantation, while advanced disease is treated by chemotherapy which can be either systemic or regional. Nano particles-based drug delivery system have been developed for the treatment of HCC, with the first FDA approved nanotechnology being liposomal doxorubicin. Colorectal cancer is the fourth commonest cancer in UK, and the second leading cause of cancer deaths. Between 14-20% of patients with colorectal cancer present with liver metastases, and a further third develop liver metastases in the course of their disease. Only a quarter of colorectal liver metastases are operable, with the rest of the patients requiring chemotherapy. Clinical translation of nanomedicine for the treatment of colorectal liver metastases is limited. Another area of unmet need in liver cancers is for better imaging technology for the intraoperative visualisation of liver tumours. Innovative ideas using nanotechnology for theranostics have been developed, though none has reached routine clinical practice yet.

Many innovative and exciting ideas in cancer treatment/ theranostics using nanoparticles have been developed in the last decade. The challenge lies in translating these concepts from the bench to the bedside. Closer interdisciplinary collaboration between academia and industry as well as between the fields of engineering, biology, chemistry and medicine are needed to make this transition from the laboratory to clinical practice.

**Clinician talks: CL-02**

**Nanoparticle-mediated immunotherapy for head and neck carcinoma: Bench-side to bedside**

**Dr Shashi Prasad MBBS PhD FRCS (Ed) (ORL-HNS) FRCS (Ed) FRCS (Glasg) MS DNB**

University Hospital of Coventry and Warwickshire, UK

<https://www.uhcw.nhs.uk/our-services-and-people/our-people/mr-shashi-prasad-rama/>

Encapsulation of tumour-associated antigens (TAA) in polymer nanoparticles (NP) is a promising approach to enhance efficiency of antigen delivery for anti-tumour vaccines. Various techniques were used to liberate TAA from cell lines. Single (gp100) and multiple (B16-tumour lysate containing gp100) antigens were encapsulated within differing molecular weight poly (lactic-co-glycolic acid) co-polymers. Differences in morphology, encapsulation/release and biologic potency were studied. Findings were adopted to encapsulate fresh tumour lysate from patients with advanced tumours and compare stimulation of tumour infiltrating lymphocytes (TIL) against that achieved by soluble lysate. The 80 KDa polymer resulted in maximal release of payload and favourable production of immunostimulatory IL-2 and IFN- $\gamma$ . NP-mediated antigen delivery led to increased IFN- $\gamma$  and decreased immunoinhibitory IL-10 synthesis when compared to soluble lysate. Findings were adopted to entrap fresh tumour lysate from five patients with advanced head and neck squamous cell carcinoma (HNSCC). To test the hypothesis that NP enhance antigen presentation, dendritic cell (DC) produced from patient blood monocyte precursors were loaded with either the un-encapsulated or NP-encapsulated versions of tumour lysates. These were used to stimulate freshly-isolated autologous CD8<sup>+</sup> T cells. In four of five patients, anti-tumour CD8<sup>+</sup> T cells showed significantly increased immune-stimulatory IFN- $\gamma$  ( $p=0.071$ ) or decreased immuno-inhibitory IL-10 production ( $p=0.0004$ ) associated with NP-mediated antigen delivery. The observations represent an enabling step in the production of clinically-translatable, inexpensive, highly-efficient, and personalized polymer-based immunotherapy for solid organ malignancies. Enhancing TAA presentation may be a viable approach to increase the efficiency of tumour cell directed-cytotoxicity via immune mechanisms. This study presents an example for this using patient-derived tumour tissue and nanotechnology-based encapsulated antigen presentation to DC. The observed CD8<sup>+</sup> T-cell response was significantly enhanced. This method may pave the way to a highly efficient cancer cell elimination method with minimal to no toxicity.

Special invited talk (SL-01)

## Tailored Rare earth-doped Upconversion Luminescence Nanomaterials for Bioimaging and Treatment

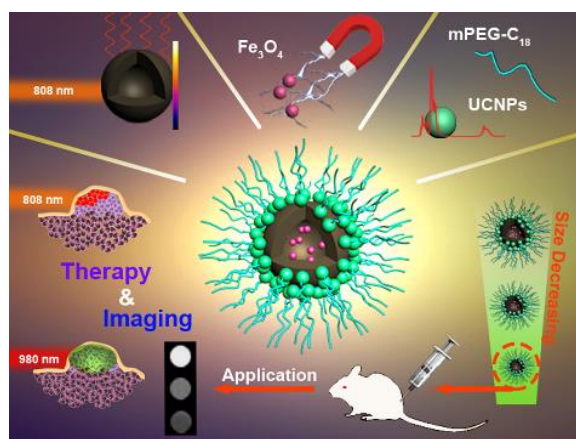
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Rare earth-doped upconversion nanoparticles (UCNPs) which could show unique upconversion photoluminescence (UCPL) under excitation with near-infrared light have attracted considerable attention due to their excellent chemical and optical characteristics.<sup>[1]</sup> UCPL shows a variety of advantages such as large anti-Stokes shifts, sharp emissions, long luminescence lifetimes, and high resistance to photobleaching. In our case, (1) several simple yet powerful methods were developed to transfer the UCNPs from hydrophobic to hydrophilic. And the resulting nanomaterials with upconversion luminescence have excellent biocompatibility and were successfully applied for bioimaging *in vitro* and *in vivo*. (2) Recently, we developed several nanomaterials to integrate both bioimaging and therapy, such as several nanosystems for dual-mode bioimaging guided therapeutic applications (Figure 1).<sup>[2,3]</sup>

**Keywords:** Rare earth-doped upconversion nanoparticles, near-infrared excitation, bioimaging, therapy



**Figure 1.** Schematic illustration of one of the theranostic nanocomposite, and near-infrared light triggered bioimaging and photothermal therapy.

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**Special invited talk (SL-02)**

**Prof. Harry Eccles**

**Professor of Nuclear Materials**

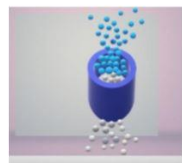
School of Physical Sciences and Computing

Director, UCLan Research Centre for Smart Materials

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[https://www.uclan.ac.uk/staff\\_profiles/professor\\_harry\\_eccles.php](https://www.uclan.ac.uk/staff_profiles/professor_harry_eccles.php)

An overview of research activity of the Centre



**UCLan Research Centre for Smart Materials**

Smart materials are and will in the future make a greater impact on business and society. From the humble beginnings of thermochromic artefacts, such as coffee mugs, smart materials are now a £multibillion global market.

I will address in UCLan's presentation:

1. Market opportunities
2. Why UCLan organised a Research Centre for Smart Materials
3. The scope of our research
4. How we manage our research projects
5. The achievements in our first year

Professor Harry Eccles

Director Centre for Smart Materials

Special invited abstract (SL-03)

## Small molecule delivery in Au-Chitosan nanoparticles to knockdown SOST gene for Osteoporosis therapy

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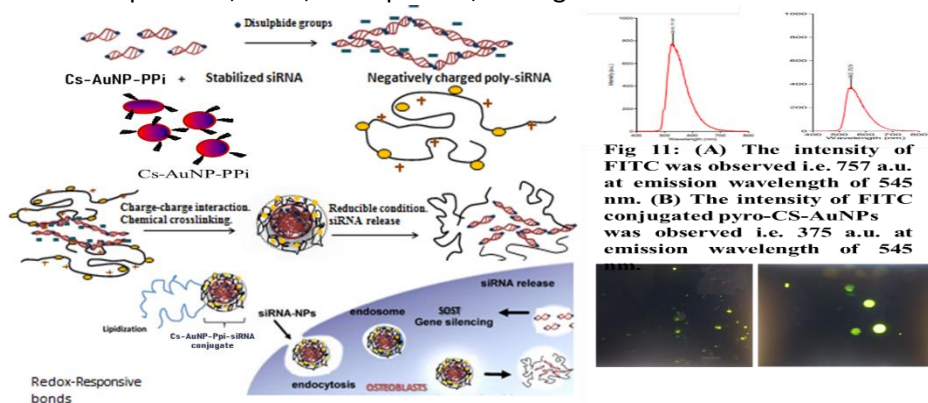
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### ABSTRACT

Osteoporosis involves bone degeneration in males and females. Existing therapies do not offer an adequate therapeutic efficacy, creating the need for developing effective therapies. siRNA delivery for gene silencing has emerged as a potential therapy in bone disorders. The SOST gene is known to inhibit the Wnt signalling cascade thereby reducing the differentiation of osteoblasts. Therefore, silencing SOST genes with a definite siRNA has given an alternative possibility to treat osteoporosis. Since siRNAs are short lived with poor half-life coupled with meagre transfection ability, it is essential to have a nanocarrier. We propose Au-chitosan nanoparticles (Au-ChNPs) biofunctionalized chitosan reduced gold nanoparticles, their physical characterization and conjugation with pyrophosphate (PPi) and siRNA. The maximum absorption ( $\lambda_{\max}$ ) of colloidal CS-AuNPs was observed at  $\sim 521\text{nm}$ , characteristic for spherical gold nanoparticles formation. Particle size, PDI, and zeta potential were observed 228nm, 0.4 and +38 mV respectively. Spherical shape of CS-AuNPs was further confirmed by TEM. Surface morphology and presence of gold metal in CS-AuNPs were confirmed by SEM-EDX. Further, characterization through XRD was confirmed the amorphous nature and through FTIR was confirmed the presence of amino and hydroxyl group at  $\sim 1640\text{ cm}^{-1}$  and  $\sim 3218\text{ cm}^{-1}$  in CS-AuNPs respectively. Furthermore, the conjugation of CS-AuNPs with PPi was confirmed through UV-Vis spectrophotometer by shifting the PPi peak towards 500nm. The conjugation of CS-AuNPs with siRNA was confirmed through gel retardation assay by shifting the conjugated band up in comparison to non-conjugated siRNA band. This established the potential utility of AuChNPs to deliver biomolecules to promote bone formation, this being a potential alternative to treat osteoporosis.

**Keywords:** Au-Ch Nanoparticles, SOST, osteoporosis, osteogenic markers



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OL-1-01

## **Structural and Physical Properties of Sodium Doped Borate Glass**

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### **ABSTRACT**

Borate glass has been considered for the technical interest due to various applications in solar energy converters, optical fibers and radiation shielding. Borate-based glasses with composition  $x\text{Na}_2\text{CO}_3(100-x)\text{B}_2\text{O}_3$ ; ( $0 \leq x \leq 20$ ) have been prepared by the conventional melt-quenching technique, where, sodium carbonate ( $\text{Na}_2\text{CO}_3$ ) acts as a network modifier. The obtained glasses were characterized by X-Ray diffraction (XRD) and Fourier transforms infrared spectroscopy (FTIR). The network structure of prepared samples depends upon the sodium content in glass compositions and also on the  $\text{BO}_3$  and  $\text{BO}_4$  units [1,2]. The variation in density, molar volume ( $V_m$ ) and crystalline volume ( $V_c$ ) indicate the substitution of the sodium atoms.

**Keywords:** borate glass, XRD, FTIR

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**Functional Nanomaterials in Industrial & Clinical Applications: Academic-Industry-  
Clinician Meet (14<sup>th</sup> to 16<sup>th</sup> July 2020), UCLan, Preston, UK**

OL-1-02 (has been considered for poster, see P-1-03 later)

OL-1-03

## Developments in Aluminium-Graphene/Ceramics Hybrid Nano-Composites

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### ABSTRACT

Strong research interest has been witnessed in graphene (G) based metal matrix composites (MMCs) due to its remarkable mechanical properties. On the other hand, Aluminium ceramic composite (Al-CMCs) have also been widely researched due to its light weight and high strength applications. It has also been seen that Al-CMCs can experience stiffness and toughness challenges that can be catered by introduction of high strength and ductile graphene in Al-G/CMCs hybrid nano-composite. Present article offers a short review on Al-G/CMCs nanocomposite with various ceramics, as secondary reinforcement, to improve mechanical properties of resulting nano-composites. Literature, especially form last 5 years, has been incorporated in the review. Graphene at interface of ceramics offers an intermediate phase that helps to overcome the challenges of stiffness and toughness. Al-G/CMCs hybrid nano-composites have substantial potential to increase, sometimes multi-fold, mechanical properties of resulting nano –composites.

**Keywords:** aluminium; graphene; ceramics; hybrid nano-composites; mechanical applications

Table 1: Al-G/CMCs based MMCs for strength applications

Sr. No.	Matrix	Reinforcement 1	Reinforcement 2	Fabrication Method	Strength Enhancement	Reference
1.	Al7075	GNP	Boron carbide B <sub>4</sub> C	Stir Casting Process	UTS: 167 MPa (46%) Hardness: 78 HV (37%) Yield strength: 260 MPa (53%) Impact Strength: 3.5J (133%)	[1]
2.	Al	GNS	Al <sub>2</sub> O <sub>3</sub>	Flake Powder Metallurgy	UTS: 359 MPa (131.6%) Yield Strength: 332 MPa (201.8%) Elongation 11.2%	[2]
3.	Al	GNP	SiC	Powder Metallurgy	Hardness: 85 HV (203%) UCS: 271 MPa (155.6%)	[3]
4.	Al6061	Graphene	ZrO <sub>2</sub>	Mix fluid metallurgy	UTS: 250 MPa (38.8%) Yield Strength: 182 MPa (42.1%) Elongation: 7.8%	[4]
5.	Al7075	Graphene	Be <sub>3</sub> Al <sub>2</sub> (SiO <sub>3</sub> ) <sub>6</sub>	Stir Casting Method	UTS: 216.6 MPa (76.9%) Hardness: 104 BHN (14.66%) UCS: 703.03 MPa (7.06%)	[5]

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OL-1-04

## **Damping Properties of Silicone Polymer/MWCNT Nanocomposites**

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### **ABSTRACT**

Silicone polymer nanocomposites (Si/MWCNT) were prepared for damping application. The mechanical, dynamic mechanical and thermal properties of the nanocomposites are studied. With the increasing content of multiwalled carbon nanotube (MWCNT), the tensile strength is increased but elongation at break is decreased. Temperature dependent visco-elastic properties of nanocomposites have also been studied. The effect of MWCNT loading on storage modulus, loss modulus and loss tangent has been observed. Thermal properties of nanocomposites have been characterized using differential scanning calorimetry (DSC) and thermo-gravimetric analysis (TGA). Thermogravimetric analysis results showed the enhanced the thermal stability. Scanning electron microscopy study showed the good MWCNT dispersion of the nanocomposites with some large filler particles.

**Keywords:** silicone; nanocomposites; thermal properties; mechanical properties.

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OL-1-05

## Mixed Zinc: Iron Nanostructures for Multifunctional Applications

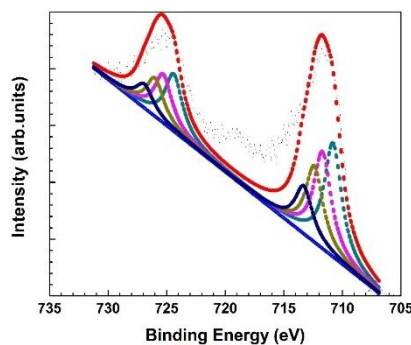
Promod Kumar<sup>a\*</sup>, Jayachandran V P<sup>b\*</sup>, Chandrashakher Kulkarni<sup>c</sup> and Pravin Kendrekar<sup>d\*</sup>

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### ABSTRACT

Transition metal oxide nanostructures are well known as attractive multi-functional nanomaterials and are among the most promising industrial materials for different science and technological applications. Mixed zinc-iron nanostructures were synthesized by a well-known combustion technique. Various approaches such as UV-Vis. absorption spectroscopy, X-ray diffraction (XRD), Photoluminescence, Transmission Electron Microscope (TEM), and X-ray photoelectron spectroscopy (XPS) were employed for the characterization of mixed zinc-iron nanostructures. X-ray diffraction studies revealed the phases of the ZnO and Fe<sub>2</sub>O<sub>3</sub>, which was well consistent with the XPS results. The Wagner plot with modified Auger parameters (MOP) was further investigated to confirm the chemical states of ZnO, Zn(OH)<sub>2</sub> and Fe<sub>2</sub>O<sub>3</sub> phases observed for the mixed zinc: iron nanostructures. The photoluminescence attributes demonstrated that the mixed zinc to iron ratio of 50:50 affected the recombination process of the electron-hole pairs produced by the photon absorption and consequently influenced the photoluminescence activity of ZnO and Fe<sub>2</sub>O<sub>3</sub> respectively. A zinc to iron ratio of 50:50 showed the best antibacterial activity among all the synthesized mixed zinc- iron nanostructures. The present study demonstrated the potential application of a simple synthesis methodology in the production of tunable nanostructures for multi-functional applications.



**Figure:** XPS analysis of pure Fe<sub>2</sub>O<sub>3</sub>.

**Keywords:** Solution combustion method, ZnO: Fe<sub>2</sub>O<sub>3</sub> NPs, XPS, PL, antibacterial activity.

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OL-1-06

## Fluorescence Active Glycopolymers Nanogel for Smart Delivery of Anticancer Drug

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### ABSTRACT

A new class of REDOX responsive glycopolymers based fluorescent nanogel was prepared for stimuli-responsive and target specific delivery of anticancer drug. A functional block copolymer (BCP) poly(pentafluorophenyl acrylate)-*b*-poly(furfuryl methacrylate) (PPFPA-*b*-PFMA) of controlled molecular weight was achieved via reversible addition-fragmentation chain transfer (RAFT) polymerization technique. The activated pentafluorophenyl ester functionality was replaced by the amine functionality of glucosamine to introduce the amphiphilic BCP poly[2-(acrylamido) glucopyranose]-*b*-poly(furfuryl methacrylate) (PAG-*b*-PFMA). [1] Furthermore, biocompatible gelatin QDs (GQDs) [2] was attached to PAG-*b*-PFMA to induce fluorescence activity in the glycopolymers. A model anticancer drug, Doxorubicin was loaded in the polymer during the crosslinking process via Diels-Alder reaction using dithio-bismaleimidoethane (DTME), a REDOX responsive crosslinker. The anticancer activity (*in-vitro*) of the drug loaded micelle was observed over MBA-MD-231, human breast cancer cell line and monitored via confocal fluorescence microscopy and flow cytometric analyses (FACS). The cytotoxicity of the prepared glycopolymers based nanogel over the MBA-MD-231 cell line was assessed via MTT assay and it was observed that the synthesized nanogel was non-cytotoxic in nature. [3]

**Keywords:** Glycopolymers, REDOX responsive, fluorescence active, nanogel, anticancer activity

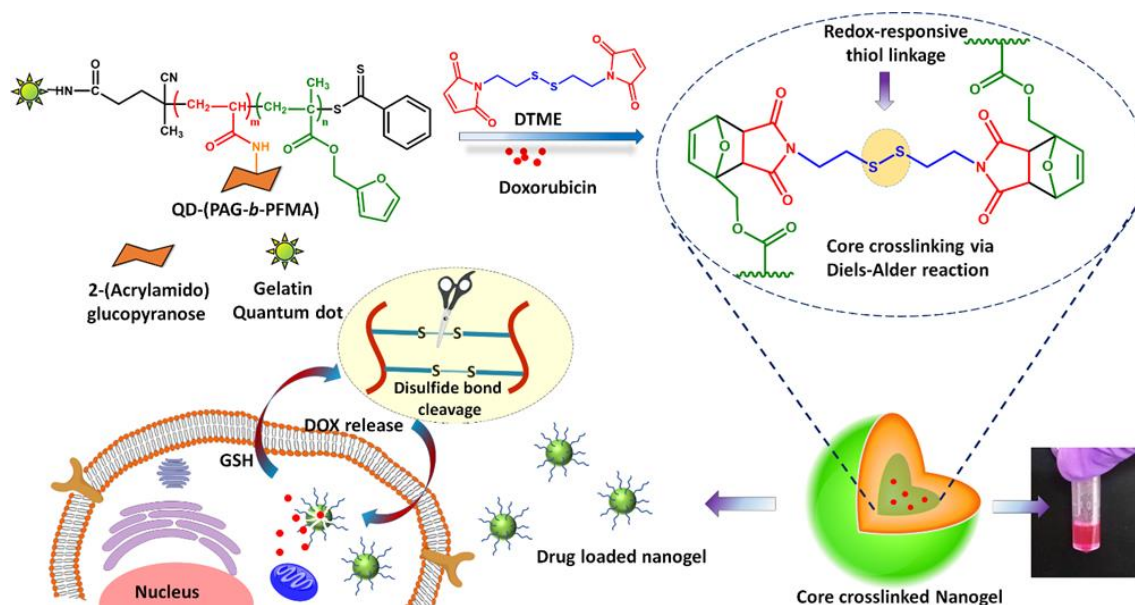


Figure: Schematic diagram of Redox responsive delivery of drug in cancer cell

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OL-1-07

## Detection of Polyelectrolytes Through Whispering Gallery Modes Based Sensor

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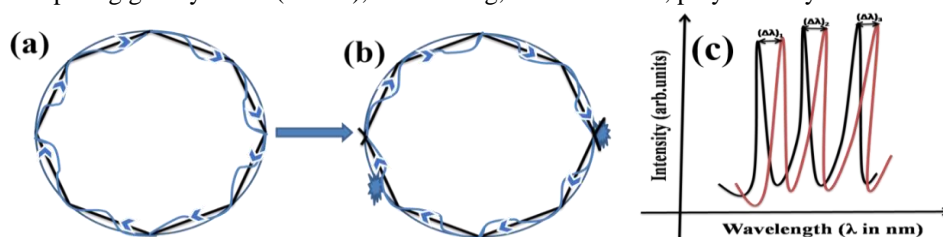
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### ABSTRACT

The development of ultrahigh biosensors to detect virus is the basic requirement to improve our health care method. Therefore, several diagnostic techniques have been proposed till date in order to collect the earliest possible information about the diseases at their initial level. Now-a-days the fluorescent labeling techniques are the most widely accepted system for detection of the certain diseases. However, the necessity of complex labeling process involves in this type of biosensors leads the researchers to find an alternative way for label free detection of biomarkers. In recent years, various label free optical transducing technologies have been introduced out of which the whispering gallery mode (WGM) based sensors have shown promising usefulness in the bio-sensing applications. WGM micro-cavities have revealed strong light confinement inside any dielectric medium due to refractive index contrast of two media through their micro-scale size, small mode volume, low optical loss, and high Q-factor. In case of WGM the light ray is traveling inside the resonator, and an integral multiple of resonance wavelength fits into the circumference of the resonator as shown in the schematic Fig.1 (a). Further, either by forming a uniform layer at its surrounding medium or attachment of any foreign analyte molecule at its surface causes a shift of the original resonance wavelength, as depicted in Fig. 1 (b). However, Fig. 1 (c) shows schematics of consecutive shifts ( $\Delta\lambda_1, \Delta\lambda_2, \Delta\lambda_3$ ), of the WGM peaks, and it is expected that the shift of WGM peaks is not the exact always. Here, we have demonstrated the WGM sensing by detecting two polyelectrolytes PSS (Polystyrenesulphonate) and PDDA (Poly diallyldimethylammonium chloride) through 2 mol.% of Li<sup>+</sup> doped ZnO microspheres, as WGM resonator.

**Keywords:** Whispering gallery mode (WGM), bio-sensing, micro-cavities, polyelectrolytes



**Fig.1** (a) Schematic diagram of confinement of light inside a spherical resonator due to total internal reflection of light. (b) shifting of resonance wavelength due to the attachment of any target analyte at the surface of the microresonator and (c) shows schematic diagram of WGM peak shift due to changes in the surrounding medium of the optical resonator. Red and black color spectra indicate the shifting of the resonance peaks before and after a change in the surrounding medium.

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OL-1-08

## **Where do we stand?**

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### **ABSTRACT**

Nanotechnology is one of the most powerful enabling technologies, in the world, providing solutions to key sectors including health, medical, space, automobile, and electronics. It, thereby, offers scope for tremendous development in number of specific sectors like semiconductors, medical imaging, drug delivery, structural materials, cosmetics, coatings, to name a few. Advancements and its implementations in these industrial areas are predicted to continue for many years and according to 2018 review report of Nanowerk, the inventory list of nanotechnology based consumer products has exceeded 4000. This implies that the employees, researchers working in this area and consumers who are utilizing these are exposed to nano-scale materials on a daily basis that might have potential health hazards and environmental issues as well. So, the importance of adequately assessing nonmaterial exposure, hazard and risk is now widely recognized. Globally, number of authorities are working towards the development of policy frameworks of nanotechnology with particular emphasis on health, safety and environmental (HSE) aspects of nanomaterials use. However, specific details for the hazard and risk assessment of nanomaterials have not been adopted in legal acts. These are being governed by their respective existing substance legislation and the authorities have issued initial guidance on the risk management in most of the countries. It is evident that the assessment and managing HSE aspects and the relevant regulatory activities are still in infancy stage. So, this work attempts to give a comprehensive overview of various regulations and the available frameworks addressing the importance, evolution and current status of safety aspects in the field of nanotechnology. Also highlights the ways to move forward for achieving cost effective and safer nano-products on the market.

**Keywords:** HSE status, nanomaterials, regulations, global status

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OL-1-09

## **Blue Photoluminescent Potassium-Doped Graphene Oxide from Agriculture Waste as a Nanocarrier in Combined Drug Delivery: The Next Medical Challenge**

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### **ABSTRACT**

In the whole world, there are remarkable resources which are invested in prevention, diagnosis, and treatment of cancer. Cancer is the most common and second leading cause of death in Europe and North America. Many efforts can be influenced the overall therapeutic efficacies and cancer treatments. Combinatorial of anticancer drugs onto the nanocarrier is one of the most promising attempts in drug delivery system. These cocktailed anticancer drugs system may provide a balanced molecular basis for novel chemotherapeutic strategies. Despite great popularity for anticancer drug combination utilizations, the hidden rules behind anticancer drug cocktails are an emerging scientific problem and pivotal topic in new era of anticancer therapy. As visualization is very important for the investigation of novel drug delivery systems (DDSs), enabling specific targeting and controlled release in diseased cells or tissue, blue photo-luminescent graphene oxides (GOs) with naturally doped potassium metal have been developed from agriculture waste for the delivery of combination of anticancer drugs. Gefitinib (GEF) and camptothecin (CPT) are effective for many kinds of cancers therapies. Therefore, we investigate the possibility that combination of these drugs could be effective against breast cancer cells. In this report, we studied the loading, release and delivery of these two anticancer drugs separately which effectively loaded onto the fluorescent nanocarrier. The loading capacity and the cell killing activity of this GEF-CPT cocktailed system loaded on fluorescent GO (F-GO) were also performed which was better than that of the individual drug system in breast cancer cells. *In vitro* cytotoxicity of the combined drugs loaded onto the nanocarrier was also performed which suggested that F-GO-CPT-GEF drug system had a significant cytotoxicity in comparison to that of the single-drug systems as well as the pure drugs. This is the first attempt to load a binary drug conjugates onto a fluorescent nanocarrier to target a specific disease with considerable therapeutic efficiency and low cytotoxicity.

**Keywords:** camptothecin, cytotoxicity, gefitinib, graphene oxide, nanocarrier.

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OL-2-01

## **Light Matter Interaction at Single Particle Level: Real Time Observation of Magnetic Field Induced Fluorescence Engineering in Fluorescent SPIONs**

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### **ABSTRACT**

Superparamagnetic iron oxide nanoparticles (SPIONs) have shown potential applications in various biomedical engineering fields because of high magnetic susceptibility. However, their applications in optical imaging were severely restricted because of the lack of fluorescence. Here, after synthesizing a novel fluorescent SPIONs nanostructure, we present a real time in situ giant fluorescence enhancement, at least an order of magnitude higher in self-assembled fluorescent SPIONs in comparison to a single fluorescent SPIONs at the single-particle level under the applied magnetic field (MF). Single particle fluorescence imaging and tracking provide the direct observation of the self-assembly and disassembly and the associated fluorescence change in SPIONs in the presence and absence of the applied magnetic field. A theoretical model was applied to calculate the dipole dipole interaction energy, drag coefficient, and quantified the dynamics of this aggregation. A light-matter interaction at single particle level that simultaneously introduced a new phenomenon of magnetic field induced gigantic fluorescence enhancement was for the first time, evident in fluorescent SPIONs in single particle fluorescence imaging and tracking studies.

**Keywords:** self-assembly, superparamagnetic iron oxide nanoparticles, fluorescence engineering, single particle fluorescence imaging and tracking.

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OL-2-02

## Novel Synthesis and Characterization of Gold: ZnO Nanoparticles and their Antibacterial Activity

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### ABSTRACT

The present work describes the study of ZnO nanostructures doped with plasmonic Au nanoparticles using a solution combustion method followed by thermal treatment in an open atmosphere. The structural, chemical, morphological and optical properties of Au doped ZnO samples were determined by XRD (X-ray diffraction), X-ray photoelectron spectroscopy (XPS), SEM (scanning electron microscopy), Transmission electron microscopy (TEM) and UV–Vis absorption spectroscopy.

The antibacterial activity of Au doped ZnO samples was further investigated against the pathogenic bacteria namely *Escherichia coli* and *Staphylococcus aureus*. Au doped ZnO samples demonstrate better antimicrobial activities against *E. coli* and *S. aureus* as compared to pure ZnO structures. These materials exhibit excellent physicochemical properties required for applications in various field of photonics, plasmonic and biomedicine.

**Keywords:** Solution combustion method, ZnO nanoparticles, antibacterial activity

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OL-2-03

# Cisplatin encapsulated Nanostructured-Lipid Carriers (CisNLC) induced sensitization of Cis-resistant ovarian cancer cells & elucidating the interlink between reactive oxygen species, glutathione and ATP7B: an *in vitro* study

**Disha Mittal**, Largee Biswas, Anita Kamra Verma\*

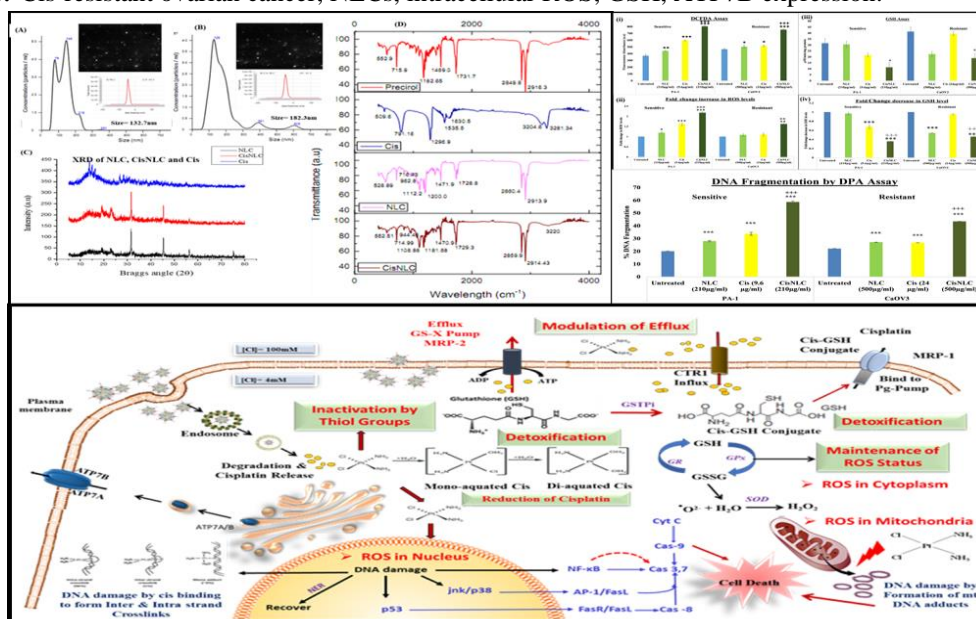
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## ABSTRACT

To investigate the potential of CisNLCs to sensitize Cis-resistant ovarian cancer cells to Cis. Identifying effective novel formulations to overcome Cis resistance with negligible side-effects is challenging. We hypothesize a strategy to modulate reactive oxygen species (ROS) and Glutathione (GSH) levels induced by Cis-NLC to inhibit ATP7B expression in *in-vitro* model, which has not been exploited so far. Synthesized CisNLCs with a size of ~182.3nm were characterized using NTA and Fourier transform infrared spectroscopy (FTIR), powder XRD and evaluated for its ability to sensitize Cis resistant ovarian cancer cells.

CisNLCs increased ROS levels and decreased GSH levels in Cis-resistant ovarian cancer cells. Using MTT, DNA fragmentation, ability of the CisNLCs to sensitize Cis-resistant ovarian cancer cells has been demonstrated. The novel biomarker ATP7B was downregulated. Further investigations of the synthesized CisNLCs can have the potential to enable efficacious Cis-based therapies for ovarian cancer.

**Keywords:** Cis-resistant ovarian cancer, NLCs, intracellular ROS, GSH, ATP7B expression.



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OL-2-04

## **Nanocrystalline Tin oxide thin film biosensor for the detection of Antibody-Antigen complex**

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### **ABSTRACT**

Biosensors are small analytical devices used for the detection of a specific analyte (enzymes, virus, bacteria, cells and DNA) in a rapid, sensitive and user-friendly manner. It combines a biological component with a physiochemical detector. The present study describes fabrication and characterization of nanostructured Tin oxide thin film based electrochemical sensor for on-site, label free, cost effective detection of antigen-antibody complex. Nanocrystalline SnO<sub>2</sub> thin film was prepared on p-type silicon substrate using Langmuir Blodgett technique. SnO<sub>2</sub> film surface was functionalized electrochemically by depositing Polyaniline (PANI) film for biomolecule immobilization. Antibody (Ab) molecules (mouse IgG) were immobilized through glutaraldehyde coupler. Electrochemical cell consisted of antibody immobilized Si/SnO<sub>2</sub> thin film as working electrode, platinum plate and wire as counter and pseudo reference electrodes, phosphate buffered saline (PBS, PH 7.2) as electrolyte. For characterization, various electrochemical techniques such as cyclic voltammetry, multifrequency impedance, static and transient capacitance at two different frequencies was used. Potentiostat/Galvanostat with Frequency Response Analyzer was used for cyclic voltammetry and impedance measurements. For detection of antigen-antibody interaction the corresponding specific antigen (Ag), goat antimouse IgG from whole serum was used. Reusability of the sensor was tested by treating the substrate with 3 M KCl for 150s to remove the bound antigen.<sup>[1]</sup>

Cyclic voltammetric experiments showed an effective current change after each process step namely, PANI deposition, Ab immobilization and Ag interaction though redox peaks were absent. After each process step, the systematic current changes were observed at positive applied bias voltage (Fig.1). Capacitance decrease after antigen injection indicates Ab-Ag interaction (Fig 2). Both cyclic voltammetric and capacitance voltage plots indicate the specific interaction of antigen with immobilized antibody <sup>[2]</sup>. The sensors were found to be reusable 3-4 times, simply by removing the antigen by treating the antibody complex with 3 M KCl for 150s. Specific binding of Ab with Ag involves hydrogen bonding and electrostatic interactions which in turn will affect the electrode/electrolyte interfacial properties. Further studies emphasize on the underlying reason for the micro interfacial pH changes occurring at electrode/electrolyte surface due to charge transfer effects along with the change in dielectric layer thickness produced by specific binding of Ab-Ag on the surface of SnO<sub>2</sub> nanostructure.

OL-2-05

## Characterization development and *in vitro* evaluation of celecoxib loaded nanoparticles-hydrogel composites for drug delivery in colorectal cancer

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### ABSTRACT

In this particular research, we prepared a pH-responsive colon targeted novel drug delivery system (CDDSNMC), which composed of mainly three parts. First, we prepared drug-loaded nanoparticles which composed of two pH-independent time-controlled release polymers Eudragit® RS100, Eudragit® RL100, and one bioactive agent of cyclooxygenase-2 inhibitor, celecoxib. After that, we loaded those nanoparticles inside a matrix system of hydrogel microsphere beads, which composed of two other pH-sensitive polymers guar gum and calcium alginate. Finally, the whole hydrogel microsphere-nanoparticle composite system was packed inside a soft gelatin capsule for oral administration [1].

Spherical celecoxib loaded nanoparticles less than 300 nm in size and spherical nanoparticle composite microspheres less than 800 µm in size were successfully developed using the solvent evaporation method and ionic gelation technique respectively. The structure and properties of nanoparticles, microspheres, and microsphere-nanoparticle composite were characterized by different biophysical methods such as UV-Vis Spectrophotometer, Differential Scanning Calorimetry (DSC), Fourier-Transform Infrared Spectroscopy (FTIR), Zeta potential, Dynamic light scattering (DLS), Scanning Electron Microscope (SEM), and Transmission Electron Microscope (TEM). TEM confirmed the distinguish structure and the crystallinity of nanoparticles, whereas SEM corroborate the size, spherical structure as well as surface morphology of microsphere beads. The average size and stability of nanoparticles were determined by DLS and zeta potential respectively. All data bolstering our research work constitutively. *In-vitro* drug release study positively indicates that formulation with 50% drug loading exhibited sustained release of 51% over 18 hours in phosphate buffer (pH 6.5). No significant burst release was observed during the *in-vitro* study.

A large number of evidence collected from several different experimental systems indicates that cyclooxygenase-2 (COX-2) may play a vital role in colorectal tumorigenesis. Large epidemiologic studies have shown a 40–50% reduction in mortality from colorectal cancer in persons taking nonsteroidal anti-inflammatory drugs (NSAIDs) regularly. Levels of COX-2 isoenzyme and certain prostaglandins like PGE<sub>2</sub>, PGF<sub>2α</sub> and PGE<sub>1</sub> are found to be higher in certain cancers like squamous cell carcinoma of head and neck, colorectal carcinoma and certain types of breast cancer. Celecoxib has recently been shown to reduce the colorectal adenoma burden in high-risk patients [2].

This unique formulation design helps us to deliver drug in specific region of our body with predetermined manner, by which we think we will successfully overcome any toxicity related problem of drug (celecoxib) during *in-vivo* and cell line (HCA-7 Colony 29) study in near future.

**Keywords:** celecoxib, cancer, microsphere-nanoparticle composite, pH-responsive, drug delivery.

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OL-2-06

## Exploring the potential of Eugenol in treating resistant melanoma in combination with first line chemotherapy: in-vivo analysis

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### ABSTRACT

Melanoma is one of the deadliest cancers with very low response and survival rates. The inherent resistance of melanoma cells towards apoptosis results in failure of chemotherapy [1]. Resistance is reported to be due to 'Survivin' [2].

In an attempt to overcome this resistance, we formulated dacarbazine and eugenol loaded liposomes and surface functionalized them with hyaluronic acid (HA) for active targeting. Anti-melanoma potential of the formulation was assessed on melanoma induced C57BL/6 mice by conduction pharmacodynamics and biodistribution studies [3].

Findings revealed that HA coating caused higher uptake of liposomes in B16F10 melanoma cells, while reduced the engulfment by macrophages. In melanoma induced C57BL/6 mice, significant difference between the tumor volumes was seen among control group and groups receiving dacarbazine solution (DS), coated liposomes of dacarbazine (DLC) and coated liposomes of dacarbazine and eugenol (DELIC). Tumor volume in DELIC treated group was least at the end of the treatment. Histopathological analysis revealed more necrosis in tumor and less damage in liver and lungs in DELIC treated group. Also, the coated liposomes were found to be more accumulated in tumor, while drug solution led to a much higher concentration in liver. Coated liposomes also stayed longer in systemic circulation as compared to solution and uncoated liposomes.

Thus, the combination of dacarbazine and eugenol holds the promise of overcoming the resistance of melanoma cells and challenges of anti-melanoma therapies.

**Keywords:** Melanoma, Resistance, Survivin, Dacarbazine, Eugenol

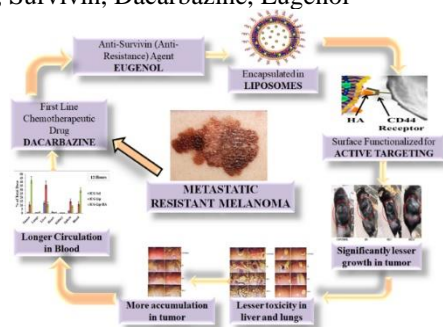


Figure 1: Role of Eugenol in Melanoma Treatment

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OL-2-07

## **Can Mesoporous Ceria be a Safer Drug Delivery Vehicle than Mesoporous Silica?**

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### **ABSTRACT**

Ever since the German physician Paul Ehrlich launched the idea of drug delivery in the form of 'magic bullet', the concept of targeted delivery has caused a paradigm shift in modern medicine. The prime objective of targeted drug delivery is to release the therapeutic drugs to a specific organ or tissue with an objective to avert drug degradation, manipulate drug pharmacological profile, and mitigate drug-originated systemic toxicity effects, including hemolysis. Hemolysis in vivo can lead to anemia, jaundice or other deleterious health conditions, e.g. hypertension and renal toxicity [1]. Hence, it is imperative to carefully evaluate the hemolytic potential of all intravenously administered pharmaceuticals.

Among the state-of-the-art vehicles for targeted delivery of therapeutics, metal-oxide nanoparticles with mesoporous structures have shown great promise [2]. Large specific surface area, tunable pore structures and excellent physicochemical stability go in favor of such nanovehicles for hosting and site-specific delivery of disparate payloads (molecular drugs, nucleic acid and proteins) [3]. In this study, we have evaluated the in vitro hemocompatibility of cerium oxide (CeO<sub>2</sub>) or ceria nanostructures as compared to SiO<sub>2</sub> nanospheres, which is the present gold standard. The hemolysis studies on SiO<sub>2</sub> nanospheres vis-à-vis CeO<sub>2</sub> nanoparticles were performed by incubating each, at various concentrations, with erythrocytes isolated from heparin-stabilized fresh human blood. Post-incubation, the absorbance value (at 570 nm) of hemoglobin in the supernatant was an indicator for the degree of hemolysis. Our study divulged the superior hemocompatibility of pristine as well as functionalized (amine and thiol) CeO<sub>2</sub> nanoparticles compared to that of mesoporous SiO<sub>2</sub> nanospheres and thus opens up new avenues for metal-oxide nanoparticle-mediated drug delivery research.

**Keywords:** mesoporous silica, cerium dioxide, surface functionalization, hemolysis

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OL-2-08

## Ormeloxifene -Hyaluronic Acid Microfibers for Breast Cancer Therapy

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### ABSTRACT

Ormeloxifene (ORM) belongs to selective estrogen receptor modulators (SERMs) class of drugs used for the treatment of breast cancer [1]. Targeted delivery of ORM can be achieved by encapsulation using hyaluronic acid (HA). Since HA-targeted receptors (CD44) are overexpressed in breast cancer, lung carcinoma and cervical cancer cells; HA has been used as a drug carrier to improve drug delivery to suppress cancer growth [2]. In this study, microfibers of ORM incorporated HA was prepared using a newly modified method and characterized for morphology, particle size, zeta potential and encapsulation efficiency using various physicochemical methods [3]. SEM images of the microfibers are given in the Figure.1. The *in vitro* drug release and cytotoxicity studies were also carried out. This study suggests that the HA-ORM microfibers could be used for breast cancer treatment in the future.

**Keywords:** ormeloxifene, hyaluronic acid, cancer therapy, encapsulation, microfibers

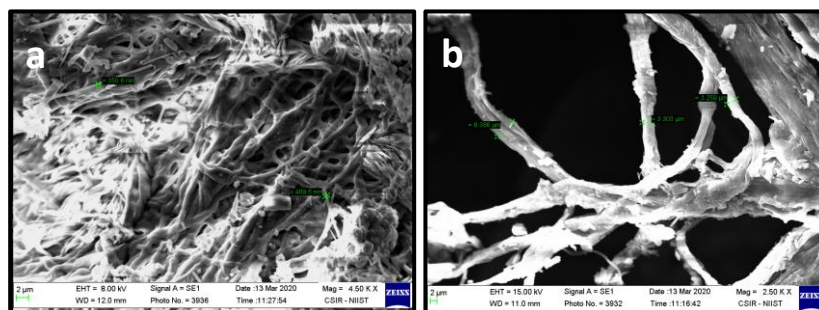


Figure 1: a) and b) SEM images of HA microfibers containing ORM

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OL-2-09

## Penetrating Peptide-Decorated Polymeric System for Improved Protein Delivery

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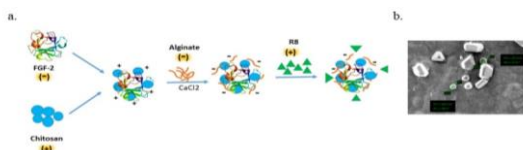
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### ABSTRACT

Various strategies have been explored to develop delivery systems able to transport biologic drugs to the diseased area by carrying targeting ligand on their surface thus improve delivery. Cell penetration peptides have been used with increasing interest in drug targeting studies in the last two decades. These peptides are advantageous because they are biocompatible and that peptide sequences can be designed to alter the hydrophobicity, affinity, load, and stability characteristics of the drug. In addition, they can be synthesized insufficient quality and quantity, at low cost and easily. In this study, an arginine-rich peptide (octaarginine (R8))-decorated fibroblast growth factor-2 (FGF-2)-carrying polymeric systems were developed as a straightforward but effective approach for improved wound healing therapy.

The improved drug delivery effect of penetrating peptides can be used in a variety of conditions, from brain diseases to skin malformations. In our previous study, we developed a cyclic peptide iRGD (CCRGDKGPDC)-conjugated solid lipid nanoparticle to deliver siRNAs against glioblastoma and we showed targeting effect of iRGD increased nanoparticle uptake in the tumor side and prolonged survival (1). In this study, FGF-2 that signal through FGF receptors regulates a broad spectrum of biological functions such as cellular proliferation, survival, migration, and differentiation was selected as a model biological drug. The electrostatic properties of FGF-2, chitosan, and alginate were utilized as advantages. Firstly, chitosan and FGF-2 were complexed through electrostatic interactions. Afterward, the obtained system was enveloped by alginate by ionic gelation in the presence of CaCl<sub>2</sub>. Thereafter, antibacterial cell penetrating peptide R8 was incorporated to the outer surface of the system (2). Acquired formulations were evaluated for their characteristics (Figure 1). According to the results, appropriate FGF-2:Chitosan:Alginate:R8 ratio was determined for further in vitro and in vivo studies. As far as we know, no previous research has investigated the incorporation of octaarginine in alginate coated-chitosan nanoparticles for enhanced protein delivery. Thus, we offer a cell-penetrating-peptide based novel therapeutic strategy to treat chronic wounds.



**Figure 1.** Construction and characterization of octaarginine decorated FGF-2 nanoparticles. (a) Schematic overview of nanoparticles, (b) Scanning electron micrograph of the optimal nanoparticle.

**Keywords:** octaarginine, cell-penetrating peptide, FGF-2, alginate, drug delivery

**Acknowledgments:** This work was supported by Ege University Research Fund [BAP, 14-ECZ-030, 2016].

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OL-2-10

## **Lignin Stabilized Bimetallic Nanoagent Doped Hydrogels for Antimicrobial Photodynamic Therapy**

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### **ABSTRACT**

Lignin has intrinsic antimicrobial and antioxidant properties, which makes it a material of potential interest. It is mainly derived as a waste from paper and pulp industries and is an underutilized biopolymer [1]. In this work, lignin was utilized as a matrix and reducing agent to synthesize gold/silver based monometallic and bimetallic nanocomplexes. Lignin was used as a sole agent for capping and stabilizing the lignin-metallic/ bimetallic nanocomplexes, using a one-pot method [2]. The synergistic antimicrobial and antioxidant properties of the lignin stabilized nanoagents were then explored. Various analytical techniques were utilized to characterize the synthesized lignin based nanocomplexes. The mechanism behind the antimicrobial activity of the nanocomplexes was also explicated. Theranostic photosensitizers were then conjugated on to the surface of the developed nanocomplexes [3]. The nanoconjugates were tested for their singlet oxygen quantum yield as well as fluorescence quantum yield. Further, the developed nanoconjugates were doped inside a biocompatible hydrogel to develop a nanocomposite hydrogel. The nanocomposite hydrogel was subjected to pH responsive study, rheological studies and scanning electron microscopy. After the characterizing the nanocomposite hydrogel, it was subjected to antimicrobial photodynamic therapy studies. This study paves a way for using agro-waste to develop value added antimicrobial products.

**Keywords:** *lignin, antimicrobial photodynamic therapy, bimetallic nanoagents, photosensitizers, hydrogels*

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## Magnetically Driven Therapies: Optimizing Performance by Mitigation of Eddy Currents

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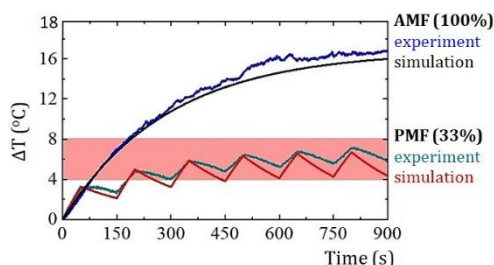
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### ABSTRACT

Cancer is one of the diseases that attracts great research interest. A very promising anticancer method is magnetic particle hyperthermia (MPH), where magnetic nanoparticles are exposed to alternating magnetic fields (AMF). This results in providing excessive heat cargo in malignant regions, resulting to temperature increase within 41 to 45°C, potentially harmful for the cancerous tissues. At the same time, surrounding healthy areas also undergo a heat shock due to eddy currents naturally occurring during electromagnetic field applications. Such a problem hinders the application of higher either in frequency and/or amplitude magnetic fields, hindering optimum performance. This is a typical problem, also in magnetic resonance imaging (MRI) systems, where it may be tackled by pulsed magnetic fields (PMF). This study initiates by evaluating field protocols, in MRI, to show the impact of pulsed magnetic fields on eddy current mitigation. As verified by simulation of a human model within an MRI setup in Sim4Life, eddy currents attenuate under typical clinical conditions. To further proceed, we attempt to apply this idea in a typical MPH protocol. Here, the field application mode consists of multiple ONs and OFFs within a tunable time interval named duty cycle. Its performance is examined both in phantom and ex-vivo samples prepared by agarose and veal tissue respectively, where magnetite magnetic nanoparticles are incubated. Specimen with magnetic nanoparticles corresponds to cancerous tissue, while specimen without magnetic nanoparticles corresponds to healthy tissue. As shown in Figure 1, there is a direct impact on temperature reduction by minimizing the duration of eddy currents flow, while a high enough temperature increase due to magnetic nanoparticles is sustained to ensure effective treatment. Theoretical simulation, by Comsol Multiphysics, of temperature evolution, has verified the beneficial role of multiple pulse instead of single pulse AC magnetic field, opening new field possibilities in magnetically driven therapy schemes, focusing on optimized performance yet considering side effects.

**Figure 1:** theoretical time (duty cycle 100%) a typical MPH applied in the agreement obvious, yet significantly,

where  $\Delta T = 4-8^\circ\text{C}$ , where  $4^\circ\text{C} = 41^\circ\text{C}-37^\circ\text{C}$  and  $8^\circ\text{C} = 45^\circ\text{C}-37^\circ\text{C}$ . Thus, eddy current generation is suppressed, while a satisfactory heat release is sustained.



Comparison between experimental and evolution temperature curves for (a) AMF and (b) PMF (duty cycle 33%) application in cycle. Both types of magnetic field are same reference phantom sample. The good between theoretical and experimental data is temperature increase in PMF is suppressed though entering easily the hyperthermia

**Keywords:** magnetic nanoparticles, magnetic hyperthermia, pulsed magnetic field, cancer therapy, MRI

### ACKNOWLEDGMENT

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## Fluorescein-entrapped magnetosomes for magnetically assisted photodynamic therapy

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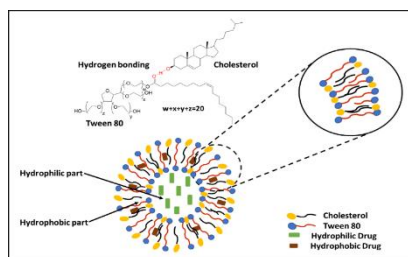
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### ABSTRACT

Here, we report the preparation of fluorescein (FL) entrapped magnetosomes, i.e. silica-coated iron oxide nanoparticles entrapped within niosomes, for application in magnetically assisted photodynamic therapy (PDT) *in vitro* [1,2]. In the synthesis of this vesicular system, the utilization of Tween-80 for niosome fabrication provides better control and stability to the self-assembled structure by forming hydrogen bond with cholesterol. The hydrogen bonding between the carbonyl group of tween-80 and hydroxyl group of cholesterol essentially governs the rigidity of the niosome. The balance of hydrophilic and hydrophobic groups provides structural integrity to the niosomes, playing a vital role in encapsulation of hydrophobic dyes/PS (fluorescence) and hydrophilic entity (IOVT) to provide dual functionality of magnetically induced photodynamic therapy, as shown in the Figure given below [3]. These magnetosomes and related controls were characterized by TEM and DLS for size, EDX for elemental composition, UV-visible and fluorescence spectrophotometry for optical properties, and VSM for magnetic behaviour. These magnetosomes were found to release entrapped FL in a sustained manner. The photoactivated conversion efficiency of molecular oxygen into the cytotoxic singlet oxygen of the photosensitizer FL is not only retained, but also enhanced, upon entrapment within these magnetosomes [4]. *In vitro* studies carried out in Panc-1 cancer cells revealed magnetically assisted enhancement in the cellular uptake of the magnetosomes. Magnetic assistance also led to enhancement in PDT efficiency in cells treated with the FL-entrapped magnetosomes and light.

**Keywords:** Magnetosomes; Fluorescein; Photodynamic therapy; Magnetic targeting; *in vitro* cytotoxicity.



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## Peroxytitanium Complex Derived Fe-doped TiO<sub>2</sub> Nanoparticles: Synthesis, Properties and Antibacterial Activity

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### ABSTRACT

The synthesis of Fe<sup>3+</sup>-TiO<sub>2</sub> nanoparticles (NPs) derived from peroxytitanium complex carried out using hydrothermal method [1]. Pure TiO<sub>2</sub> and Fe<sup>3+</sup> doped TiO<sub>2</sub> powders were characterized to study their structural, compositional, morphological and optical properties [2-3]. The X-ray diffraction patterns shown in Fig.1 were of crystalline pure anatase TiO<sub>2</sub> and crystallite size decreases from 10.17 to 8.25 nm with addition of Fe<sup>3+</sup> ion [4]. FE-SEM micrographs reveal well diffused aggregates with nanograin morphology. The efficiency of antibacterial activity against *E. coli* was studied under different physicochemical parameters [5]. The antibacterial activity varies with concentration of Fe<sup>3+</sup> in TiO<sub>2</sub> matrix against *E. coli* bacteria. The antibacterial activity was increased with increasing Fe<sup>3+</sup> content in TiO<sub>2</sub> NPs and the highest antibacterial activity was observed for 2.15 wt. % Fe<sup>3+</sup>-TiO<sub>2</sub>.

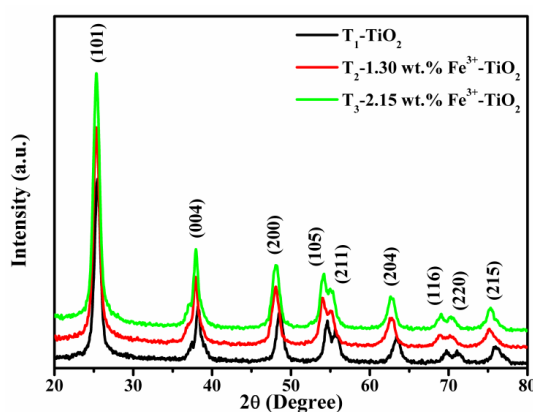


Fig.1 X-ray diffraction patterns T<sub>1</sub>, T<sub>2</sub> and T<sub>3</sub> nanoparticles.

**Keywords:** Fe<sup>3+</sup> doped TiO<sub>2</sub>; XRD; FE-SEM; Antibacterial activity

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OL-2-14

## Polyunsaturated fatty acid-based targeted nanostructured lipid carrier system with enhanced brain permeability: a novel approach for treating breast to brain metastatic cancer

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### ABSTRACT

Brain metastases (BM) are the common type of intracranial tumour and the most frequent complications of systemic breast cancers [1]. Unfortunately, most of the available chemotherapy options do not effectively cross the blood-brain barrier (BBB), rendering the brain as a true sanctuary site for disease relapse. In this study, we report the enhanced therapeutic efficacy of docetaxel (DTX) when combined with polyunsaturated fatty acids (PUFA) appended nanostructured lipid carrier for effective treatment of breast cancer metastasised to the brain. Lipid-based nanocarrier (NLCs) was developed following a detailed optimisation of critical factors including product and process parameters, and 3<sup>2</sup> factorial design, resulted in a stable formulation with high drug loading, entrapment efficiency and uniform particle distribution. The NLCs was further surface modified with two PUFAs, Gamma (GLA) and Alpha-linolenic acids (ALA). ALA-DTX-NLCs synergistically improved the anticancer efficacy of DTX, cell uptake, and apparent permeability Papp through metastatic blood-brain tumour barrier (BBTB) mode developed from MDA-MB-231 cells.

On the other hand, GLA-DTX-NLC improved DTX efficacy with no significant effect on cell uptake and permeability through the model. Therefore, we propose ALA as a successful ligand to improve drug transport and uptake by MDA-MB-231 cells. Further studies are required to recognise these data and progress to *in-vivo* and clinical testing.

**Keywords:** metastatic breast cancer, brain tumour barrier model, docetaxel, nanostructured lipid carrier, Polyunsaturated fatty acids.

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OL-2-15

## Assessments of solid lipid nanoparticle formulations for the delivery of CRISPR / Cas9 Genome editing plasmids as an alternative to viral vectors

OL-2-15

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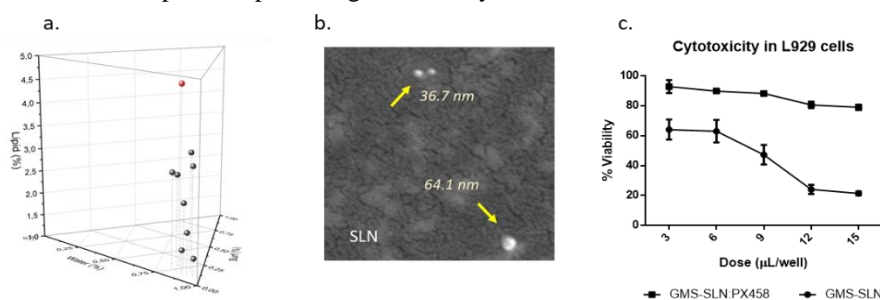
### ABSTRACT

The CRISPR/Cas9 system is a promising gene editing tool with wide-ranging applications, however a biocompatible and efficient delivery of CRISPR/Cas9 expression systems remains a challenge [1]. To overcome this phenomenon, we have developed a solid lipid nanoparticle (SLN) based delivery system for a widely used plasmid DNA encoding Cas9 protein as an effective alternative to viral vectors.

Primarily, SLNs were produced by microemulsion dilution technique based on the pseudo-ternary phase diagrams and 3D tetrahedral plots [2]. Electrophoretic mobility assays were carried out and optimal complex formation ratio was determined. DLS measurements were performed in order to investigate the physicochemical properties of SLNs and complexes. Obtained SLNs and complexes with PX458 CRISPR-Cas9 plasmid have particle sizes of 68.15 and 112.8 nm, respectively [3]. Zeta potential values have dropped after complex formation and polydispersity index values are less than 0.3 for all formulations. Particles are found to be stable up to 90 days. DNase I protection and serum stability assays showed that developed formulation is able to protect the PX458 plasmid from degradation. According to cytotoxicity test results, no significant cytotoxicity was observed on HEK293T and L929 cells for the transfection doses. Furthermore, the developed SLN system revealed similar transfection efficiency with commercial Lipofectamine in HEK293T for PX458 plasmid ( $P > 0.05$ ).

Overall, our findings reveal that we have achieved a good SLN basis for a non-viral delivery system and have the potential to produce SLNs with desired properties by modifying production parameters and components to facilitate translating CRISPR/Cas9 into pre-clinical and clinical studies [4].

**Keywords:** cationic solid lipid nanoparticle, gene delivery, CRISPR/Cas9, PX458, transfection



**Figure 1.** a. 3D tetrahedral plot of microemulsion, b. SEM image of the SLN, c. Viability results

This study was funded by the Scientific and Technological Research Council of Turkey (TÜBİTAK-SBAG-218S682).

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OL-2-16

## Design and Development of Uncooled Terahertz Detector Arrays as On-chip Integrated Medical Device

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### ABSTRACT

Modern explorations for thermal radiation detectors fueled by advancement in nanofabrication technologies and newer understanding of materials for various on-chip integrable devices in Terahertz (~300 GHz –3 THz) range offers remarkable potential for biomedical applications. In this study the schemes of design, development and fabricated of uncooled terahertz detector arrays with potential application as on-chip integrated terahertz medical systems, is elaborated. These unit devices are fabricated with integrated heater/thermistor/half-wave dipole gold (Au) antenna with a titanium (Ti) heater, a SiO<sub>2</sub>/SiN<sub>x</sub> interlayer, on SiO<sub>2</sub> and SiN<sub>x</sub> substrates, using nanoscale meander-shaped (design width~100 nm) Ti thermistors, with reasonably high electrical and optical responsivity and moderate noise-equivalent power (NEP). Device parameters such as the temperature coefficient of resistance (TCR) and resistivity plays critical role in the design while device miniaturization. The reduction in thermistor width leads to higher responsivity, but detrimental to the noise response (NEP) of the devices, which validates our previous investigation into narrow width effects [1,2], and may be linked to smaller grain size in thinner metal interconnects (thermistors) responsible for the lower TCR. Hence increased resistivity of the devices and enhancement in responsivity in the design was largely due to the nanoscale meander design among other. Schemes of improvement of electrical and thermal properties of the microbolometer by Joule heating and other effects of annealing have also been explored.

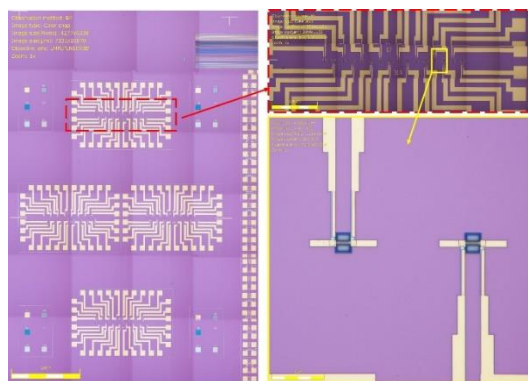


Figure.1. shows optical microscope images of Ti based uncooled antenna-coupled THz microbolometer arrays with design width of the thermistor ~ 0.1 and 0.2  $\mu\text{m}$  with enlarged optical microscope images of a set of microbolometer device with heater and the meander structured thermistor floating above the cavity.

**Keywords:** THz Detectors, Biomedical Systems, TCR, Responsivity, Narrow Width Effect,

### ACKNOWLEDGMENTS

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OL-2-17

## Cancer Nanomedicine Developed from Total Human Serum: A Novel Approach for Making Personalized Nanomedicine

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### ABSTRACT

Albumin nanoparticle (nab<sup>TM</sup> technology) is one of the most successful nanomedicine platforms used in clinics for cancer drug delivery. Abraxane® is the first albumin-bound paclitaxel nanomedicine (size ~130nm) approved by US-FDA for advanced breast cancer, non-small cell lung cancer, and pancreatic cancer [1]. Abraxane® also uses highly purified recombinant human albumin which involves a laborious, proprietary process, and high cost of production [2].

Here we report a very simple, bed-side, method of making anti-cancer drug-loaded protein nanomedicine using the patient's own serum or from a matched donor. In-vitro studies using peripheral blood mononuclear cells (PBMCs) and in-vivo studies conducted in rat models showed no adverse cytokine-chemokine release indicating the immune compatibility of the TSN platform. Total serum nanoparticles (TSN) were prepared by simple co-precipitation with hydrophobic chemo-drugs such as paclitaxel (PTX) and piperlongumine (PL). The nanoparticles loaded with PTX and PL showed sizes of 100nm and 30nm with an encapsulation efficiency of 42.6% and 51% respectively. Considering the approval of Abraxane® for pancreatic cancer, we tested the efficacy of TSN-PTX and TSN-PL in human pancreatic cell lines. TSN-PTX tested on MIA Pa Ca -2 retained ~20% cells, while TSN-PL showed cytotoxicity of 100% at the highest treated concentration. Further, we tested the efficacy of TSN-PL in *in vivo* xenograft models of pancreatic cancer. Compared to free PL, TSN-PL showed promising efficacy in inhibiting MIA Pa Ca -2 tumor in vivo, without causing any significant hematological toxicity. In effect, we report a unique protein nanomedicine platform technology using the patient's blood serum, which with further optimization can be developed into personalized nanomedicine at an affordable cost.

**Keywords:** pancreatic cancer, total serum nanoparticles, paclitaxel, gemcitabine, drug delivery

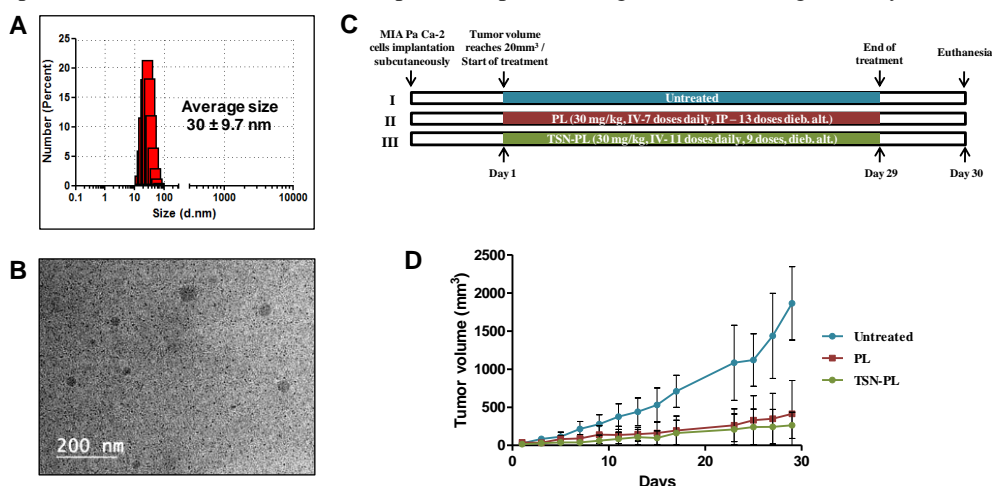


Figure 1: (A) Particle size distribution of TSN-PL nanoparticles, (B) TEM image TSN-PL, (C) Schematic diagram of the study design of in-vivo anti-tumor studies. Animals were subcutaneously injected with MIA PA Ca-2 cells and when the tumor volume reached around 20mm<sup>3</sup>, treatment was started (20 doses) till day 29. Animals are euthanized on day 30. (D) The tumor volume treated with PL and TSN-PL [Volume = (Width)<sup>2</sup> x Length / 2]

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OL-2-18

## Multifunctional magneto-plasmonic Fe<sub>3</sub>O<sub>4</sub>/Au nanocomposites for photothermal therapy

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### ABSTRACT

There is a growing interest toward the magneto-plasmonic nanocomposites due to their potential use for targeted drug delivery, nanoparticle-based diagnostic and therapeutic applications [1]. The nanocomposites with magnetic iron oxide core and gold shell possess magnetic and optical (plasmonic) properties inherent to both individual components.

Herein, we report magneto-plasmonic Fe<sub>3</sub>O<sub>4</sub>/Au core/shell nanocomposites prepared via green approach: chemical reduction of Au ions by tryptophan, as well as photochemical under UV-C LED irradiation, in the presence of nanosized magnetite. This approach allowed us to obtain dynamic Fe<sub>3</sub>O<sub>4</sub>/Au nanosystems that exhibit optical properties of nanoscale gold (plasmon absorption band peaked at ~ 550 nm) and can be reversibly attracted/aggregated by external magnetic field, with aggregation accompanied by an increase in absorption in near infrared (NIR) spectral region (Fig. 1, A and B).

To assess photothermal therapy of cancer cells in vitro, cancer cells were incubated with magneto-plasmonic Fe<sub>3</sub>O<sub>4</sub>/Au nanocomposites and irradiated by laser at 593 nm. The formation of irradiation induced microbubbles on the cell surface was revealed by a confocal microscopy imaging (Fig. 1C).

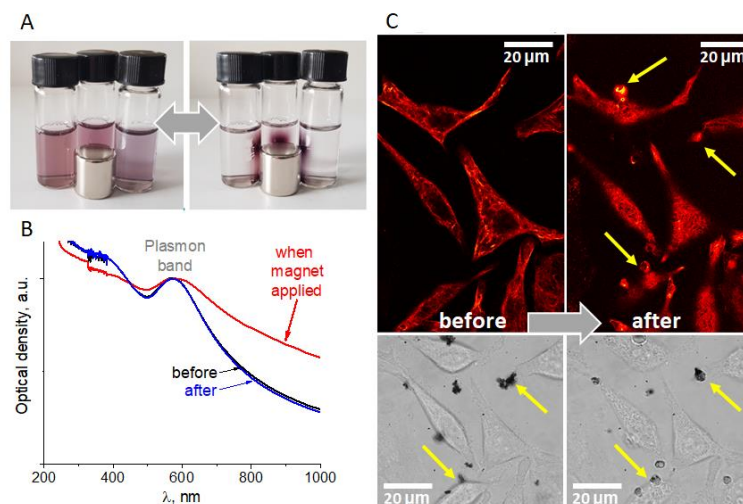


Figure 1. A. Magnetophoretic effect on Fe<sub>3</sub>O<sub>4</sub>/Au nanocomposites. B. Fe<sub>3</sub>O<sub>4</sub>/Au absorption spectra with magnetic field induced reversible change. C. Laser irradiation initiated formation of microbubbles on Fe<sub>3</sub>O<sub>4</sub>/Au treated HeLa cells visualized by confocal fluorescence (top) and transmission (bottom) microscopy images.

**Keywords:** magneto-plasmonic nanocomposites, Fe<sub>3</sub>O<sub>4</sub>/Au, photothermal effect, microbubbles, HeLa cells.

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OL-2-19

## Investigating the potential of a nano-formulation for intra-vaginal drug delivery system of an insulin sensitizing agent as a tool for treatment of polycystic ovarian syndrome (PCOS)

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**Background:** PCOS, a highly prevalent endocrinopathy in women of reproductive age is majorly due to Insulin resistance [1]. Mechanically, metformin, (MTF) not only improves the insulin signal, but also controls the hyperandrogenism whereas myo inositol (MYO) improves the FSH signal, guides GLUT4 channel and controls the androgen level [2]. However, oral administration of these drugs in combination is often associated with impaired bioavailability and adverse effects leading to poor patient compliance. Intravaginal drug delivery system is capable of penetrating via mucus deeply into the vaginal rugae and delivery the drugs thereof and allowing high concentrations to reach the target ie ovarian tissues through the uterovaginal blood vessels [3,4].

**Aims and objective:** To design, develop and characterize an intra-vaginal pH sensitive gel constituting of MET and/or MYO loaded nanoparticles coated with low molecular weight polymer.

**Method:** *In-silico* studies were performed elucidating drug interaction with IP3 kinase and insulin receptors, IVDD nanoparticles were fabricated by solvent evaporation method and duly characterized and optimized.

**Result:** Molecular docking reveals that MYO bound tightly at the active site of inositol receptor protein by forming hydrogen bonding with Lys521 and Gln524 while MET molecules were bound tightly on the insulin receptor protein forming strong hydrogen bonds with Arg1136, Asn1137 and Asp1083. The pH sensitive gel containing MTF and MYO PLGA nanoparticles were successfully prepared. Characterization revealed an average particle size and surface charge as  $198 \pm 15.5$  and  $205 \pm 16.8$  nm ( $p < 0.05$ ); average surface charges were  $-22 \pm 6.8$  and  $-20 \pm 5.6$  respectively. The average encapsulation efficiency and drug loading were  $86 \pm 9.5\%$  and  $18.06 \pm 5.4$ .

**Conclusion:** *In-silico* studies facilitate the strong interaction of drugs with the related receptors on the surface of the ovary, the target site. The proposed intra-vaginal drug delivery particles potentially exhibit promise for alteration, development of normal follicles, regular menstrual cycle, ovulation, improved insulin and FSH signals to ameliorate PCOS.

**Keyword:** *In-silico* study, intra-vaginal, myo-inositol, metformin and polycystic ovarian syndrome.

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OL-2-20

## Synthesis of Silver Nanoparticles in Starch-based Hydrogel: Antipseudomonal activity and Potential for Tackling Wound Infections

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### ABSTRACT

Silver nanoparticles (AgNPs) are reported to possess significant antibacterial activity. *Pseudomonas aeruginosa* is an epitome of nosocomial agent causing increased morbidity and mortality among patients hospitalized with traumatic wounds. Effective treatment of *P. aeruginosa* infections can be problematic because the organism is intrinsically resistant, and readily acquires resistance, to multiple antibiotics [1]. Therefore, scientific community is in search of an efficacious drug option for tackling *Pseudomonas* mediated wound infections. Silver nanoparticles loaded hydrogel is anticipated to provide protection against *P. aeruginosa* by the slow release of silver ions as well as due to their broad-spectrum antimicrobial efficacy [2]. Here we explored the *in-situ* synthesis AgNPs and the development of starch-based hydrogel loaded with them. The synthesis involves the use of silver nitrate, gelatin/starch, honey and water as the silver precursor, stabilizing agent, reducing agent and solvent respectively. Honey being a natural product with antibacterial as well as wound healing properties underlines its application as reducing as well as capping agent. The colloid obtained at a pH of 8.5 is found to consist of nearly spherical AgNPs of size approximately 15-20 nm. The AgNPs were characterized using UV-vis absorption spectroscopy, Fourier transform infra-red spectroscopy (FTIR), X-ray diffraction (XRD), and transmission electron microscopy (TEM). Antipseudomonal activity of AgNPs as well as the AgNP-loaded hydrogel was investigated by agar well diffusion method. Furthermore, the minimum inhibitory concentration was studied by microtube broth dilution method showed that AgNPs as well as the AgNP-loaded gels possess better antipseudomonal efficacy than the existing antibiotic imipenem belongs to the carbapenem a 'last-resort' treatment option for multidrug resistant Gram-negative infections [1]. This work demonstrates that AgNP-loaded hydrogel exhibits great potential in tackling one of the most prominent wound infecting nosocomial pathogen.

**Keywords:** Silver nanoparticles, nosocomial agent, antipseudomonal activity, wound infections, minimum inhibitory concentration

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OL-2-21-SL

## Fabrication of Dual-plasmonic Ag@CuS nanostructures for Theranostic applications with Improved SERS Performance.

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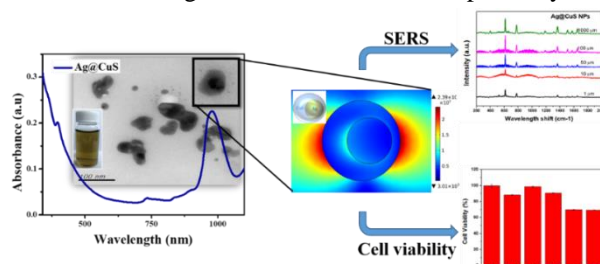
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### ABSTRACT

Complex nano hybrids show a new class of materials with improved physicochemical properties which have greater potential as sensors, drug carriers, bioimaging agents etc. The metal-semiconductor nanocomposites with extraordinary opto-electric properties are more effective than their individual elements for biophotonics applications. The intense near fields are the primary reasons to choose Silver and the self-doped copper chalcogenides for their optical properties around the near-infrared spectral region (750–2500 nm). Moreover, the CuS NPs have shown better photothermal (PT) conversion efficiency which is useful for carcinogenic tumour tissue ablation. Herein, we report a simple hydro-thermal synthesis for core-shell Ag@CuS nanoparticles (NPs) with plasmon resonance bands at around 400 nm and 975 nm. Transmission Electron Microscopy (TEM), X-Ray powder diffraction (XRD) and X-Ray Photoelectron spectroscopy (XPS) were performed to get the structural as well as elemental confirmations. The as-synthesised dual Plasmonic NPs were used as Surface Enhanced Raman Spectroscopy (SERS) substrate for the detection of Rhodamine 6G dye with concentration variation. Also for our better understanding towards the electromagnetic field confinement across NPs and heating effect due to light irradiation, theoretical study was done using COMSOL Multiphysics simulation tool. Again, we found that our experimental results have good agreement with the simulated data. We performed the cell viability test using HeLa cells which confirms the biocompatibility nature of the NPs. It was found that Ag@CuS NPs exhibit an improved SERS activity with good biocompatibility which can be a promising candidate for fabrication of SERS substrate as well as photothermal therapy (PTT) application.

**Keywords:** metal-semiconductor, electromagnetic. Plasmonic, biocompatibility, SERS.



OL-2-22

## Polysaccharide modified nanomaterials used as an electroactive material: application in clinical diagnostics

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### ABSTRACT

In current study, ZnO and ZnO nanocomposites and Ag Nanoparticles-ZnO nanocomposite (ZnO/PS/Ag) were synthesized and further characterised. Zinc oxide has a very broad and versatile range of application including, cosmetics, and pharmaceutical uses and chemical sensing etc. Zinc oxide nanoparticles (ZnO NPs) are one of the most important metal oxide nanoparticles popularly employed in various fields due to their peculiar physical and chemical properties. These NPs and nanocomposites were studied for different characterisation techniques such as FTIR SEM, XRD etc. Electrochemical behaviour of these nanoparticles were studied and can be further used as a transducer to modify electrode surface for further studies in detection of pathogenic bacteria. ZnO can be used as a promising material in electrochemical studies. Zn NPs were modified by different polysaccharides and compared its effectiveness as an electroactive material. Polysaccharides like chitosan and LBG were used for modification of ZnO Nps. This study shows the comparative analysis of ZnO and Nanocomposites for further use as a transducer. This material can be used as a transducer in diagnostic assays as well.

**Keywords:** nanocomposite, pathogen, electrochemical, transducer

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OL-2-23

## **Nanoemulsion based Gel of Fluconazole for Topical Delivery**

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### **ABSTRACT**

The goal of any drug delivery is to provide a therapeutic amount of drug to a proper site so that the drug concentration can be achieved promptly and then maintained. Drug delivery via nanoemulsion based gel formulation has been proposed to be prevailing in the type of controlled drug delivery device both in present and future. The idea behind developing a topical nanoemulsion based gel formulation was for delivering fluconazole sustained release pattern for an extended period of time to reduce frequency of application and improve the patient compliance by reducing dosing frequency. Fluconazole is a triazole and is a potent broad - spectrum antifungal activity in fungal infection of hairs and skin [1-3].

For preparation of nanoemulsion, oleic acid was selected as the oil phase. Acrysol EL135 and propylene glycol were selected as the surfactant and co-solvent respectively, and were mixed (Smix) in different weight ratios (1:1, 2:1, 3:1, 4:1). Pseudoternary phase diagrams were developed and oleic acid and Smix were mixed in different weight ratios ranging from 1:9 to 9:1. Based on the nanoemulsion region of each diagram, the formulae were selected. The formulated nanoemulsions were characterized and evaluated for globule size, zeta potential, viscosity, drug content. Optimized nanoemulsion were incorporated into Carbopol gel which were examined for *ex vivo* skin permeation study and antifungal activity which was compared to the marketed product Flucos<sup>®</sup> gel.

The size of nanoemulsion was found in the range of 84.8 - 430.4 nm (PDI: 0.260 -0.385). The pH was ranged from 5.00 to 5.50. The *in vitro* drug release was found to be 51.43% in 6 h. The results of nanoemulsion based gel containing fluconazole showed better antifungal activity against *Aspergillus niger*. Hence, it can be concluded that prepared nanoemulsion based gel containing fluconazole may be a good formulation for topical delivery.

**Keywords:** Nanoemulsion, gel, topical, fluconazole, antifungal

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OL-2-25

## Antibacterial properties of highly magnetic monodispersed FeCo nanoparticles

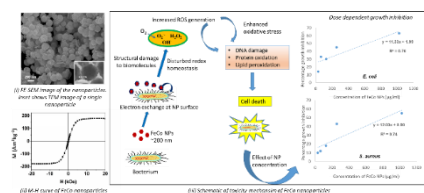
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### ABSTRACT

FeCo nanoparticles have been synthesized by the polyol reduction process and characterized for their structural, morphological, magnetic and potential antibacterial properties. X-Ray Diffraction (XRD) pattern indicates formation of BCC phase of the alloy without any impurity phases [1]. Electron microscopy images taken using Field emission scanning electron microscope (FE-SEM) and Transmission electron microscope (TEM) reveal formation of uniform spherical structures of ~ 200 nm diameter, as shown in Fig. (i). Magnetic properties investigated using a Vibrating sample magnetometer (VSM) suggests the nanoparticles to be highly magnetic with a saturation magnetization ( $M_s$ ) of ~ 180 Am<sup>2</sup>kg<sup>-1</sup> and coercivity ( $H_c$ ) of ~ 150 Oe. The corresponding hysteresis curve is depicted in Fig (ii). Antibacterial activity of the synthesized nanoparticles was investigated qualitatively by measuring the zone of inhibition (ZOI) of bacterial growth, by disc diffusion assay, for two test bacteria namely *S. aureus* and *E. coli*. At a nanoparticle concentration of 10 mg/ml, this was determined to be 0.5 mm for both the species, suggesting nearly similar susceptibility to the synthesized nanoparticles. Further quantification of antibacterial performance was done by standard broth dilution tests, where dose dependent inhibition of the bacterial growth was investigated. A positive linear correlation ( $R^2 = 0.74$  for *S. aureus* and  $R^2 = 0.76$  for *E. coli*) was observed between nanoparticle concentration and percent bacterial growth inhibition, that was indicated by the decrease in solution turbidity. The MIC values for both the strains were accordingly ascertained to be >1024 µg/ml. An attempt has been made to understand the underlying bacterial toxicity routes of the synthesized nanoparticles by relating with their physical and chemical properties. These have been summarised in Fig (iii). Owing to the ability of FeCo to undergo changes in oxidation state in the bacterial culture medium; reactive oxygen species (ROS) induced damage, direct structural damage to bio-molecules or damage to cell wall due to physical adherence at the bacterial cell wall have broadly been speculated to be the possible inhibitory mechanisms. Thus, synthesized FeCo nanoparticles can potentially act as single-entity magnetic antibacterials, where the ease of field-assisted targeting and retrieval [2] can answer the current medical needs against increasing number of multi-drug resistant bacterial strains [3] and also can be used for environmental remediation [4].



**Keywords:** FeCo, antibacterial, zone of inhibition, reactive oxygen species, minimum inhibitory concentration

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OL-2-26

## Vitamin C Induced Perturbation of Redox Balance Downregulates the Expression of Nrf-2 in Cisplatin-Resistant Ovarian Cancer Cells

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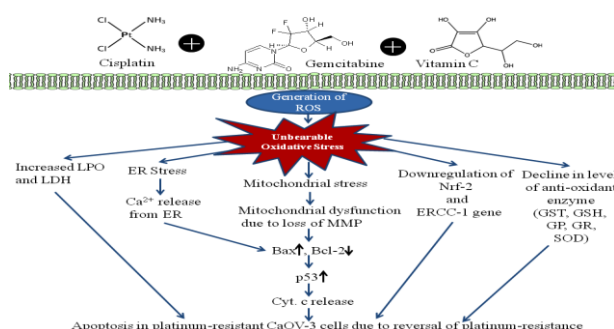
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### ABSTRACT

Cisplatin resistance is detrimental in the successful management of ovarian cancer. Since, Vitamin C (VC) has the potential to reverse chemo-resistant phenotypes, we investigated the impact of VC sensitization followed by combinatorial therapy with conventional chemotherapeutic agents in platinum-sensitive (PA-1) and resistant (CaOV-3) ovarian cancer cells. Differential dose priming with VC in PA-1 cells (2mM VC) and in CaOV-3 cells (4mM VC) for 24hrs with a constant dose of Cisplatin (4.5 $\mu$ M) in combination with Gemcitabine (31.25 nM) in PA-1 cells and 62.5 nM in CaOV-3 cells caused DNA damage, reduction in MMP and mitochondrial CytC release, upregulation of p53 and Bax gene. Increased downregulation of genes contributing to CR i.e. ERCC-1, Nrf-2, Bcl-2 gene were observed in CaOV-3 cells as compared to PA-1 cells. ROS generation post-VC sensitization was responsible for ER stress induced intracellular Ca<sup>2+</sup> release and mitochondrial apoptosis pathway activation. Reduced anti-oxidant enzymes (GST, GSH, GP, GR, SOD) levels were reported post-combination treatment. Perturbation of redox balance results in irreversible oxidative damage causing unbearable metabolic insults in ovarian cancer cells. Interestingly, by preferentially protecting the normal cells, VC exhibits remarkable specificity and pro-oxidative potential for reversal of cisplatin resistance in cancer cells.

**Keywords:** Ovarian Cancer, Cisplatin Resistance, Vitamin C, Oxidative stress, p53, Pro-oxidant, Apoptosis.



OL-2-27

## POSS Functionalized Star Glycopolymers; A Lectin Binding Ligand

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### ABSTRACT

A new class of organic-inorganic hybrid star glycopolymers based on polyhedral oligomeric silsesquioxane (POSS) was prepared to study its interaction with carbohydrate binding proteins, lectins. The POSS-polycaprolactone (POSS-PCL)-cored octa-arm star-shaped glyco block copolymer (BCP), poly( $\epsilon$ -caprolactone)-*b*-poly(glucopyranose) (Star-POSS-PCL-*b*-PGlc) was successfully synthesized via the combination of ring opening polymerization (ROP) and MADIX (macromolecular design by interchange of xanthate) polymerization technique. Octa(3-hydroxy-3-methylbutyl dimethylsiloxy) POSS (Star-POSS) was utilized to initiate the ROP of the  $\epsilon$ -caprolactone to achieve octa-arm star-shaped Star-POSS-PCL.[1] A successive bromination followed by xanthation[2] of the synthesized Star-POSS-PCL polymer promoted further polymerization of 3-O-acryloyl-1,2:5,6-di-O-isopropylidene- $\alpha$ -D-glucopyranose (AIPGlc) via MADIX polymerization to fabricate Star-POSS-PCL-*b*-PGlc of different block lengths. The synthesized star-shaped block copolymers (BCP) were characterized using <sup>1</sup>H NMR, FT-IR and DSC analyses. The morphology and aqueous solution behavior of the Star-POSS-PCL-*b*-PGlc were analyzed using FESEM, HRTEM and DLS analyses, respectively. The binding efficiency of Star-POSS-PCL-*b*-PGlc with lectin having different glycopolymers block length was studied using turbidimetry assay and fluorescence quenching titration (FQT) using photoluminescence spectroscopy (PL).[3] Here, FITC labeled concanavalin A (FITC-Con A) was used as a model lectin. The cytotoxicity study of the star-shaped BCPs over the human fibroblast cells revealed the non-toxic nature of the BCPs which open up its great potential towards drug delivery vector.

**Keywords:** Star glycopolymers, octa(3-hydroxy-3-methylbutyl dimethylsiloxy) POSS, RAFT polymerization, lectin-binding.

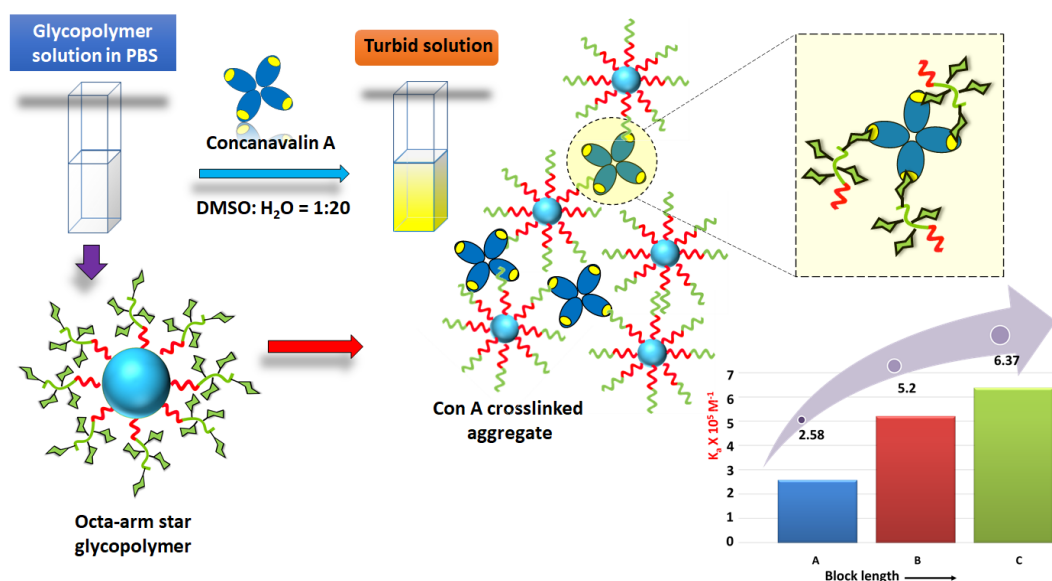


Figure: Schematic diagram of interaction between star glycopolymers and Con A.

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OL-2-28

## Hydrothermally synthesized pristine and Sr-doped $\text{CuBi}_2\text{O}_4$ for antimicrobial and photokilling applications

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### ABSTRACT

**Abstract:** Copper bismuth oxide ( $\text{CuBi}_2\text{O}_4$ ) nanoparticles are known for their optoelectronic and photocatalytic properties. It is well known that doping these materials can significantly enhance their physicochemical and structural properties leading to better applications. Pristine and Strontium (Sr)-doped CBO i.e. copper bismuth oxide ( $\text{CuBi}_2\text{O}_4$ ) nanoparticles were synthesized by a low temperature chemical route and structural phase confirmed by X-ray diffraction (XRD) patterns. XRD results show that pristine and Sr-doped CBO has been crystallized with a spinel-type structure in tetragonal crystal system shown in fig.1. Sr-doped CBO absorbs strongly in UV-Visible region of an electromagnetic spectrum. Also, nanostructured thin films of pristine and doped CBO are grown on conducting i.e. fluorine doped tin oxide (FTO) glass substrate using seed assisted hydrothermal method and schematic is shown in fig.2. Antimicrobial activity of doped and pristine samples was studied with *E. coli* and *S. aureus* and confirmed with the repetitive analysis. Disc diffusion assay and MTT assay were performed to study antimicrobial effects and cell viability. The photokilling effect of these materials were tested using visible light illumination. We observed about 65% cytotoxicity within 15 min of exposure to visible light.  $\text{CuBi}_2\text{O}_4$  was doped with 1%, 2% and 4% Sr.  $\text{CuBi}_2\text{O}_4$  doped with 4% of Sr was found to be most effective as compared to the pristine  $\text{CuBi}_2\text{O}_4$ . We have also tried to reveal the possible mechanism for the enhanced antimicrobial and photokilling effects. We are exploring it further in the areas of surface sterilization, water purification and waste water treatment.

**Keywords:** Copper Bismuth Oxide, hydrothermal, photokilling, cytotoxicity

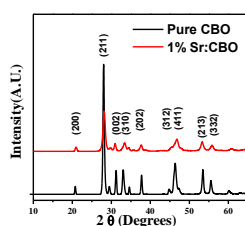


FIG.1: XRD ANALYSIS OF CBO

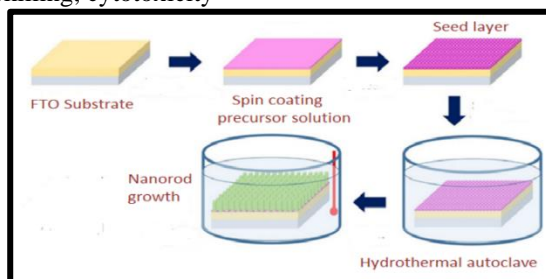


FIG. 2: SCHEMATIC DIAGRAM

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## Quantitative macromolecular magnetic resonance imaging of normal endothelial barrier disruption via bio-philicity interaction

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343-4139*

### ABSTRACT

Macromolecular therapeutics have shown promise for the enhanced passive permeation and retention Maeda effect selective transcapillary permeability into diseased tissue, however which varies with nanocarrier molecular weight [1] or size [2] and shape [3], in addition to surface charge [2, 4] with the associated potential for toxicity. Temporal determination of effective transvascular delivery at voxel-by-voxel spatial resolution is possible with the application of paramagnetic  $T_1$ -weighted NMR imaging with *in vitro*  $r_1$  relaxivity being  $2.8 - 3.6/T \cdot \text{msec} \cdot \text{molar concentration}^{-1}$  at 3 Tesla [5; Table 1], in contrast to that of ferromagnetic iron oxide core-based agents with higher intramolecular interaction affinity and  $r_2$  relaxivity, which are  $T_2$ -weighted signal enhancement agents [6, 7]. With the linear normalization of  $T_1$ -weighted signal intensity by longitudinal relaxivity conversion and application of the  $r_1$ -adjustment to *in vivo* imaging signal data, it becomes possible to determine blood plasma and tissue Gd concentration *in vivo* for agents with extended half-lives [2, 8], in addition to pharmacokinetic modeling of smaller size agents comparable to that of quantitative autoradiography [9, 10]. Therefore,  $r_1 \cdot T_R^{-1}$ -adjusted dual-flip angle dynamic contrast-enhanced  $T_1$ -weighted MRI can be utilized to quantifiably detect alterations in blood brain barrier endothelium permeaselectivity by Gd concentration space mapping with or without kinetic modeling (Figures 1 and 2) [8], in addition to imaging blood-brain tumor barrier (BBTB) permeability to  $[(\text{Gd}^{3+})\text{-DTPA}]^{2-}$ -conjugated PAMAM dendrimers (poly 1<sup>+</sup>) with neutralized exteriors upto 11.8 nanometers in diameter with effective peak concentration approaching 0.1 mM in intra-axial brain tumors [2]. For spheroidal nanoparticles with near neutral surface charge, the effective size range is 7 – 10 nanometers that results in extended blood plasma circulation matched to molecular size-selective biodistribution dynamics across arterially-supplied endothelial barriers of pathologic tissue (ie solid tumor, anaplastic ; nl < 6 – 7 nm), which however is increased to  $\geq 14$  nanometers for poly 1<sup>+</sup> insufficiently charge separated (IS) rhodamine (Rh) or Doxorubicin (Dox) exteriorly functionalized Gd-DTPA conjugated G5 and G8 PAMAM dendrimers (poly 2<sup>-</sup> IS 1<sup>+</sup>) as examples (Figure 1, panels A and B). Furthermore, there appears to be cationo-biophilicity toxicity to the normal blood brain barrier (BBB; Figure 1, panel C [2]), as evidenced by the positive contrast enhancement on functionalized dendrimer concentration mapping with respect to Gadolinium (Figure 2, red arrows), which implies toxicity of additional overlaying chemotherapeutic charge hydrophilicity per nanometer ( $\text{nm}^{-1}$ ) that is comparable to that of surface un-neutralized polyamidoamine core dendrimer (poly IS<sup>1+</sup>) toxicity *in vitro*. Theranostic part structures with chelated cationic paramagnetic heavy metal possess favorable biocompatibility, some of which are approved for clinical diagnosis

**Keywords:**  $T_1$  weighted, paramagnetic, contrast enhancement, theranostic, cationotoxicity

OL-3-01

## Mesoporous Perovskite of interlocked nickel titanate nanoparticles for electrochemical supercapacitor electrode

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### ABSTRACT

We have synthesized mesoporous nickel titanate (NTO) rods encompassing interlocked nanoparticles with clearly visible textural boundaries via sol-gel route, as an excellent working electrode for the supercapacitor. The mesoporous NTO rods assembled in the hexagonal shape of average diameter  $\sim < 1 \mu\text{m}$  and  $\sim 3$  to  $6.4 \mu\text{m}$  long, are composed of nanoparticles of diameter  $\sim 30 \text{ nm}$ . The well crystalline NTO rods of hexagonal phase to the space group of R-3H possess average (mean) pore size distribution of  $17.48 \text{ nm}$  throughout the rod body. The stoichiometric mesoporous NTO rods with increased textural boundaries played a significant role in the larger diffusion of ions, and delivered the specific capacitance ( $C_s$ ) of  $542.26 \text{ F/g}$ , energy density of  $8.06 \text{ Wh/kg}$  and a power density of  $4320 \text{ W/kg}$  in an aqueous KOH electrolyte, is significantly better than Ni, Mn, Fe, Cr and Ti-based perovskites or their mixed-phase accompanied by metal oxides as impurities. Moreover, the diffusion-controlled easy/faster and enhanced access to the  $\text{OH}^-$  ions ( $20.4 \mu\text{s}$ ) deep inside the rod body, delivered long life cycle, high stability up to 2100 cycles, and excellent retention of 91 %. Overall, mesoporous NTO rods hold potentials as an electrode material for long cycle lifetime supercapacitor and holds possibilities for further improvement after forming the nano-hetero-architecture or hybrid structures with other prominent materials such as  $\text{NiO}$ , and  $\text{Mn}_2\text{O}_3$ , etc.

**Keywords:** Mesoporous perovskites, Nickel titanate, Nanoparticles, Supercapacitor, Cyclic stability, XPS, Wettability, etc.

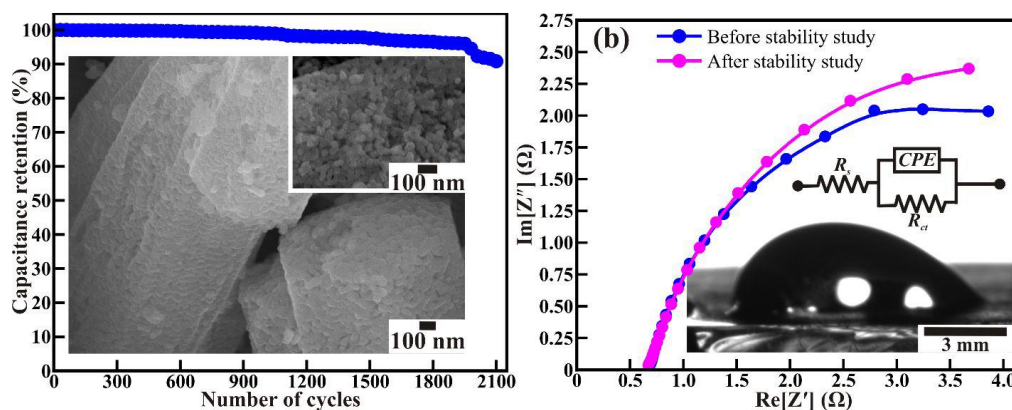


Fig.1 Graphical abstract

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OL-3-02

## **Activated Carbon and Waste Plastics Derived Graphene Nanosheets Composite for High Performance Supercapacitor Application**

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### **ABSTRACT**

Energy is an essential part of every living organism, especially for human being. Presently, more than 80% of the energy demands fulfill by fossil fuels but the use of these fuels creates a lot of environmental issues. Therefore, we need greener and alternative energy sources to fulfill world energy demands. In this regard, supercapacitors exhibit as the promising energy storage devices which have a lot of charming properties such as high capacitance value, faster charging and discharging rate and longer life cycle than the other energy storage devices.

In addition, plastic turns into a fundamental component of the human lifestyle. Due to this, over the past years, the production and influence of non-biodegradable plastics have amplified dramatically. The production of plastics reached more than 150 million tons per year. Its production increases day by day to fulfill the demand of the increasing world population. After using the plastics, they discard in our surrounding and create the vast deposition of plastic wastes which spoil the beauty of our cities, contaminate the water bodies and create environmental pollution. After examining the adverse effect of the waste plastics, many efforts have been made by the scientist to overcome the plastic waste by using recycling technique. Recycling of waste plastics evolves as the emerging technique from the other methods such as incineration and landfill, but as recycled plastics are generally devalued products. Thus, we need some upcycling techniques for the conversion of waste plastics into some value-added products.

Due to the aforementioned problems, here we report the mass production of graphene nanosheets from the waste plastics by using degradation agent at high temperature. Further, we synthesized activated carbon and graphene nanosheets composite for the high supercapacitor application. The developed materials were characterized by various spectroscopic and microscopic techniques. The electrochemical performance of as-prepared materials evaluated under the cyclic voltammetry, electrochemical impedance spectroscopy and galvanostatic charging-discharging. The as-synthesized composite showed the highest specific capacitance of 834 F/g with excellent cyclic stability. The results of this work definitely give the paves an alternative and best pathway for remediation of plastic waste and further its use for energy application.

**Keywords:** Graphene, Waste plastics, Activated carbon, Supercapacitor

## Towards the development of rechargeable high performance Zinc-air batteries

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### ABSTRACT

'Rechargeable batteries' is one of the promising energy storage technology that can meet the future energy demand for smart grid energy storage and electric vehicles (EVs) [1]. Among all energy storage devices, Lithium ion batteries (LIBs) technology lead the consumer market, however, limited energy density ( $250 \text{ WhKg}^{-1}_{\text{cell}}$ ), volume expansion on charge-discharge and safety issues limit their application in automobile industry. Recently, Metal air battery technology has been recognized as a potential power source for future generation of EVs. Among several other Metal-air batteries, Zinc-air battery (ZAB) has been extensively studied due to its comparatively high energy density ( $1084 \text{ WhKg}^{-1}$ ) which is almost four times of what LIBs provide. Moreover low cost ( $\$10 \text{ kW}^{-1}\text{h}^{-1}$ , much less than LIBs), environment friendliness and safe operation also adds to its advantages over other types of batteries [2]. Recently we have shown that long performance ZABs can be developed with a novel bifunctional catalyst called Co@NGS-NSs where cobalt (Co) nanoparticles are dispersed over graphitic spheres of 300 nm diameter [3]. After the half-cell studies using this catalyst for oxygen reduction and oxygen evolution reactions, ZABs are constructed using this catalyst as air electrode and Zn metal as anode. The ZAB showed an open circuit voltage of 1.36 V having a maximum power density of  $\sim 52 \text{ mWcm}^{-2}$  and energy density of  $876 \text{ Wh/Kg}$ , and these values are on par with Pt/C system while much better in terms of long term stable performance ( $>48$  hours) where Pt/C is found to be failing. Synergistic activities of cobalt and nitrogen doped graphitic carbon in the catalyst towards catalytic processes are proven both experimentally and theoretically.

**Keywords:** Bifunctional Catalysts; Zinc Air Battery; Rechargeable Battery; Nitrogen Doped Carbon; Oxygen Reduction Reaction; Oxygen Evolution Reaction; Cobalt Nanoparticles

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OL-3-04

## Triazine Based Secondary Amine Linked Polyphenolic Porous Organic Polymers for High CO<sub>2</sub> Capture and Selective CO<sub>2</sub> Adsorption

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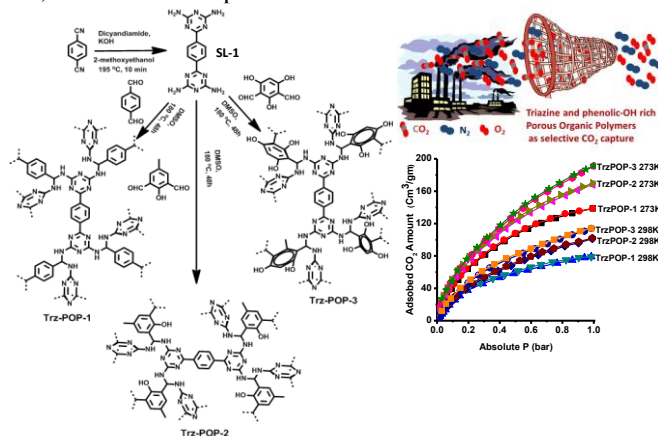
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### ABSTRACT

Design and successful synthesis of porous organic polymers<sup>1</sup> as adsorbent for postcombustion CO<sub>2</sub> uptake from flue gas mixtures along with high CO<sub>2</sub>/N<sub>2</sub> selectivity is a very demanding research area in the context of developing a suitable adsorbent to mitigate the greenhouse gas CO<sub>2</sub><sup>2</sup>. We report three triazine-based porous organic polymers TrzPOP- 1, -2, and -3 through the polycondensation of two triazine rings containing tetraamine and three dialdehydes. These porous organic polymers possess high Brunauer-Emmett-Teller (BET) surface areas of 995, 868, and 772 m<sup>2</sup> g<sup>-1</sup>, respectively. Out of the three materials, TrzPOP-2 and TrzPOP-3 contain additional phenolic-OH groups along with triazine moiety and secondary amine linkages. At 273 K, TrzPOP- 1, -2, and -3 displayed CO<sub>2</sub> uptake capacities of 6.19, 7.51, and 8.54 mmol g<sup>-1</sup>, respectively, up to 1 bar pressure, which are considerably high. Despite the lower BET surface area, TrzPOP-2 and TrzPOP-3 containing phenolic-OH groups showed higher CO<sub>2</sub> uptakes. To understand the CO<sub>2</sub> adsorption mechanism, we have further performed the computational studies to analyze noncovalent interactions between CO<sub>2</sub> molecules and different polar functionalities<sup>3</sup> present in these porous polymers. TrzPOP-1, -2, and -3 have the capability of selective CO<sub>2</sub> uptake over that of N<sub>2</sub> at 273 K with the selectivity of 61:1, 117:1, and 142:1 by using the initial slope comparing method. On the other hand, at 298 K, the calculated CO<sub>2</sub>/N<sub>2</sub> selectivities in the initial slope comparing method for TrzPOP-1, -2, and -3 are 27:1, 72:1 and 96:1. Cost effective and scalable synthesis of these porous polymeric materials bearing phenolic-OH and amine-functionalized pore surfaces reported herein for selective CO<sub>2</sub> capture has a very promising future for environmental clean-up.<sup>4</sup>

**Keywords:** POPs, Surface area, Selective CO<sub>2</sub> uptake.



**Figure 1.** Synthetic pathway of TrzPOP-1, TrzPOP-2 and TrzPOP-3 and their selective CO<sub>2</sub> uptake capacity.

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**Functional Nanomaterials in Industrial & Clinical Applications: Academic-Industry-Clinician Meet (14<sup>th</sup> to 16<sup>th</sup> July 2020), UCLan, Preston, UK**

OL-3-05 (has been considered for poster presentation, see poster section P-3-05)



[1].

OL-3-06

## **Meet the All-Carbon Solar Cells for Renewable Applications**

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### **ABSTRACT**

Rapid deployment of renewable energy and technological diversification of energy sources would indeed result in significant energy security and economic benefits. Among all the renewable energy forms, solar energy has its advantages and potential for power generation as it directly converts solar energy into electrical power, leaving no adverse environmental effect. The development of perovskite solar cells (PSCs) has resulted in a "catfish effect" for other photovoltaic technologies with a high power conversion efficiency and low-cost fabrication [1]. Inevitably, the cell performance limitations are now linked with other parameters, where progress is required to enable the full potential of the technology to be realized such as (i) poor moisture stability of the perovskite, limiting device lifetime; (ii) toxicity of lead perovskite, which could preclude some application areas for the devices; (iii) unstable structure of Pb-based perovskites for UV-curing (high-energy light sensitive) [2]. At present, PSC devices are reaching their storage and processing limit, causing a significant push to find new materials for solving these issues in their next-generation devices. In this regard, new nanostructured materials designing for next-generation solar cell development have been an extensive area of research. Recently, carbon has been gained considerable attention because of its cost-effectiveness, environmental superiority, abundant, and excellent photo-electrochemical catalytic activity towards the redox species. The self-assembling characteristics allow carbon nanomaterials to be readily explored environmentally benign, solution-processed, low-cost and efficient solar light-harvesting materials [3]. Therefore, we have inspired from the PSC research and thus replaced the regular PSC layers by different carbon allotrope based layers to fabricate a novel solar cell architecture. Sequential fabrication of carbon solar cells was further tested under an ambient condition, where FTO/graphene/single-walled carbon nanotube/graphene quantum dots-fullerene/carbon black paste layers were assembled with poly(methyl methacrylate) (PMMA) as an encapsulating layer (Figure 1). The PMMA layer provides significant improvement towards the ingress of water vapour, and hence leading to exhibit stability up to 1000 h. The photo-conversion efficiency of the PMMA encapsulated carbon solar cell has been increased by ~105% and the stability decreased by only ~10% after 1000 h of moisture ambient exposure [4]. The added benefits as low-cost materials and solution-based manufacturing route are therefore expected to integrate the carbon allotropes for this type of new solar cells. The carbon solar cell showed 38% visible transmittance that made suitable future building-integrated photovoltaic (BIPV) window application. This work strongly encourages employing solution-processed photovoltaic materials fabrication.



**Figure 1.** Digital image of the carbon solar cell as fabricated by solution-processed layer deposition of different allotropes of carbon (as a single source).

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OL-3-07

## Environmentally Friendly and Sustainable Synthesis of Carbon nanomaterials from Solid waste materials for Solar cell and Supercapacitor Applications

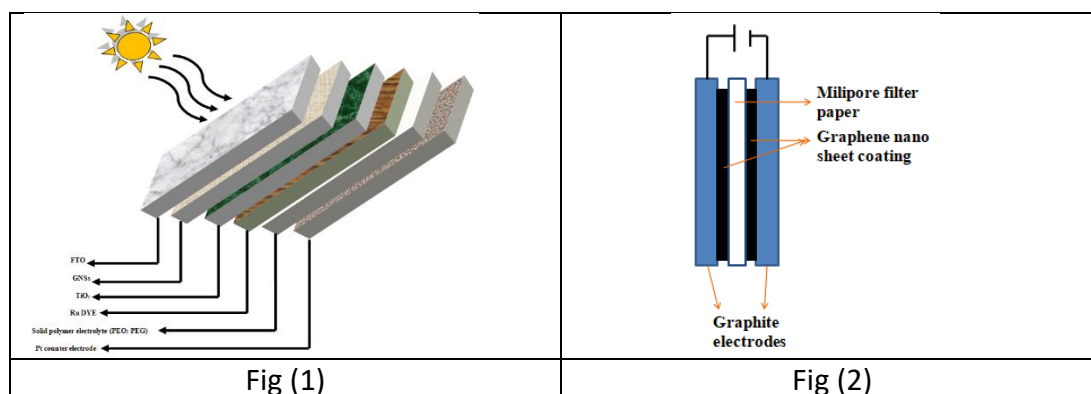
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### ABSTRACT

Today, world is looking for environmental friendly and sustainable technology for the cheaper and cleaner energy for the conservation of mother earth. However, still the production of cleaner energy has become a serious issue because of unavailability of potential materials for energy conversion and energy storage devices. At the same time, alarming situation of solid waste density showed critical condition for the sustainability of ecology and biodiversity in the developing countries. The density of the solid waste is not only affected the ecology and biodiversity of the nation, but it is also equally affected economy and energy output of the country. Therefore, an urgent solution is needed in order to save ecology, energy and economy at the same time. In this regard, graphene is considered to be 21<sup>st</sup> century wonder material due to its extraordinary electrical, mechanical and optical properties. The unbeatable properties of graphene nanosheets have shown tremendous interest for the application of the energy conversion and storage devices. However, the expensive cost and critical synthesis process of this wonder material has limited the industrial application. So, in order to confront the problem of energy crises and solid waste management, we developed an effective and potential technology by upcycling solid waste materials including plastic waste [1-2], paper waste, agriculture waste and food waste into graphene nanosheets. Graphene nanosheets thus obtained are characterized by number of spectroscopic and imaging techniques showed 2-5 nm thick graphene nanosheets. Further, the graphene nanosheets thus obtained are exploited for the application of dye sensitized solar cells and supercapacitor applications. Moreover, the graphene nanosheets thus obtained are also employed for the fabrication of transparent conducting electrodes. Reports suggested that the graphene nanosheets act as band tuner and successfully increase the efficiency of the DSSCs with solid polymer electrolytes **fig (1)**, while as active layer in supercapacitors showed a specific capacitance of 98 F/g to 377 F/g with PVDF-HCF binders **fig (2)**. In addition to it, first time solvent-antisolvent technique was investigated to fabricate transparent conducting electrodes by using waste derived graphene nanosheets. Graphene based transparent electrodes thus fabricated showed more than 80% transmittance and lower sheet resistance for optoelectronic applications. Thus, the overall work showed the conservation of “EEE” i.e. economy, energy and ecology at the same time with environmental friendly techniques.



**Keywords:** Solid waste materials, Upcyclization, Carbon nanomaterials, DSSCs, Supercapacitors

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OL-3-08

## ENHANCED PERFORMANCE OF GRAPHENE DOPED P3HT BASED PHOTOVOLTAIC DEVICE

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<sup>b</sup>CSIR- National Physical laboratory, New Delhi, India

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### ABSTRACT

Because of low cost manufacturing organic photovoltaic cell (OPV) is a promising technology. Enhancing power conversion efficiency (PCE) of OPV is major work to be done for commercial applications and photocurrent generation in OPVs is key factor to enhance the efficiency of such devices [1]. The light illuminate on photoactive material and upon absorption of photon bound electron and hole pair (called as Exciton) generates. The formed excitons then require dissociating and collected, which could only be possible at the junction of semiconducting material of different ionization potentials or electron affinities. However, at heterojunction interface, this dissociation of Exciton and thus charge transfer can occur very rapidly that photo induced excitations produced far from the interface recombine before diffusing to the heterojunction. As organic active material possess extremely short length of exciton diffusion which confine its true practical utility. Therefore, avoid any other interface effects, blends of soluble conjugate polymers as donar and fullerene as acceptor are used as bulk heterojunction (BHJ) to form organic active layer. This maximize the exciton dissociation by matching the typical exciton diffusion length (~10 nm) nanoscale phase separation of donors and acceptors within the exciton diffusion length increases the opportunity for excitons to dissociate into charge carriers, resulting in better PCE [2]. Structural advances in BHJs are continuous in order to maximize the exciton dissociation by matching the typical exciton diffusion length, increase the carrier mobility in the phase-separated layers, and enhance light absorption, proper alignment of donor and acceptor energy levels to enhance the charge transfer. In this regard, a material with extremely high carrier mobility is needed in blends which cooperate conductive pathways in the active layer [3]. Graphene, can promote more efficient charge-carrier transport because the two-dimensional (2-D) planar structure and large specific surface area, excellent charge-carrier mobility, thermal and chemical stability. Also, it provides compatibility with organic materials and can be solution processed [3]. Therefore, in the present paper, we subject the study of the effect of graphene doing on the charge conduction of Poly(3-hexylthiophene) (P3HT) polymer which is used as electron donar in BHJ organic photovoltaics. For this purpose, two devices have been fabricated in the following configuration: Device 1: ITO/PEEDOT: PSS/P3HT/Al and Device2: ITO/PEEDOT: PSS/P3HT+G/Al. P3HT is hole transposing layer with the HOMO level around 5.18 eV and with graphene doing its HOMO level switches 5.5eV (calculated using Cyclic Voltametry). The schematic of both devices and their energy level diagram have been shown in figure 1. This diagram suggests that the both devices have been acting as a hole only device. Because of the large energy gap between Al and LUMO of P3HT/P3HT+G, the probability of electron conduction is negligible. So, in the present case we will discuss the transport properties of holes in pure and graphene doped P3HT.

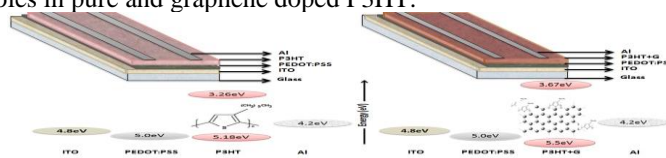


Figure 1: Schematic of device and their energy level diagram for Device 1: ITO/PEEDOT: PSS/P3HT/Al and Device2: ITO/PEEDOT: PSS/P3HT+G/Al.

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OL-3-09-SL

## Simulations of the band- gap changes of carbon nanotubes (CNTs) and graphene nanoribbons (GNRs) and a preliminary review on future ultra-thin transistors

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### ABSTRACT

This research presents simulations of CNTs and GNRs to study the density of the states, electronic band structure, and the effect of different types of strains on GNRs. I also present simulation results of one of the important physical and fundamental parameters, i.e. band-gap changes of CNTs and GNRs by way of application of different types of strains (hydrostatic, uniaxial, and arbitrary) and doping. In particular, because it is known that the effect of strain on the electronic structure of GNRs depends on its edge shape and structural indices, I consider both armchair GNRs (AGNR) and zigzag GNRs (ZGNR) structures to study their band-gap changes. Owing to their relatively small dimensions (~50 nm) and extremely high performance (current range > 3 milliamperes/micrometer), these two-dimensional (2-D) GNRs are highly sought after materials for research and material engineering communities to fabricate ultra-thin transistors (UTTs). This research also presents a preliminary review of future UTTs and, interestingly, few research efforts are currently being in pipeline to fabricate such devices<sup>1</sup>, which could replace conventional nanometer transistors (those made of silicon) or of the currently popular transition metal dichalcogenides.

**Keywords:** simulations; ultra-thin nanomaterials; carbon nanotubes; graphene nanoribbons.

### RESULTS

With the ever-increasing demands of customers that their electronic gadgets to be small, yet powerful, the research and engineering fraternity is striving hard to miniaturize them. Nevertheless, it is almost impossible even with the current nanometer-scale transistors made of silicon to meet Moore's scaling law<sup>2</sup> owing to various quantum effects<sup>3</sup>. In these circumstances, few prospective low-dimensional materials (monolayer and a channel length of as small as 5 nm) such as graphene nanoribbons and carbon nanotubes have been proposed that could overcome additional leakage currents in a tiny transistor<sup>4</sup>, which are primarily due to quantum effects. These nanoscale carbon derivatives including GNRs and CNTs have excellent electronic properties, along with outstanding elastic, optoelectronic, and thermal properties, to name a few<sup>5-7</sup>. To further understand the band-gaps of these 2-D materials including AGNR and ZGNR under various strains, as shown in Figures 1a and 1b, we have sought a tight-band Hamiltonian method, with which it has become possible for us to simulate the band-gaps, density of states and effect of various strains on them and yielded very interesting results. Once I present simulation results, I also review the most recent trends in the field of UTTs.



**Figures 1a)** Molecular structures of AGNR and **1b)** ZGNR [source: nanoHub].

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OL-03-10-SL

Si nanowire arrays with over-layer of camphor based graphene for sensing applications

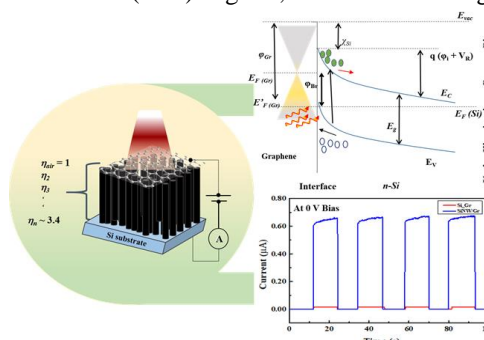
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ABSTRACT

Semiconductor nanowires, especially Si nanowires arrays (SiNWAs) have attracted much attention due to its high broadband absorption, high density and extra ordinary surface/volume ratio. These opto-physical properties demonstrate their high potential for practical applications in advanced devices such as transistors, photodetectors, light-emitting-diodes, solar cells and bio/chemical sensors. The application of Si-based photodetectors in light detection demonstrates low sensitivity in the ultraviolet and near infrared (NIR) regime, due to its low light absorption coefficient. Moreover, Si has an indirect band gap which results in low light sensitivity and it is mainly restricted in visible to NIR light. Graphene on the other hand, exhibits an extremely high charge carrier mobility, a very broad spectral range of detection from ultraviolet to terahertz and quasi wavelength independent absorption, which is a result of its gapless band nature. Recently, solid carbon source such as camphor as a natural precursor has taken much attraction for the synthesis to form a large area monolayer graphene by very facile and novel approach. Compatibility of Graphene with Si



**Figure 1:** (a) Schematic diagram of Gr/SiNWAs schottky junction device, (b) The band bending alignment of Gr/SiNWAs Schottky junction and (c) photoresponse

or SiNWAs makes it a promising candidate for large-scale and cost effective ultrafast photodetection. The growth of high-quality CVD graphene from camphor and its high performance optical device has not been addressed so far. We have presented high performance near infrared (NIR) photodetectors by using camphor as solid source of carbon for developing mono-bi layer Gr/SiNWAs schottky heterojunction [1]. The nanowire arrays show excellent optical light trapping properties and on the other hand, graphene act as transparent and conductive sheet. Hence a combination of graphene over SiNWAs serves as an excellent NIR light trapping system. Few recent results towards the development of such nano-network based heterojunction device will be discussed.

**Keywords:** silicon nano-wire, nanowire arrays, graphene, camphor, NIR sensor.

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OL-4-01

## **NanoFarming In Industry**

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### **ABSTRACT**

The use of nanomaterials in agriculture has been very popular in recent years. Nanomaterials have started to be used as fertilizers and pesticides in agriculture. Nano-forms of metals are highly effective in providing essential nutrients for the plant compared to convection fertilizers and are stable against changing climatic conditions. They are also applied less and more effectively than traditional fertilizers when applied as fertilizers. Studies show that when Nano (Ca, P, Mg, K, Zn, Mn etc.) materials are applied to the plant, it increases the amount of photosynthesis that promotes plant growth. It has been observed that super paramagnetic iron nanoparticles increase leaf chlorophyll content even under hydrophobic conditions, and that molybdenum-containing nanoparticles promote beneficial microorganisms in the plant root zone. In this study, ZnO nanoparticles were immobilized and their suppressive effects against the maize pest *Cytophilu Zeamaise* were determined by the enzyme chitinase. We also found that nanoparticles together with plant growth promoting Bacteria (PGPB) can lead a synergistic life. Thus, we anticipate that nano-bio fertilizers, regulators and pesticides will be more effective and effective in the future.

As a result, nanomaterials are likely to play a more effective role in agriculture in the future. these nanomaterials can be rapidly gained into the agricultural sector by providing fabrications with the necessary equipment for synthesis as industry. It is strongly recommended that toxicological investigations of nanomaterials be conducted before they are applied to nature.

**Keywords:** nanofarming, industry, fertilizers, nanoparticles

OL-4-02

## **Nano-based slow releasing fertilizers for enhanced agricultural productivity**

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### **ABSTRACT**

Nanotechnology is an emerging technology with a potential to improve agricultural yield by taking advantage of the salient features of nanostructured materials. Nano-encapsulated conventional fertilizers help in slow and sustained release of nutrients over an extended period of time. In this work, we report synthesis and application of a slow releasing nanocomposite fertilizer (SLRNF). Comparative studies on the performance of the SLRNF and a conventional Nitrogen, Phosphorus and Potassium (NPK) fertilizer were done. The nanocomposite fertilizer was characterized using Field Emission Scanning Electron Microscopy (FESEM) for surface studies and particle size analysis, Fourier Transform Infrared Spectroscopy (FTIR) for chemical composition studies, Powder X-ray Diffraction (P'XRD) for structural analysis and Energy Dispersive Spectroscopy (EDAX) for elemental composition analysis. The SLRNF exhibited a superior performance over the bulk or conventional fertilizers for instance, phosphate leaching tests conducted for a period of 50 minutes showed a leached phosphate concentration of 0.002 mol/dm<sup>3</sup> and 0.008 mol/dm<sup>3</sup> respectively for the SLRNF and conventional NPK fertilizer respectively. The research work has revealed the huge capability of nano-based slow releasing fertilizers in improving plant nutrient availability for enhanced growth. It was realized that nanotechnology can stimulate the generation of much more cost effective and smarter fertilizers for improved crop yield.

**Keywords:** nanotechnology, agriculture, slow release fertilizer, plant nutrient availability

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**Functional Nanomaterials in Industrial & Clinical Applications: Academic-Industry-Clinician Meet (14<sup>th</sup> to 16<sup>th</sup> July 2020), UCLan, Preston, UK**

OL-4-03 (accepted for poster presentation, see poster section (P-4-03))

**Functional Nanomaterials in Industrial & Clinical Applications: Academic-Industry-Clinician Meet (14<sup>th</sup> to 16<sup>th</sup> July 2020), UCLan, Preston, UK**

OL-4-04 (accepted for poster presentation, see poster section (P-4-05))

OL-4-05

## Ga-Doped and Pt-Loaded Porous TiO<sub>2</sub>-SiO<sub>2</sub> for Photocatalytic Nonoxidative Coupling of Methane

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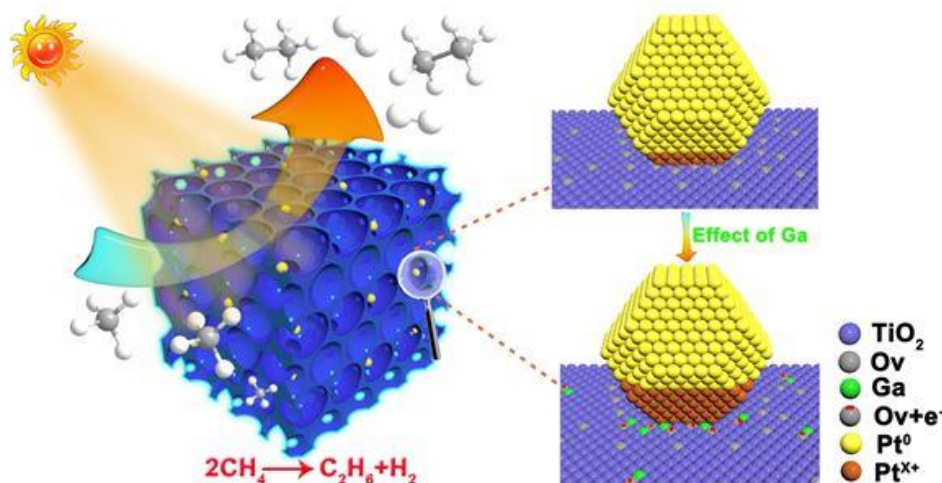
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### ABSTRACT

Photodriven nonoxidative coupling of CH<sub>4</sub> (NOCM) is a potential alternative approach to clean hydrogen and hydrocarbon production.<sup>1</sup> Herein, a Mott-Schottky photocatalyst for NOCM is fabricated by loading Pt nanoclusters on a Ga-doped hierarchical porous TiO<sub>2</sub>-SiO<sub>2</sub> microarray with an anatase framework, which exhibits a CH<sub>4</sub> conversion rate of 3.48  $\mu\text{mol g}^{-1} \text{h}^{-1}$  with 90% selectivity toward C<sub>2</sub>H<sub>6</sub>.<sup>2</sup> This activity is 13 times higher than those from microarrays without Pt and Ga. Moreover, a continuous H<sub>2</sub> production (36  $\mu\text{mol g}^{-1}$ ) with a high CH<sub>4</sub> conversion rate of ~28% can be achieved through a longtime irradiation (32 h). The influence of Ga on the chemical state of a surface oxygen vacancy (Vo) and deposited Pt is investigated through a combination of experimental analysis and first-principles density functional theory calculations. Ga substitutes for the five-coordinated Ti next to Vo, which tends to stabilize the single-electron trapped Vo and reduce the electron transfer from Vo to the adsorbed Pt, resulting in the formation of a higher amount of cationic Pt. The cationic Pt and electron-enriched metallic Pt form a cationic-anionic active pair, which is more efficient for the dissociation of C-H bonds. However, the presence of too much cationic Pt results in more C<sub>2+</sub> product with a decrease in the CH<sub>4</sub> conversion rate due to the reduced charge-carrier separation efficiency. This study provides deep insight into the effect of the doping/loading strategy on the photocatalytic NOCM reaction and is expected to shed substantial light on future structural design and modulation.

**Keywords:** photocatalysis, methane conversion, platinum, TiO<sub>2</sub>



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OL-4-06

## Redox-sensitive nanotrident: eco-friendly warriors for aqueous sustainability

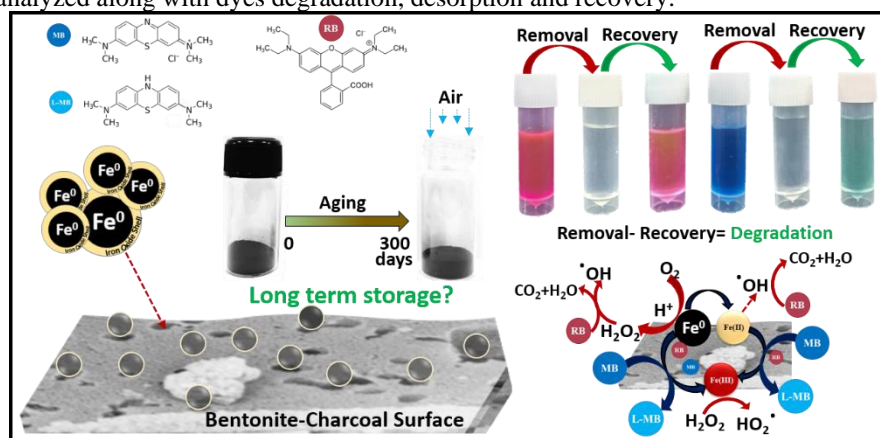
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### ABSTRACT

Clean water, the elixir of life, is of tremendous importance in achieving environmental sustainability. For decades, several anthropogenic activities have contributed to a frightening increase in the concentration of toxic pollutants in water bodies. Redox-sensitive nanoparticles like nZVI, Fe<sub>3</sub>O<sub>4</sub>, reduced graphene, and zero-valent aluminum, etc. are of particular interest for their eco-friendly nature and higher contaminant removal capacities due to their electron transferring ability along with high surface area. Owing to their non-stability in the environment, various surfaces have been explored for the preservation of redox state of such particles. It includes either porous surfaces like- charcoal, zeolite, MOFs, COFs, etc. or layered surfaces like clays, graphene, etc. Here we report the combined layered-porous surface for the preservation of redox nature of supported nanoparticles. This system with two adsorbent surfaces and one redox-sensitive nano-adsorbent can be pronounced as nanotrident. Here, in this work, porous charcoal, layered bentonite clay and their mixture with different bentonite: charcoal ratios have been comparatively evaluated as surfaces for supporting redox-sensitive nanoscale zero valent iron (nZVI) particles. A 300 days of air exposure was given to investigate the impact of long term storage on composites reactivity for dyes. FT-IR spectra of various reaction precipitates, before and after washing were also recorded and analyzed along with dyes degradation, desorption and recovery.



**Fig.1** Graphical overview of the work

Results conclude that a change in the surface composition towards mixed porous charcoal- clay for supporting nZVI particles resulted in the removal of methylene blue and Rhodamine-B dyes. Spectroscopic observations suggested a surface dependent variation in the dye degradation mechanisms of nZVI on the clay-charcoal surfaces. Highly porous surfaces with limited layering (charcoal enriched) have shown organic degradation of both the dyes, whereas layered surfaces with limited porosity (clay enriched) were strongly chemisorbing the dyes. No significant impact of aging was observed for charcoal enriched composites which have good environmental applicability, high efficiency with minimal impact of long-term storage for removal of different dyes [1].

**Keywords:** redox-sensitive nanoparticles, nZVI, dyes removal, nanotrident, organic degradation

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OL-4-07 (accepted for poster presentation, see poster section P-4-04)

OL-4-08

## Charge transfer do play a role in antimicrobial activity of Graphene oxide against gram negative bacteria, *Escherichia Coli*

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### ABSTRACT

The communication enlightens that charge transfer also play a pivotal role in the death mechanism of bacteria (*E. coli*) when interacted with graphene oxide (GO). GO has already been shown to possess very good antimicrobial properties [1,2]. The physical mechanisms such as cutting, wrapping, trapping etc. has been established already to reconcile the antibacterial activities of GO [3]. The term, charge transfer was just a hypothetical term on the antibacterial activities of GO until our experiment has proved that such a mechanism during bacteria death do exist as evidenced by the surface potential change as measured with the help of Kelvin Probe Force Microscopy (KPFM) [4]. The KPFM deals with giving a bias to the conducting AFM tip by creating a threshold potential at the tip apex. When such a tip comes in contact with any surface having conducting properties, the difference in potential can be calculated as contact potential difference (CPD) by using an established algorithm [5]. The gram negative *E. coli* bacterial cell wall is surrounded by a thin peptidoglycan layer which carries the ionic charges of bacteria due to the presence of a thin layer of lipopolysaccharides [6]. GO, on the other hand, is also assigned electronegativity because of the presence of the unsaturated double bond unlike the neutral graphene sheets. The experiment was carried out by tuning the charge property of GO by incorporating the zinc-phthalocyanine (ZnPc) physically. Heating could change the conducting properties of ZnPc (transition from  $\alpha$ -phase to  $\beta$ -phase) and thus changes the electronic properties of ZnPc-GO nano-hybrids [7]. Thin films of ZnPc are grown with thermal evaporation and the thickness was calculated to be 30 nm. GO thin layers are deposited by homemade dripping method [8] over the thermally grown ZnPc layer where thickness of the former is found to vary from 1.5 – 4.0 nm. *E. coli* cells are allowed to get in contact with the electronically tuned ZnPc-GO nano-hybrids. The gradual death of the bacteria was measured with in-situ CPD change and then by mapping with KPFM. The result certainly demonstrates an establishment of charge communication between the bacteria cell and the composite structure. The present work aimed at exploring the surface potential change due to the ionic transfer occurring at the interface of ZnPc-GO nano-hybrids and the bacterial cells. We believe this communication will pave the way for new dimensional study of electrostatic interaction by elucidating the biophysical events happening at the interface of ZnPc-GO nano-hybrids and bacteria cells.

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OL-4-09 (accepted for poster presentation, see poster section P-4-02)



OL-4-10

**Investigation of the Effect of Chitinase Enzyme Isolated from *Lactobacillus coryniformis* Bacteria on Zinc Nanoparticles Immobilization and the Effect of Storage Harmful Corn Bits (*Sitophilus zeamais*) on Development**

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**ABSTRACT**

Biotechnological and nanotechnological methods which have increased rapidly in the recent years have been frequently used in various fields in the agriculture. These methods have become the focus of researchers due to their superior properties to traditional methods. Taking advantage of these methods, it has been planned to minimize the yield and quality degradation by the pests seen in seed corn, which is heavily cultivated in Turkey, under the storage conditions. In this context, it was aimed to control the growth of Maize Weevil *Sitophilus zeamais* Motschulsky using the nano formulation that will be developed in the study. In the preliminary study phase of our project, the chitinase enzyme was partially purified from *Lactobacillus coryniformis*. In the second phase, zinc oxide (ZnO) nanoparticles were immobilized. Then, this formulation was applied to the corn pest, *Sitophilus zeamais*, at 0, 2, 4, 6, 10 mg/L doses and the results were presented as the preliminary study in the project. In the first phase of our project, the activity of the enzyme chitinase obtained from *Lactobacillus coryniformis* will be spectrophotometrically examined. In the second step, the chitinase enzyme obtained from the bacteria will be purified by HPLC Fraction collector column method. In the third phase, a nano formulation will be formed by immobilizing chitinase in zinc oxide (ZnO) nanoparticles. For the optimization of the formed formulation, the effects of pH, initial concentration and temperature will be examined. Fourier Transform Infrared Spectrophotometer FTIR, SEM, AFM and EDX Analysis will be performed to test the stability of the immobilization. At the end of all these procedures, in the fourth phase, five different nano formulation doses (0, 2, 4, 6 or 10 mg/L) will be generated and the formulation will be applied to the corn beads by forming an application dose on 25 adults with 5 different nano formulation doses in 4 repetitions by spraying method and its ingestion by the beetle's metabolism will be maintained. In the fifth step, insect intestinal tissues will be cut using a microtome device and removed for enzyme analysis. In the sixth phase, samples will be taken from the intestines of the insects, will be analyzed for the determination of alkaline phosphatase, adenosine triphosphatase, lactate dehydrogenase activities and the results will be compared to those obtained in the control samples. Our basic theory in this formulation is the socioeconomical benefit. Accordingly, it will provide a direct and indirect contribution to the country's economy by obtaining product that can compete with chemical insecticides (malathion, etc.) used in the market at a high rate. This study will also lead the scientists for the related future studies and research articles that will be published on this subject will contribute to the related literature.

**Keywords:** Nano, bio, pesticide, Zinc oxide

OL-4-11-SL

## Enhanced Drug Adsorption and Anti-Microbial Activity of Functionalized Multiwalled carbon nanotubes (MWCNTs)

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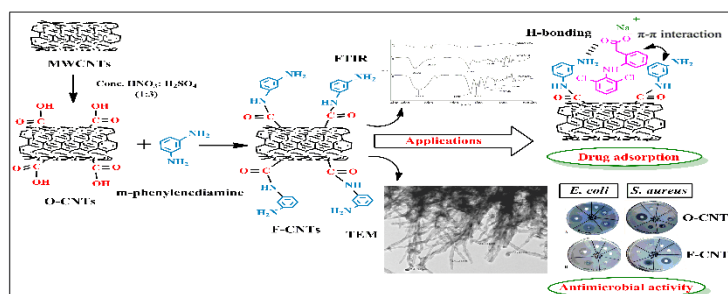
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### ABSTRACT

The inherent unique properties of Carbon nanotubes (CNTs) offer an exciting platform to enable significant research opportunities. Surface functionalization of CNTs improves its hydrophilicity and makes it biocompatible for biomedical applications. Functionalization further facilitates the complex formation capability of CNTs, thereby enhancing its selectivity. In this work, MWCNTs were first oxidized (O-CNTs) to introduce carboxylic group and then further functionalized (F-CNTs) with m-phenylenediamine, which was confirmed by FTIR and TEM. It was used as an effective adsorbent for the adsorptive removal of Diclofenac from water. To estimate the maximum potential of functionalized nano-adsorbent, various parameters that affect the adsorption such as contact time, pH, stirring speed, and initial drug concentration were optimized. Under optimum conditions of pH 6, stirring speed 600 rpm, the maximum adsorption capacity obtained was 532 mg g<sup>-1</sup> which is superior to the values reported in literature. The adsorption was quite rapid as 25 mg L<sup>-1</sup> drug solution was adsorption in only 3 minutes of contact time. The adsorption kinetics and isotherms were studied to evaluate the adsorption process. Results suggested that data showed best fit in kinetics pseudo-second order and Langmuir isotherm model. This indicates monolayer adsorption of drug on functionalized MWCNTs. Furthermore, the oxidized and functionalized MWCNTs were applied on gram-negative *Escherichia coli* and gram-positive *Staphylococcus aureus* using agar disc diffusion assay to validate their anti-microbial activity. Results were unique as both oxidized and functionalized MWCNTs were equally active against both *E. coli* and *S. aureus*. The pronounced polarity and presence of functional groups allows both O-CNTs and F-CNTs to show increased antimicrobial activity. It can be predicted that the functional groups further increase their affinity for adsorption of bacteria which causes structural damage and oxidative stress, eventually leading to death. The newly synthesized F-CNTs have great potential in water treatment, with their dual action of removing diclofenac drug and pathogens from water samples. Since, drug adsorption was significantly higher in functionalized MWCNTs, it successfully established their application in biomedical applications.

**Keywords:** adsorption, antimicrobial, diclofenac, functionalized multiwalled carbon nanotubes, m-phenylenediamine.



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## Post-synthetic amine functionalized SAPO-5 & SAPO-34 molecular sieves: Important catalysts for epoxide ring opening reaction

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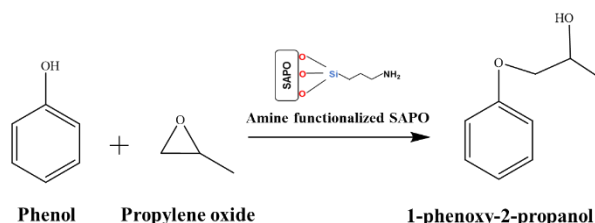
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### ABSTRACT

Microporous zeolite types molecular sieve materials such as AlPOs and SAPOs are of great interest for their prominent applications in catalysis, adsorption and ion-exchange processes. Inspired by the application of microporous materials, SAPO-5 and SAPO-34 materials were synthesized according to literature procedure [1] and modified via post-synthetic amine functionalization using aminopropyltriethoxysilane (APTES) [2]. Functionalized materials were thoroughly characterized using powder XRD, N<sub>2</sub> adsorption-desorption isotherm, FT-IR, FE-SEM, TGA and <sup>13</sup>C-CP MAS NMR. Industrially important synthesis of  $\beta$ -amino alcohol and  $\beta$ -phenoxy alcohol implicates the ring opening of epoxide with nitrogen containing (amines) or oxygen containing (alcohols) nucleophiles [3]. Amine functionalized SAPO-5 and SAPO-34 materials were found to be important catalysts in epoxide ring opening reaction of propylene oxide with phenol for the production of  $\beta$ -phenoxy alcohols. Reaction conditions were optimized to achieve better conversion and selectivity of product. Prepared materials were also found to be efficient with higher selectivity and conversion for other ring opening reactions using various epoxides and amines for the synthesis of  $\beta$ -amino alcohols.

**Keywords:** amine functionalized SAPO-5, amine functionalized SAPO-34, epoxide ring opening reaction

**Figure 1.** Epoxide ring opening reaction using amine modified SAPO materials as a catalyst



**Table 1.** Epoxide ring opening reaction using amine functionalized SAPO materials as a catalyst

Reactants	Conversion (%)	Selectivity (%)
Phenol- Propylene oxide	60	90
Morpholine- Propylene oxide	86	100
Aniline- Propylene oxide	29	99
Piperidine- Propylene oxide	95	100
Pyrrolidine- Propylene oxide	95	100
Aniline- Styrene oxide	90	100
Piperidine- Cyclohexene oxide	30	98
Pyrrolidine- Cyclohexene oxide	70	100

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OL-5-02

## Amorphous Zeolites for CO<sub>2</sub> to Fuel and Plastic to Chemical Transformation

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### ABSTRACT

In this work, we report the synthesis and application of a new class of material, called “Amorphous Zeolites (AmZe)” [1], which possesses Brønsted acidic sites like in zeolites and textural properties like ASAs. This was achieved by controlling the hydrolysis and condensation reaction kinetics between silica (tetraethyl orthosilicate) [2,3] and alumina (aluminum acetylacetonate) precursors in a bicontinuous microemulsion template [4-7]. The synergy between strong acidity and accessibility was reflected in the fact that AmZe catalyzed eight different catalytic processes (styrene oxide ring-opening, vesidryl synthesis, Friedel–Crafts alkylation, jasminaldehyde synthesis, m-xylene isomerization and cumene cracking) which all require strong acidic sites and larger pore sizes, with better performance than state-of-the-art zeolites and amorphous aluminosilicates (Figure 1). Notably, AmZe efficiently converted a range of waste plastics to hydrocarbons at significantly lower temperatures. A Cu-Zn-Al/AmZe hybrid showed excellent performance for CO<sub>2</sub> to fuel conversion with 79% selectivity for dimethyl ether. Performance of AmZe for plastic degradation and CO<sub>2</sub> conversion was found to be superior to conventional zeolites. The catalytic activity and selectivity of AmZe was then investigated by conventional and DNP-enhanced solid-state NMR to provide molecular-level understanding of the distinctive Brønsted acidic sites of these materials. Due to their unique combination of strong acidity and accessibility, AmZe will be a potential alternative to hierarchical zeolites.

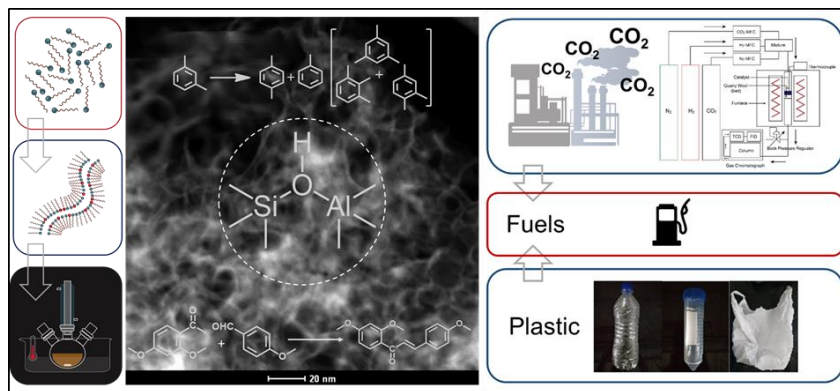


Figure 1. Synthetic Scheme and application of Amorphous Zeolites (AmZe) in CO<sub>2</sub> to fuel and plastic to chemical conversion.

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OL-5-03

## Triazine based POPs for heterogeneous catalysis in syntheses of chromene and HMF

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### ABSTRACT

Heterogeneous catalysis has become a hot field of research for its carbon efficiency and ease of utility along with energy saving and low usage of volatile organic solvents. Porous organic polymers (POPs) have very high prospect in that regard owing to its robustness, high surface area and wide range of functionality [1]. Herein, a new N-rich triazine-thiophene based microporous polymer TrzDBTH was prepared using Friedel-Craft reaction and used as a solid basic heterogeneous catalyst for one-pot synthesis of biologically important 4-H-chromene derivatives. TrzDBTH was sulphonated to make another hyper-crosslinked porous polymer viz. STrzDBTH. This was used as solid acid catalyst for the synthesis of 5-hydroxymethylfurfural (HMF) from different biomass sources. HMF is a value added platform chemical for bio-fuel, polymer industry and fine chemicals. As a base catalyst, chromene yield with TrzDBTH was from 88 to 93% and STrzDBTH provides the HMF yields from 57 to 97% for different carbohydrates with high recyclability [2].

**Keywords:** POPs, Heterogeneous catalysis, Chromene, HMF

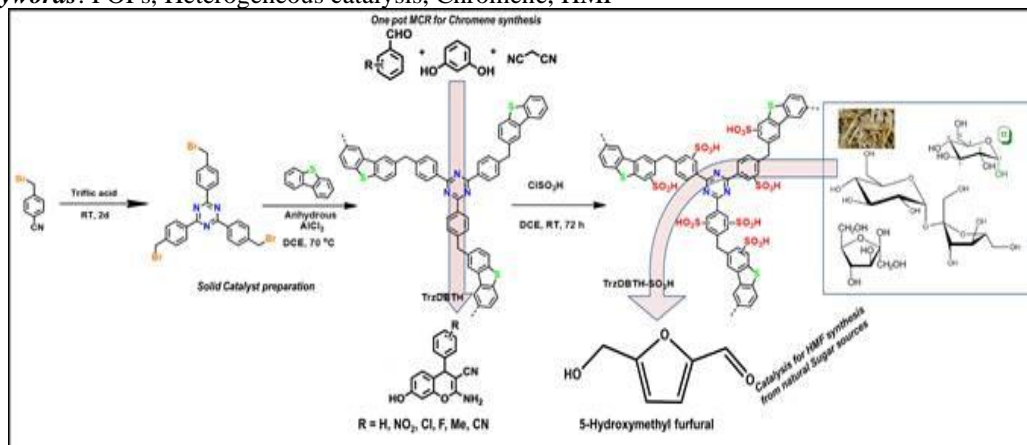


Figure 1. Schematic diagram of catalysis for synthesis of chromene and HMF

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OL-5-04

## Visible Light-Driven Selective Organic Degradation by FeTiO<sub>3</sub>/Persulfate System: the Formation and Effect of High Valent Fe(IV)

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### ABSTRACT

There is a long debate about the existence and role of high-valent Fe(IV) and hydroxyl radical (OH<sup>•</sup>) in H<sub>2</sub>O<sub>2</sub> system,[1] but the study about the possible contribution of high-valent Fe(IV) in PS system still remains in its infancy,[2] especially for the heterogeneous reaction system. The role of high-valent Fe has rarely been explored in persulfate-based heterogeneous reaction. Herein, the existence of Fe(IV) is verified in a visible light-assisted FeTiO<sub>3</sub>/persulfate system by Mossbauer Spectra and using methyl phenyl sulfoxide as the probe. The FeTiO<sub>3</sub>/persulfate/light system is capable of selectively degrading aromatic compounds with a higher ionization potential including tetracycline and bisphenol A by photo-generated high-valent Fe(IV). The contributions from SO<sub>4</sub><sup>•-</sup>, OH<sup>•</sup> and <sup>1</sup>O<sub>2</sub> are excluded. The comparable efficiency in the dark requires higher dosages and suffers from a rapid deactivation. Based on XPS, Raman and EPR analyses, the poor dark activity is caused by the formation of a complex between *in situ* formed Fe(III) and SO<sub>4</sub><sup>2-</sup> on the FeTiO<sub>3</sub> surface; this complex is, however, the key intermediate for Fe(IV) production under the light irradiation. This study reveals SO<sub>4</sub><sup>2-</sup> plays a vital role in the formation of surface Fe(IV) because its formation promotes the hole-electron separation and form surface complex with Fe(III), which as an abundant species in PS-based systems has long been neglected.

**Keywords:** FeTiO<sub>3</sub>, persulfate, high valent Fe(IV), irradiation, selective degradation

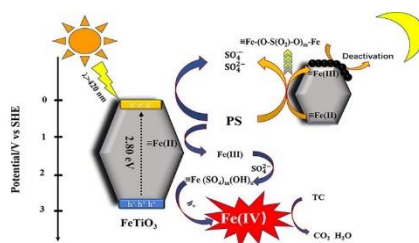


Figure 1. The proposed mechanism of FeTiO<sub>3</sub>/PS system.

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OL-5-05

## An efficient and rapid synthesis of 1, 4-dihydropyrano [2, 3-c] pyran and 1, 4-dihydropyrano [2, 3-c] quinoline derivatives using copper nanoparticles grafted on carbon microsphere

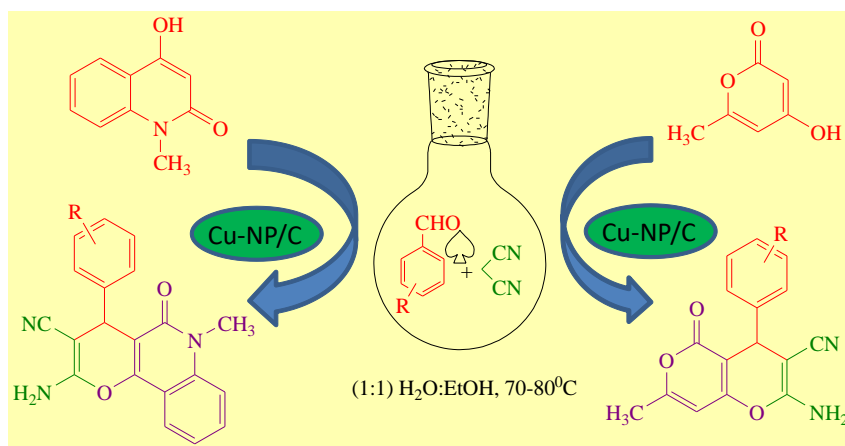
Nitishkumar S. Kaminwar<sup>1</sup>, Sunil U. Tekale<sup>2</sup>, Rajkumar U. Pokalwar<sup>3</sup>, Pravin S. Kendrekar<sup>4\*</sup>,  
Chandrashekhar V. Kulkarni<sup>5</sup>, László Kótai<sup>6</sup>, Rajendra P. Pawar<sup>2\*</sup>

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### ABSTRACT

A rapid and efficient three component synthesis of 2-amino-3-cyano-4-aryl-7-methyl-5-oxo-4, 5-dihydro-pyrano [3, 2-c] pyran and 2-amino-3-cyano-4-aryl-6-methyl-5,6-dihydro-5-oxo-4-H-pyrano-[3, 2-c]-quinoline derivatives catalyzed by copper nanoparticles grafted on carbon microsphere (Cu-NP/C) is developed. Mild reaction condition with excellent yield of the product is the key features of the method.



**Scheme-1:** One-pot synthesis of pyrano-pyran and pyrano-quinoline derivatives

**Keywords:** Cu-NP/C, pyrano pyran, pyranoquinoline, multicomponent reaction

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P-1-01

## CO<sub>2</sub> Absorption in Ionic Liquid Thin Films: an *in situ* XPS and NEXAFS Study

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### ABSTRACT

Carbon dioxide (CO<sub>2</sub>) capture and separation has become an important process in reducing CO<sub>2</sub> emissions in fossil fuel-fired power plants. Currently, alkanolamine solvents such as monoethanolamine (MEA) are typically used for CO<sub>2</sub> capture but incur unwanted long-term costs due to the energy required to regenerate them [1]. Recently ionic liquids (ILs) have been researched as potential green alternatives for CO<sub>2</sub> capture in post-combustion power plants owing to their high CO<sub>2</sub> capacity, very low volatility, high thermal stability and lower regeneration temperatures compared to MEA [2–4]. ILs are liquid salts with melting points below 100°C, consisting of pairs of anions and cations held together by strong Coulomb forces [5]. It is vital to understand the effect of a mixture of gases on the IL and how they compete for absorption since industrial flue streams typically consists of many gases such as CO<sub>2</sub>, H<sub>2</sub>O, and acidic gasses.

In this work we report a combined *in situ* X-ray photoelectron spectroscopy (XPS) and near edge X-ray absorption fine structure (NEXAFS) study into the ordering and interactions of multilayer and electrosprayed thin film depositions of the superbasic ILs [P<sub>66614</sub>][benzim] and [P<sub>66614</sub>][124Triz] on rutile TiO<sub>2</sub> (110) before, during, and after exposure to CO<sub>2</sub>.

Angle-resolved NEXAFS measurements taken over the Carbon K edge at X-ray incidence angles ( $\theta$ ) of 30° and 70° from the substrate surface provide an insight into the ordering of [P<sub>66614</sub>][benzim] thin films before and after exposure to 1 mbar of CO<sub>2</sub>. Prior to CO<sub>2</sub> exposure the relative intensities of the  $\pi^*$  and  $\sigma^*$  peaks suggest that the ring of the anion preferentially orients towards the surface normal (i.e. upright from the surface). Upon exposure to CO<sub>2</sub>, the [benzim]<sup>−</sup> anion reorders on the surface and lies closer to the plane of the substrate.

Depth profiling XPS reveals that competitive absorption between CO<sub>2</sub> and H<sub>2</sub>O in electrosprayed thin films of [P<sub>66614</sub>][124Triz] varies with sampling depth. Upon absorption of CO<sub>2</sub>, the [124Triz]<sup>−</sup> anion chemically reacts with CO<sub>2</sub> at deprotonated amine sites to form carbamate, resulting in carbamate features in the XPS spectra. Results suggest that carbamate primarily forms in the bulk layers and the reaction is reversible. To a lesser extent, carbamate binds at the surface and does so irreversibly. Water adsorbs in greater concentrations at the surface than in the bulk and does not inhibit further CO<sub>2</sub> absorption.

**Keywords:** ionic liquids, x-ray photoelectron spectroscopy, gas capture, thin films, energy

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P-1-02

## Polymer Doping of SWCNT Fluid Suspensions as a Machinery to Control Laser Light Harvesting

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### ABSTRACT

Fluid suspensions of single-walled carbon nanotubes (SWCNT) tantalize researching owing to their application as optical filters, the effect of optical power limiting (OPL) of laser radiation being in focus. Previously [1, 2] we have shown that addition of polyvinyl alcohol (PVA) in SWCNT suspensions effects the bleaching, a phenomenon detrimental regarding the OPL and observed at pulse-periodic regime of irradiation. We studied the OPL of SWCNT aqueous suspensions stabilized by sodium deoxycholate (SDOC; 1% wt.) with varying additions of PVA by Z-scanning ( $\lambda = 532$  nm,  $I_{00} = 180$  MW/cm<sup>2</sup>) at pulse repetition rates 0.05 and 1 Hz. All suspensions demonstrate OPL at 0.05 Hz, which can be quantified by an extinction coefficient,  $\beta_{ext}$ , in the intensity  $I$  vs. displacement ( $z$ ) reciprocity:  $dI(z)/dz = -\alpha_{ext}I(z) - \beta_{ext}I^2(z)$ , a linear extinction being  $\alpha_{ext} = 3.237$  cm<sup>-1</sup> in all cases. Our experiment evinces that PVA addition can provide a two-fold increase in  $\beta_{ext}$ . At a rate of 1 Hz the OPL competes with bleaching. These two phenomena were juxtaposed in terms of  $\beta_{ext}$  and extinction saturation:  $dI(z)/dz = -\alpha_{ext}I(z)/(1 + I(z)/I_{sat}) - \beta_{ext}I^2(z)$ . Since the minimal  $I_{sat}$  values are greater than the maximal input intensity,  $I/I_{sat} \ll 1$ , a bleaching coefficient holds:  $\beta_{bl} = \alpha_{ext}/I_{sat}$ . Consequently, the result of the competing processes will be optimal at a minimum of  $\beta_{bl} - \beta_{ext}$ , whose values in our study point at the suspension SWCNT-60' (60 min ultra-sonication in dispersion processing, diameter of SWCNT bundle is several nm) with 1.5% of PVA as the least disrupted by bleaching ( $\beta_{bl} - \beta_{ext} = 0.247$  cm/GW). Bleaching in SWCNT-5' suspension (bundles over 10 nm) is stronger than in SWCNT-60', so the use of PVA in the former is not advantageous with respect to the OPL. Suspensions of carbon nanoparticles *per se* are not stable in water, so one needs to employ finer particles and stabilize them by surfactants. We studied aggregation properties of SDOC in mixed aqueous matrixes with concentrations of PVA 0, 1, 2 and 3% wt (temperature spanning 20 - 37°C). The enthalpy and entropy increments into the Gibbs energy of micellization appeared to be commensurable. It gives grounds to assert a superiority of SDOC as a dispersant for SWCNT in aqueous-polymer solutions: it operates via both inter-molecular hydrogen bonding and a hydrophobic effect. Doping of a fine-bundle SWCNT suspension by small amounts of PVA enhances resistibility of the composite regarding light-induced bleaching. This feature is interpreted basing on the viscosity-transport properties of fluid aqueous polymer matrixes.

**Keywords:** single-walled carbon nanotubes (SWCNT), optical limiting, surfactant, water-polymer matrix

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P-1-03

## A Review on Engineered Nanomaterials in Antimicrobial Paints and Coatings

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### ABSTRACT

In order to mitigate the global concern of bio-deterioration of buildings, heritage monuments, etc [1],[2], nano-additives have been gradually evolving as alternatives to conventional eco-toxic biocides [3] and weakly efficient biodegradable additives [4], for antimicrobial paints and coatings. This review proposes a comprehensive summary of various nanomaterials for prevention of biofilm formation on indoor and outdoor surfaces. The representative materials have been categorized into organic nanomaterials [5], inorganic nanomaterials [6] and hybrid nanocomposites [7] - their morphologies, synthesis techniques and performance have been evaluated herein. This review will contribute to further knowledge and advanced applications of nanomaterials for healthier buildings and structures, in terms of, unharmed mechanical strength, preservation of aesthetic appearance and improved indoor and outdoor air quality.

**Keywords:** bio-deterioration, nanomaterials, paints, coatings, building health.

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P-2-01

## Mangiferin mediated Nano-therapeutic efficacy for chronic wound treatment through magnetic or photodynamic effect

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### ABSTRACT

Chronic wound related severity are leading concerns worldwide because of poor quality of life, enhanced health care burden to overcome morbid survival index, distress related to pathogen persistence (adaptive survival strategy by pathogen) as biofilm structures and chronic inflammation at wound site are the major contributors thus, amplifying the chronicity towards more severe and life threatening situation. Mangiferin, being a polyphenol glucosyl xanthone obtained from *Mangifera indica* exhibit forthcoming potential as a phytochemical against chronic wound severity, because of its antimicrobial, antibiofilm anti-inflammatory properties along with wound healing nature that can potentially be subjugated for a better therapeutic approach for healing chronic wounds. We hypothesize mangiferin-loaded magnetic nanoparticles that will provide easy and enhanced penetration, retention and efficient targeting under the influence of applied magnetic field/or by photodynamic therapy targeting chronic wound related biofilm infections. Its synergistic/additive effect as advanced targeting approaches can probably introduce altered pathways *via* nano-therapeutics for chronic wound management. It can revolutionize the treatment prospective by penetrating and targeting the biofilm immune interaction, thereby reducing chronic wound inflammation and pathogenic persistence to ensure timely revival minimizing risk associated with conventional methods to tackle the non-penetrating biofilm structure, poor detachment inducers, impaired biofilm signal blocking.

**Keywords:** Mangiferin; chronic wound; biofilm; chronic inflammation; nano- loaded magnetic formulation; magnetic field; photodynamic effect.



Fig. 1: Diagrammatic illustration of Mangiferin mediated Nano-therapeutic efficacy for chronic wound treatment through magnetic or photodynamic effect

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P-2-02

## Lysophosphatidic acid (LPA) as a potential biomarker to envisage cardiovascular disease (CVD) in *Rheumatoid arthritis* patients

Vikas Shukla and Anita Kamra Verma\*

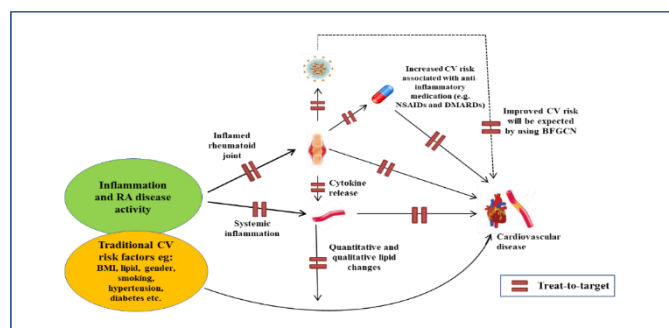
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### ABSTRACT

Rheumatoid arthritis (RA) an autoimmune chronic inflammatory disease and Cardiovascular diseases (CVD), are the major cause of death worldwide. Cells like macrophages and Fibroblast-like synoviocytes (FLS) are the main effector cells because there are many escalating evidences that shows the imbalances of M1/M2 macrophages and FLS have been noted down during the course of disease development. In addition, these secretory cells release matrix proteases which disrupts the inflammatory cascade. It has been found that RA patient's usually have a high inflammatory burden, dyslipidemia and increased risk of CVD. In comparative epidemiological studies between diseased and normal population, it has been evidenced that 50-60% of RA patients exhibit a greater chance of CVD dependent mortality. Lysophosphatidic acid (LPA) is an effective biomarker for lipid-signaling that is produced during inflammation. In normal circumstances, alterations in lipid levels occur during inflammation, but the effect of lipids on arthritis is not fully understood yet. Therefore, Berberine, an alkaloid could be envisaged as a therapeutic strategy in reduction of inflammation induced lipidemia by targeting the macrophages and modulating the LPA function. However, the biopharmaceutical limitation of Berberine is its poor aqueous solubility, wherein encapsulating berberine in nanoparticles would offer an extremely viable option to enhance its efficacy. Hence, a novel berberine loaded folate-conjugated glycol chitosan nanoparticles (BFGCN) could be a hypothesized as a three-pronged approach to target activated macrophages, fibroblasts of synovial fluid for down-modulation of LPA.

**Keywords:** RA, CVD, Berberine, LPA, Berb-FGCN, Macrophage Polarization



**Figure 1:** Schematic representation of downmodulation of LPA by Berberine loaded Folate-conjugated Chitosan Nanoparticles

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P-2-03

## Stealth lipid polymer hybrid nanoparticles encapsulated with paclitaxel for effective brain delivery

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### ABSTRACT

Brain targeting is by far the most challenging as Blood–brain barrier (BBB) the physiological hindrance, impedes the passage of neuro-therapeutics to gliomas. Nanotechnology applications efficiently facilitate transport of molecules overcoming BBB. Lipid polymer hybrid nanoparticles, consisting of a polymeric core coated by a layer of lipids, are a class of highly scalable, biodegradable nanocarriers that have shown great promise in drug delivery applications. Although they have generated sufficient interest, they are yet to be exploited. This report the designing of lipid polymer hybrid nanoparticles (LPHNPs), consisting of the polymeric core and an outer phospholipid shell and stabilized by various surfactants like tween 80, poloxmer 188, solutol HS 15 and TPGS, with an aim to boost brain delivery and avoid opsonization. LPHNPs would be synthesized using modified single-step nanoprecipitation technique, loaded with paclitaxel (PTX), and are an efficient delivery vehicle. Low-density lipoprotein (LDL) receptors are over expressed on the surface of glioma as well as on the endothelial cells of BBB. We will explore the LDL receptors for delivering the chemotherapeutic molecule especially to the brain cancer cells. Innovatively, we have conceptualized the coating of LPHNP with surface active agents instead of classical PEG-lipid layer aiming to manage comparable furtiveness character to the hybrid nanoparticles followed by encapsulation with PTX. The LPHNP resembles the LDL, as apolipoprotein E present in blood gets adsorbed on the surface of hybrid nanoparticles as a fact of surfactants and interact with LDL receptors on BBB that will help in increasing site-specific drug delivery especially to the brain tumor cells *via* crossing the BBB. The PTX encapsulated LPHNPs (PTX-LPHNPs) are biodegradable and biocompatible indicating slow sustained release of the drug targeted to brain tumor. The PTX-LPHNPs have an enhanced *in-vitro* cytotoxicity activity when compared to the free PTX. The present study consents the efficacious designing of LPHNPs confirming the potential applicability in enhancing the therapeutic brain delivery.

**Keywords:** Lipid–polymer hybrid nanoparticle, Paclitaxel (PTX), BBB, Low density lipoprotein

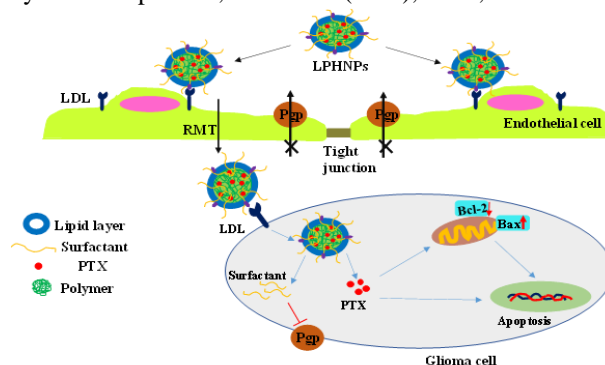


Figure 1: Drug-delivery mechanism of LPHNPs *via* crossing BBB

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P-2-04

**Development and characterization of a sequentially delivered system for amelioration of periodontitis**

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**ABSTRACT**

**Aim** - Periodontitis is the most prevalent inflammatory disease of the periodontium accompanied by bleeding gums, connective tissue destruction, formation of periodontal pocket and irreversible loss of alveolar bone. Periodontal connective tissue destruction and alveolar bone loss occurs primarily through the host response of bacterial plaque and its byproducts [1]. Hence the present work is mainly targeted to develop and optimize a novel formulation of sol to gel system containing microcapsule in which nanoparticles are embedded. Also, multi-therapeutic agents such as minocycline, celecoxib, doxycycline hyclate and hydroxyapatite will be incorporated in different compartments of sol to gel system for circumvention of all stages of periodontitis [2]. **Materials & Methods**- Doxycycline was adsorbed on the surface of hydroxyapatite by dissolving the two in aqueous solvent and uniform adsorption was ensured by scanning electron microscopy (SEM). The complex loaded alginate-chitosan nanospheres were prepared by the ionic gelation method and optimized by varying different process variables. Further dried nanoparticles along with the celecoxib were incorporated inside the PLGA microcapsules [3]. And these microcapsules with doxycycline hyclate were suspended in the chitosan gel. **Results**-The size of the optimized nanospheres was 290 nm with polydispersity index (PDI) of 0.142. Scanning electron microscopy (SEM) and Transmission electron microscopy (TEM) revealed spherical shape particles with smooth surface. The optimized system revealed a cumulative drug release of 74.23% for doxycycline in 72 hours. Further microcapsules were developed and characterized by the TEM which revealed the presence of nanospheres inside them. And the gel was successfully characterized. **Conclusion**- Novel polymeric particulate system was successfully developed and optimized for periodontitis.

**Keywords**- Periodontitis; host modulation therapy; nanospheres, scanning electron microscopy, transmission electron microscopy.

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P-2-05

**A machine learning approach for polymer nanoparticles and metal nanoparticles designed in antiviral drug delivery**

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**ABSTRACT**

Nanomaterials provide unique biochemical properties which is usually tailored to adjust in our physico-chemical environment for targeted drug delivery. Different nanomaterials with different properties have been known to show proven biomedical applications including anticancer as well as antiviral activities. Currently, many of these nanomaterials such as nanoparticles, nanofibers, nanospheres, nanotube, liposomes, etc. are being studied widely either as an antiviral/anticancer drug itself or as vehicle for targeted delivery. A wide variety of data from the researches of different nanomaterials that show antiviral property and beneficial activities of targeted delivery can be harnessed together and orchestrated in algorithms with the help of machine learning to facilitate different outcomes in the field of antiviral nanotherapeutics. There are still rooms to improve our understandings of binding sites of a nanomaterial to drug or its reaction to physicochemical environment. Using machine learning methods with their ability in classifying diverse structures and complex mechanisms, we will be able to predict the best/optimized nanomaterials system for any specific viral infection or antiviral activities. To these days, machine learning methods are well known and have been applied effectively to reduce the time, costs and risks in advanced drug development field. Combining nanotherapeutics and machine learning to facilitate antiviral-drug development systems through automation in the analysis and other relationships in bio-pharmaceutical networks would eventually help us to reach a complex goal very easily. In this study, we used machine-learning approaches to provide a new avenue to explore antiviral drug delivery system on polymer nanoparticles and metal nanoparticles such as PLGA, PEG and Gold.

Keywords: nanoparticles, antiviral, drug delivery system, machine learning

P-2-06

## Differently Sized Drug Loaded Chemo Responsive Mesoporous Silica Elicits Differential Gene Expression: Implications for Breast Cancer Therapy

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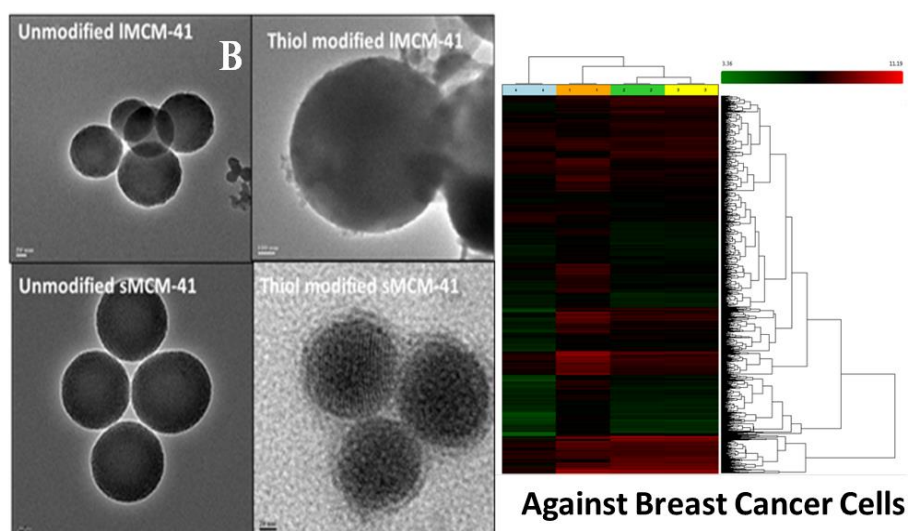
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### ABSTRACT

Changes in the size of the mesoporous silica carrier alter the drug release profiles as well as their internalization in cells. The difference in the localization of the carriers will result in differences in the molecular targets acted upon by the drug released. The differential expression of genes from the mesoporous silica treated cells was compared with those treated with the free drug. Out of the total 49,372 genes that were analyzed, the smaller dimensioned thiol-functionalized sMCM-41 loaded with the drug up-regulated 517 genes and down-regulated 2595 genes when compared with the cells treated with the free drug. In comparison, the larger sized drug-loaded thiol-functionalized MCM-41 enhanced the expression of 4520 genes and suppressed the expression of 1136 genes. Analysis of these target genes reveals that the smaller samples were more effective in suppressing oncogenes and nuclear transcription factors involved in cancer cell proliferation, invasion as well as survival. The findings were further validated using an *in vivo* model. This study is the first of its kind to be performed using two different sized chemo-responsive mesoporous carriers in breast cancer cells.

**Keywords:** Microarray analysis, thiol-functionalized mesoporous silica, breast cancer, chemo-responsive drug delivery systems, size

### GRAPHICAL ABSTRACT



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P-2-07

## **Functionalized Graphene Oxide as a Vehicle for Site-Specific Drug Delivery**

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### **ABSTRACT**

The demand of targeted drug delivery has increases day by day due to the lack of biocompatibility, bioavailability and cytotoxic index of various aromatic drugs. Therefore, the indiscriminate application of GO has grown exponentially towards biomedical field due to its intrinsic physico-chemical properties such as surface to volume ratio, pH and temperature sensitivity, unique structure and shape, aspect ratio, extent of oxidation, composition and various functional group linkages. Due to these extraordinary properties, various biological entities can linked to the single GO based system and targeted to their specific site. Synergistic combinations of multiple biomolecules can overcome toxicity and other side effects associated with high dosage of single drugs countering biological compensation, allowing reduced dosage of each compound or accessing site specific multi target mechanisms. In this present work, we have successfully synthesized GO via modified Hummer's method and functionalized it with biocompatible polymer, polyethylene glycol (PEG) and Folic acid (FA). An aromatic anticancer drug SN-38 and a biotin binding protein Avidin attached non covalently with the functionalized GO. The functionalized GO as a nanocarrier helps to improve not only the solubility but also the cellular uptake of drug by enhancing its ability to go across the target cell membrane which was confirmed by *in vitro* cytotoxicity test. The *in vitro* cytotoxicity confirms the synergistic effects of the both biomolecules.

**Keywords:** Graphene Oxide, biocompatible, cytotoxic index, FA, SN-38, Avidin.

**Acknowledgements:** The author(s) are greatly thankful for the financial assistance from the National Mission of Himalayan Studies (NMHS), Kosi Kataramal, Almora, India.

P-2-08

## Optimization and characterization of drug loaded lignin nanoparticles for combating solid tumor

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### ABSTRACT

Lignin is a plant based aromatic polymer which is available in abundance. Developing lignin as an alternative to available polymers has numerous benefits including biodegradability, renewability, cost effectiveness, ease of forming self-assembling nano-structures and also clearing of industrial biomass separation waste[1]. This study aims at developing a simple method for formulating drug loaded lignin nanoparticles along with optimization of process and formulation parameters for better control on final formulation. We have formulated drug loaded lignin nanoparticles by dialysis method based on solvent displacement principle. In this method, lignin and irinotecan were dissolved in DMSO and after filtration were dialyzed against an anti-solvent leading to the self-assembling of the lignin molecules into nanoparticles and entrapment of drug within[2]. The developed formulation was optimized by face centered central composite design (FCCCD) where concentration of lignin and concentration of irinotecan were selected as two independent variables whereas particles size and % drug loading were taken as dependent variables. Optimized drug loaded lignin nanoparticles (DLNPs) were characterized for particle size, PDI and surface charge, %entrapment efficiency and %drug loading. Shape and size of nanoparticles were observed by microscopic technique of TEM. *In vitro* drug release and release kinetic model were also observed. The efficacy of DLNPs against solid tumor was determined by performing MTT assay and cytotoxicity was established in various solid tumor and normal cell lines including MCF-7, A549 and HEK-293 [3]. The results of this research work demonstrate the self-assembling nature of lignin and bio safety of nanoparticles thus indicating their potential as substitute to synthetic polymers. The optimized formulation (DLNPs) was found to be within acceptable nano range and PDI indicates almost monodispersed formulation. Surface charge of DLNPs was found to be  $-25.43 \pm 2.41$  mV. The % entrapment efficiency was observed as  $67.65 \pm 1.95\%$  and %drug loading was observed as  $29.88 \pm 3.71\%$ . TEM image suggest that nanoparticles are spherical in shape and size is in corroboration with the DLS data. *In vitro* drug release studies for 72h indicates sustained mode of drug release and kinetic model studies shows that DLNPs follow Peppas Korsmeyers model i.e. drug diffuses out due to difference in concentration gradient. MTT assay suggest that DLNPs has higher %cytotoxicity against solid tumor cell lines like MCF-7 and A549 when compared to drug suspension. However, on normal cells of HEK-293, DLNPs were found to be safer.

**Keywords:** self-assembling, irinotecan, solvent displacement, cytotoxicity, optimization

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P-2-09

## Therapeutic potential of oral resveratrol chitosan drug delivery system in VCD induced osteoporotic mice model by activation of SIRT1.

**Largee Biswas & Anita K Verma\***

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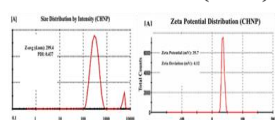
### ABSTRACT

Post-menopausal osteoporosis being a multifactorial ailment affecting both men and women causing morbidities and continued treatment, hospitalization and frequent osteoporotic fractures. The estrogen deficiency induced oxidative stress on bone has not yet been elucidated, and resveratrol, having exceptional antioxidant capacity, can affect bone tissue through SIRT1, NF $\kappa$ B pathways. Its clinical efficacy is limited owing to its low solubility in water coupled with quick metabolism of resveratrol that causes low bioavailability. Our goal was to exploit the therapeutic potential of Resveratrol, an agonist for the estrogen receptor that exhibits enhanced free radical scavenging activities for oral delivery in a chemically induced osteoporosis model in C57BL/6 mice. For oral delivery, Chitosan nanoparticles (ChNPs) were synthesized by ionic gelation crosslinked with sTPP having a size 299nm (PDI=0.437), zeta potential of +35.7mV.

C57BL/6 mice were injected with 4-Vinylcyclohexenediepoxy (VCD) (160mg/kg) intraperitoneally for 15 days and incubated for 6 weeks. After 6 weeks, mice were administrated with resveratrol (40mg/kg/day) for 10 weeks and then calcein (25mg/kg) and alizarin (30mg/kg) intraperitoneally for 6 days, followed by sacrificing of mice. The ovaries and femur bone were isolated to study the morphology of ovary followed by bone histology. Blood samples stored for evaluation of ALP, OPG and sirtuin 1 (SIRT1). Gradual depletion of ovarian follicles with irregular shape of granulosa cells by accelerating atresia confirmed menopause in VCD treated mice. Low intensity of green fluorescence (calcein) and high intensity in alizarin red were observed in VCD treated mice probably due to reduced calcium levels and matrix mineral in bone.

**Keywords:** Oral delivery, ChNP, Resveratrol, VCD model osteoporosis, Pharmacokinetics, SIRT1

### Oral resveratrol (RSV) drug delivery systems.



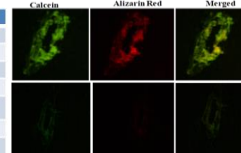
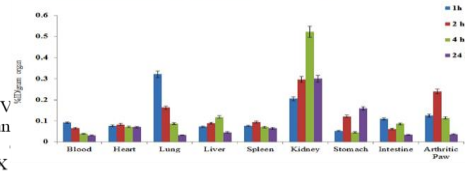
**[A] Size distribution of CHNP (Size 299.4 nm, PDI 0.437)**  
**[B] Zeta potential of [A] CHNP (+35.7 mV)**

**SEM of CHNP as measured by EV LS 10 (Carl Zeiss, Brighton, German at a working accelerating voltage 20.0kV and at amplification of 15000X**

### Pharmacokinetics of Chitosan nanoparticles

Parameter	Unit	Value
Absorption Rate Constant ( $K_a$ )	1/h	2.12
Elimination Rate Constant ( $K_e$ )	1/h	0.272
Half Life Time ( $t_{1/2}$ )	h	0.761
Maximum Time ( $T_{max}$ )	h	3
Maximum Concentration ( $C_{max}$ )	Counts	6.363
Area Under Curve ( $AUC_{0-\infty}$ )	Counts*h	18.89
Mean Residence Time (MRT $_{0-\infty}$ )	h	2.496

### Biodistribution of <sup>90</sup>Tc-CHNP



### Establishment of in-vivo osteoporotic model



**Bone histo-morphometric:**  
Significant bone weakening post treatment VCD (160mg/kg) in mice model was observed

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P-2-10

## Photo-Enhanced Singlet Oxygen Generation of Chitosan coated Prussian Blue Nano-assembly for Augmented Photodynamic Therapy

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### ABSTRACT

The fact that MDR (multi drug resistant) bacterial strains are becoming more prevalent in community-acquired infections [1] and a lack of development of new potent broad-spectrum antibiotic or immunosuppressive medication calls for implementation of optimal and safe strategy such as photo dynamic therapy (PDT) [2]. Herein, we report a newly fabricated chitosan nano-assembly (CHPB-FD), for endogenous oxygen generation and enhanced PDT. CHPB-FD nano-assembly, is prepared by loading photosensitizer (fluorescein isothiocyanate-dextran, FITC-dextran) to chitosan coated Prussian blue (CHPB). The interior PB core acts as a nanocatalyst (catalase), facilitating the decomposition of hydrogen peroxide speeding up the oxygen supply synergistically amplifying the O<sub>2</sub> dependent therapeutic effect of photo dynamic therapy due to blue light irradiation. In addition to this the PB core also acts as a photothermal agent increasing the local temperature upon red light irradiation [3]. The electro statically glued FITC-dextran to the positively charged CHPB can immediately transform the formed molecular oxygen (due to catalase-like activity of the nano-assembly) to generate cytotoxic singlet oxygen upon blue light irradiation and it does not interfere with the photothermal activity of the PB core irradiated with red light. This dual light irradiation obviates the competition at molecular level for the single light source and ensures complete photodynamic and photothermal efficiency. Photodynamic chitosan nano-assembly caters to the urgent need for biocompatible nanocatalysts, showcasing stimuli-responsive O<sub>2</sub> supply and simultaneously converting molecular O<sub>2</sub> to cytotoxic <sup>1</sup>O<sub>2</sub> for amplified therapeutic efficacy of PDT. CHPB-FD nano-assembly explores the alternative strategy against the traditional anti biotics as an antibacterial PDT agent eradicating the need of broad- spectrum anti biotics for MDR microorganisms.

**Keywords:** Antibacterial Photodynamic therapy, chitosan nano-assembly, FITC-dextran, nanocatalyst, Photothermal therapy, Synergistic effect.

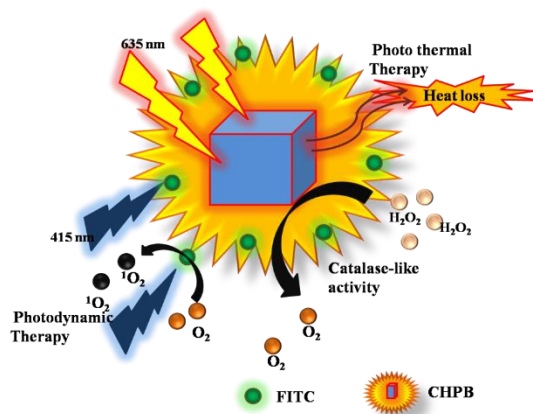


Fig1: Photo-enhanced endogenous O<sub>2</sub> generation of CHPB-FD for augmented photodynamic therapy

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P-2-11

### Artificial Intelligence in Drug Development and Delivery

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#### ABSTRACT

Artificial intelligence (AI) and AI-enabled technologies (AIET) are set to digitally transform the pharmaceutical, biologic, and wearable device industries (Fig.1) [1]. The huge investment of time and money in drug research and development requires the application of more innovative techniques and customized strategies. AI-assisted techniques offer tremendous opportunities for solving the complex algorithms associated with designing of functional drug delivery systems, accelerated drug discovery, identifying potential drug targets and lead drug candidates, predicting the bioactivities and interactions of drugs and treatment outcomes [1,2]. For health care, big datasets and complex algorithms will integrate the development and delivery of small- and large-molecule drugs, genetic therapies, and medical devices tailored to specific user profiles and even to individual consumers, with dynamic, real-time updates and adjustments [2,3]. The machine learning (ML) and disruptive management have taken over the world by storm and are now becoming a part of digital health sciences. The AI, ML, Internet of things (IoT), Cloud, High speed quantum systems (HSQS) and fast internet connectivity are the catalyst for disruptive innovations [1,3]. They can confer speed and sensor capacity to data processing and forecast large scale data analysis to extract the limited and highly accurate information, which is beyond of the capacity of human mind [4]. This high level of computation in milliseconds is possible by AI only. Moreover, it is foreseen that the future of drug development and delivery may point towards AI-based approaches. As the researchers investigate various new applications to benefit humanity, AI has not been explored considerably regarding drug development delivery [3,4]. By narrowing down the application of AI research and challenges, it is possible to bring translational benefits. Herein, we enclose a holistic view of AI applications in healthcare, particularly concerning drug designing and targeted drug delivery approaches. In brief, the significance of AI in the development of new drugs and delivery systems and related challenges will be highlighted, including the advances of organ-on-chips, 3D Bioprinting, pharmacogenomics and gene therapy, wearable devices, nanorobots, nanomachines and the new insights into the molecular mechanisms of diseases and related factors, towards the development of more effective drugs and drug delivery systems.

**Keywords:** artificial intelligence, artificial neural networks, 3D printing, organ-on-a-chip, drug delivery



**Fig. 1.** A variety of drug development and drug delivery approaches driven by artificial intelligence and nanotechnology

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P-2-12

## **Superparamagnetic Iron Oxide Nanoparticles Containing Photosensitizer for Cancer Theranostics Application**

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### **ABSTRACT**

With the increasing mortality rate in line with incidence, the diagnostic procedures and treatments on liver cancer needs to be advanced. <sup>[1]</sup> In this context, a new paradigm in cancer theranostics is achieved by using multifunctional biocompatible nanoparticulate system. This project aims to utilise the properties of magnetic and optical nanoparticles specifically for liver cancer by targeting cancer cells under the influence of an external magnetic field with multimodal properties of hyperthermia, photothermal (PTT) and photodynamic therapy (PDT).

Herein, we report synthesis and characterisation of mesoporous silica-superparamagnetic iron oxide nanoparticles loaded with optical Indocyanine Green (ICG) as a photosensitizer for multifunctional nanoparticulate system (MSN-SPIONs-ICG). Two types (hydrophilic and hydrophobic) of iron oxide nanoparticles synthesised by co-precipitation were coated with mesoporous silica of pore diameter around 3.5 nm. The overall size of MSN-SPIONs varied from 25 - 200 nm as observed from Transmission Electron Microscope (TEM). A characteristic FT-IR peak at around 550 and 1000 cm<sup>-1</sup> indicated Fe-O vibration of core Fe<sub>3</sub>O<sub>4</sub> and silica shell, respectively. The mesopore ordering of silica shell and crystallinity of iron oxide was further confirmed by a characteristic low angle and high angle XRD patterns. Loading capacity of ICG on mesoporous nanocomposites was around 3.4%. The ability to heat the suspension of MSN-SPIONs-ICG under AMF was observed to the set hyperthermia temperature of 42 °C. Similarly, a temperature change of around 6 °C in 6 minutes of NIR laser irradiation (808nm, 120mW) was observed on ICG loaded nanocomposites. Furthermore, the formation of singlet oxygen after irradiation of laser light was confirmed using the decay profile of 9,10-anthracenediyl-bis (methylene) dimaleonic acid (ABMDMA) dye.

With the initial encouraging results, we plan to use commercial liver cancer cell lines (HepG2) to perform *in-vitro* hyperthermia and PTT/PDT studies.

**Keywords:** Superparamagnetic iron oxide nanoparticles, Indocyanine green, Mesoporous silica, Hyperthermia, PTT/PDT

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P-2-13

## Redox-activated targeted mesoporous silica nanoparticles (MSN)-based nano-delivery platform for co-delivery of doxorubicin (NH<sub>2</sub>MSN-DOX-CpG/FA) against Lung cancer

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### ABSTRACT

Lung Cancer remains a lethal disease, associated with second highest cause of cancer related death in developing countries. Nano-theranostics has gained considerable interest in cancer treatment, as it represents a highly stable nanoplatform using self-assembly to incorporate a wide variety of cargos with precise functions of immunotherapy and chemotherapy.

Here, we propose a stimuli-sensitive redox-activated mesoporous silica nanoparticles (MSN)-based nano-delivery platform for co-delivery of doxorubicin (DOX/CpG). In this drug-delivery system (DDS) loaded with Doxorubicin (NH<sub>2</sub>MSN-DOX) and CpG oligodeoxynucleotide as effective immunotherapeutic agents, that activate the macrophages to release cytokines/chemokines to further activate T-effector cells causing trafficking at tumor site thereby stimulating both innate and immune responses. We conceptualized the synthesis of amine-functionalized Mesoporous silica nanoparticles (NH<sub>2</sub>MSNs) loaded with doxorubicin drug and CpG ODN(NH<sub>2</sub>MSN-DOX-CpG) subsequently modified with targeting moieties like - Folic acid (NH<sub>2</sub>MSN-DOX-CpG/FA) as a combinatorial delivery device of multiple ligands with specific functions of immunotherapy and chemotherapy. This nanoplatform-mediated combinatorial based therapy will contribute an efficient regulation on cancer microenvironment by increasing infiltration of immune cells to tumor site; down regulation of immunosuppressive cells may further enhance anti-tumor efficacy leading the cells to apoptosis. Nanoparticles can selectively release DOX and eliminate cancer cells, while they will have negligible effect on the healthy breast cells, due to the acidic and redox microenvironment in cancer cells. Overall, the designed nanoplatform, exhibits high selectivity between cancer cells and healthy cells and can be exploited simultaneously for tumor-selective drug targeting and for immunotherapy.

**Keywords:** Immunotherapy, chemotherapy, tumor microenvironment, Mesoporous silica materials, Doxorubicin.

### GRAPHICAL ABSTRACT

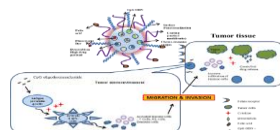


Fig 1: Schematic representation of proposed MSNs for co-delivery against Lung Cancer

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P-2-14

## Biogenic Selenium Nanoparticles Produced by the Probiotic *L. casei* and Selenium Nanoparticles-enriched *L. casei* as Bioactive Dietary Compounds Against Colon Cancer

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### ABSTRACT

Selenium (Se) is an essential trace element that exerts multiple and impressive health-promoting effects including immunoregulatory [1], anticancer [2] and chemopreventive [3] activities. There is though, a very narrow window between the beneficial/therapeutic dose of Se and the dose that exerts toxicity [4]. Nanomaterials, due to the enhanced role of surface interactions and weak intermolecular forces, display different physicochemical properties compared to bulk materials [4]. As such, Se nanoparticles (SeNps) possess distinct physicochemical characteristics compared to other selenium forms. Noteworthy, SeNps are less toxic and have better bioavailability [5].

Herein, we achieved green synthesis of SeNps utilizing the probiotic *Lactobacillus casei* ATCC 393 (LC), a bacterial strain previously shown to exert antitumor effects against colon cancer [6,7]. We studied the potential of LC-derived SeNps as well as SeNps-enriched LC as bioactive compounds against colon cancer employing *in vitro* and *in vivo* pre-clinical colon cancer models. SeNps exerted cancer-specific growth inhibitory activity and increased immunogenicity in colon cancer cells. Noteworthy, oral administration of SeNps or SeNps-enriched LC, induced a significant 50% or 75% respectively, inhibition in tumor volume compared to control animals, in the CT26 syngeneic BALB/c colon cancer model. The observed *in vivo* tumor growth inhibition was accompanied by higher levels of serum IFN $\gamma$ , a critical regulator of innate and adaptive immunity [8], and IL-12, a cytokine with a protective role against colon cancer [9]. Moreover, SeNps, downregulated the expression of cytochrome c in HT29 human colon cancer cells -an effect that has been linked with increased immunogenicity- and induced the translocation of calreticulin to the cell surface, a process associated with immunogenic cell death.

We provide evidence that SeNps produced by LC and SeNps-enriched LC could be good candidates for the development of oral formulations or dietary supplements for the chemoprevention of colon cancer. Our results demonstrate the strong potential of nanoparticles-enriched probiotics for cancer prevention while highlighting the exciting prospects of their exploitation in pharmaceutical and food industries.

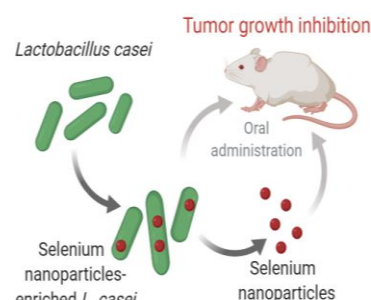


Figure 1. Biogenic selenium nanoparticles synthesized by the probiotic *Lactobacillus casei* inhibit colon cancer cell growth *in vitro* and *in vivo* when administered orally in ...

**Keywords:** selenium nanoparticles, biogenic, *Lactobacillus casei*, colon cancer

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P-2-15

## **Zinc–alendronic acid nanoscale coordination polymers in drug delivery**

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### **ABSTRACT**

Bisphosphonate (BP) drugs have shown potent therapeutic potential in the treatment of osteoporosis and bone metastasis from several cancers [1]. They are pyrophosphate analogues which are known to directly target bone cells (osteoclast) and inhibit osteoclast mediated bone resorption, with no known side effects. In addition, these drugs also show indirect therapeutic effects via inhibition of tumor metastasis to visceral organs (lung, liver), probably via immunomodulation [1,2]. However, free BP drugs are prone to capture and degradation by the reticuloendothelial system (RES), have poor pharmacodynamics and biodistribution, and sub-optimal targeting potential. Therefore, formulation of a nanocarrier for the delivery of high amounts of BP drugs can significantly improve their bioavailability, pharmacokinetics and targeting ability.

Herein, we report the fabrication of a novel nanoscale coordination polymers (NCPs), containing high amount of the bisphosphonate drug alendronic acid (AL) as the organic ligand, and zinc ions, using using template-free chemical precipitation method. The elemental composition (EDS) and thermogravimetric analysis (TGA) data of the Zn-AL NCPs confirmed their composition. TEM and FESEM micrographs of the as-synthesized Zn-AL NCPs showing the average size to be around 30 and 40 nm, respectively. The average hydrodynamic radii obtained with the help of DLS was found to be 180 nm, with polydispersity index (PDI) of 0.132. Drug release studies showed an initial burst effect, followed by a slow and steady release of about 73 % in a span of 5 days. Cell viability (MTT) assay in pancreatic cancer (Panc-1) cells showed higher cytotoxicity for the Zn-AL NCPs as compared to that of free AL. These studies show the promise of Zn-AL NCPs in cancer therapy applications.

**Keywords:** nanoscale coordination polymers (NCPs), zinc-alendronic acid nanoscale coordination polymers (Zn-AL NCPs), chemotherapy, immunotherapy

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P-2-16-SL

## Antibacterial properties of highly magnetic monodispersed FeCo nanoparticles

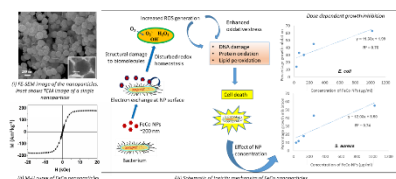
Moditma<sup>1</sup>, Priyanka Singh<sup>2</sup>, Raksha Sharma<sup>3</sup>, A.K. Verma<sup>2</sup> and S. Annapoorni<sup>1</sup>

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### ABSTRACT

FeCo nanoparticles have been synthesized by the polyol reduction process and characterized for their structural, morphological, magnetic and potential antibacterial properties. X-Ray Diffraction (XRD) pattern indicates formation of BCC phase of the alloy without any impurity phases [1]. Electron microscopy images taken using Field emission scanning electron microscope (FE-SEM) and Transmission electron microscope (TEM) reveal formation of uniform spherical structures of ~ 200 nm diameter, as shown in Fig. (i). Magnetic properties investigated using a Vibrating sample magnetometer (VSM) suggests the nanoparticles to be highly magnetic with a saturation magnetization ( $M_s$ ) of ~ 180 Am<sup>2</sup>kg<sup>-1</sup> and coercivity ( $H_c$ ) of ~ 150 Oe. The corresponding hysteresis curve is depicted in Fig (ii). Antibacterial activity of the synthesized nanoparticles was investigated qualitatively by measuring the zone of inhibition (ZOI) of bacterial growth, by disc diffusion assay, for two test bacteria namely *S. aureus* and *E. coli*. At a nanoparticle concentration of 10 mg/ml, this was determined to be 0.5 mm for both the species, suggesting nearly similar susceptibility to the synthesized nanoparticles. Further quantification of antibacterial performance was done by standard broth dilution tests, where dose dependent inhibition of the bacterial growth was investigated. A positive linear correlation ( $R^2 = 0.74$  for *S. aureus* and  $R^2 = 0.76$  for *E. coli*) was observed between nanoparticle concentration and percent bacterial growth inhibition, that was indicated by the decrease in solution turbidity. The MIC values for both the strains were accordingly ascertained to be >1024 µg/ml. An attempt has been made to understand the underlying bacterial toxicity routes of the synthesized nanoparticles by relating with their physical and chemical properties. These have been summarised in Fig (iii). Owing to the ability of FeCo to undergo changes in oxidation state in the bacterial culture medium; reactive oxygen species (ROS) induced damage, direct structural damage to bio-molecules or damage to cell wall due to physical adherence at the bacterial cell wall have broadly been speculated to be the possible inhibitory mechanisms. Thus synthesized FeCo nanoparticles can potentially act as single-entity magnetic antibacterials, where the ease of field-assisted targeting and retrieval [2] can answer the current medical needs against increasing number of multi-drug resistant bacterial strains [3] and also can be used for environmental remediation [4].



**Keywords:** FeCo, antibacterial, zone of inhibition, reactive oxygen species, minimum inhibitory concentration

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P-2-17

**Magnetic field triggered peptide covered mesoporous silica coated superparamagnetic iron Oxide as drug carriers**

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**Abstract**

An ideal drug delivery system must be able to have their own therapeutic efficacy, encapsulating the higher doses of payload, targeted to specific site and exhibit the tuneable physicochemical properties and biocompatibility. It remained a tremendous challenge itself to engineer a single drug delivery system, possessing all above characteristics. To address this possibility, here, we developed the superparamagnetic core that can be guided to target sites and can trigger the disassembly for payload release under Alternate Current Magnetic Field (ACMF). This core was further coated with mesoporous silica to achieve increased drug encapsulation and the mesopores of silica were capped with biocompatible dipeptide self-assemblies for triggered and controlled release of drug molecules. This delivery system under ACMF has shown hyperthermia response to kill the targeted cells. Moreover, this study revealed a new paradigm for a controlled release using ACMF trigger system that does not need any ligand modification or physical property modulation and can be produced in multilayers, which is expected to have variety of applications to treat wound healing, pulmonary, drug-eluting vascular grafts and stents and skin disorders.

**Keywords;** SPIONs, Peptide Self-assemblies, Drug Delivery Sytem, Core-shell, Coating



P-3-01

**Structural characterization of composites of activated carbon and solid waste plastic driven graphene for supercapacitive application**

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**ABSTRACT**

The plastic was improvised to improve the standards of day to day life of human, but now days it raises the worse situation for our eco-system. The main hazard is due to its non-biodegradable nature. Therefore, waste plastic management and its conversion to some useful goods is one of the main challenges. This challenge can complete under the three R's i.e. Reuse Reduce Recycle. Therefore, in order to reduce the waste plastic garbage, we need to reuse or recycle it. Some time it is not possible to reuse some old plastic like polybags, water bottles, stationary cover etc. so it is highly needed to recycle them to make some new thing. To this aspect, our group already had done a key experiment for the conversion of solid plastic waste into graphene nanosheets using pyrolysis and heating at high temperature under nitrogen atmosphere [1]. Further, other environmental wastes like rice husk, sugar cane husk, etc. is also utilized by recycling them form the synthesis of activated carbon. The activated carbon has been used in number of wide variety application ranging from cleaning, filtering, energy devices, etc. Another big challenge in front of environmentalist and scientist is the sustainable energy storage [2]. Fortunately, supercapacitor provides a bench mark solution for this as they are the most promising and versatile energy storage device for the various applications such as hybrid electric vehicles, portable electronics and uninterruptable power supply. As activated carbon provides low production cost, great adsorbitive property and high packing density, thus choosen as best material for supercapacitive devices [3]. But its low conductivity and low energy density curtail its commercial application. Therefore, increasing its conductivity and hence specific capacitance, can be appropriate route to achieve high performance supercapacitor. To this ground, Graphene, a two-dimensional sp<sup>2</sup> hybridized single atomic sheet of graphite can be utilized to make a composite with AC in order to enhance the surface area as well as conductivity [4-5].

In this regard, we endeavour to synthesis the composites of graphene nanosheet driven from waste plastic with activated carbon. The structure characterization of the prepared composites has been done using X-ray diffraction (XRD) technique, Fourier Transform Infrared (FTIR) spectroscopy and Scanning Electron Microscopy (SEM). Change in microstructure behavior has been observed after increasing the graphene concentration has been observed which may relate to change in supercapacitive behavior of the composite material.

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P-3-02

## **Characterization and electrical conductivity of Lithium doped Borate**

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### **ABSTRACT**

In the present work, the lithium oxide (Li<sub>2</sub>O) doped borate glass (B<sub>2</sub>O<sub>3</sub>) with composition xLi<sub>2</sub>O.(100-x)B<sub>2</sub>O<sub>3</sub> (x = 0, 10 and 20 in mol %) has been prepared by using the quick melt-quench method [1,2]. The effect of lithium has been investigated on the structural and electrical properties of the samples by means of X-Ray Diffraction (XRD), Fourier Transform Infrared (FTIR) spectroscopy and dc conductivity measurements. Also, the density and molar volume of these glasses are found to increase with increase in lithium content.

**Keywords:** borate glass, XRD, FTIR

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P-3-03

## Single-Component White Light Emitting Semiconductor Nanocrystals

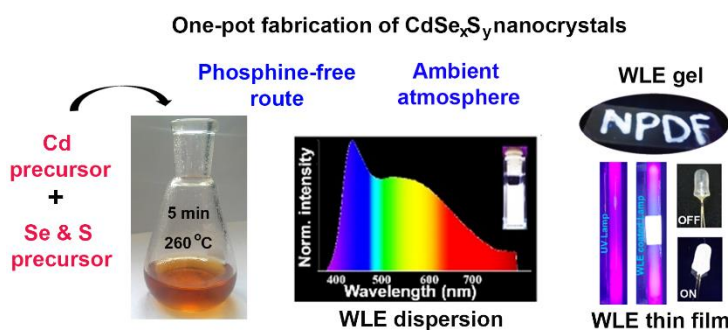
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### ABSTRACT

White light emitting materials are promising for lighting devices. Generally, white light is produced by mixing red, green, and blue emitting materials or by mixing two complementary colors in a definite proportion.<sup>1</sup> But the multi-component systems may lead to possible undesirable changes causing the loss of color purity and decrease in quantum efficiency. Thus, the single-emitting systems are advantageous over multiple component systems.<sup>2</sup> Herein, we report a facile one-pot fabrication route to prepare white light emitting CdSe<sub>x</sub>S<sub>y</sub> nanocrystals with enhanced quantum yield using cadmium oxide, sulphur powder and selenium powder as starting materials employing a long chain hydrocarbon solvent, paraffin. The phosphine-free reagents are used in the fabrication of the nanocrystals. The optical properties of nanocrystals can be effectively tailored by controlling the reaction time, reaction temperature, and the molar ratio of Se to S.<sup>3</sup> The lattice parameters of the crystals were estimated through powder X-ray diffraction (PXRD). The PXRD data revealed the formation of homogeneous alloy nanocrystals on changing the molar ratio of Se and S.<sup>4</sup> The emission of pristine CdSe<sub>x</sub>S<sub>y</sub> nanocrystals can be tuned across the visible region by changing the molar ratio of Se : S. The band-edge and trap-state emissions were observed covering a whole visible range leading to a single-component white light emission. The longer wavelength emission was found to be originated through trap states. The fine tuning of the Se/S ratio and the reaction time led to the efficient generation of the white light emitting semiconductor nanocrystals in solution, hydrogel and polymer-embedded thin film with Commission Internationale de l'Eclairage (CIE) coordinates of (0.30, 0.31), (0.31, 0.32) and (0.31, 0.33), respectively. The high color rendering index (CRI) and correlated color temperature (CCT) values of WLE thin film suggest promising use for solid-state lighting applications.



**Figure 1:** The schematic illustration of the properties and applications of white light emitting CdSe<sub>x</sub>S<sub>y</sub> nanocrystals.

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P-3-04

## Waste Plastic Generated Graphene Nanosheets for Next Generation Building Materials and Supercapacitors

N. G. Sahoo<sup>1</sup>, G. Tatrari<sup>1\*</sup>

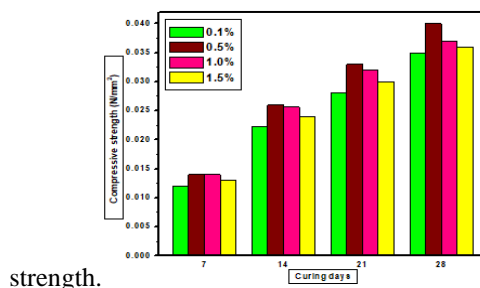
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### ABSTRACT

The demands of extra strengthen additives for concrete materials and cost-effective energy storage devices are increasing with increase the global population. The waste plastic is another issue that needs to be dealt within certain timeline, thus a parallel qualitative and productive approach is required to deal with this critical issue. The waste plastic due to presence of high carbonic content can be converted into different carbon nano-materials likewise graphene, carbon nanotubes etc. These nanomaterials possess excellent mechanical and electrochemical properties that can be applied into various applications. Here we report, an innovative approach to convert waste plastics into graphene sheets for extra strengthen concrete materials and cost-effective supercapacitor devices. In brief, the plastic waste was collected, dried, chopped and washed before placing into pyrolysis chamber where the high temperature pyrolysis i.e. 800 °C, results synthesis of black charred residue. Advanced characterization techniques like RAMAN, FT-IR, TEM, SEM/EDX, XRD evaluated and identified the black charred residue as graphene nanosheets. The obtained graphene was used as the nanofiller for the concrete blocks. The strength of these blocks was tested by using Universal Testing Machine (UTM) and result showed 43% enhancement in the compressive strength along with 30% enhancement in the tensile strength with the addition of 0.5 wt % graphene into cement. Further, the electrochemical performance testing was done after fabricating graphene sheets based device. The result of Cyclic Voltammetry (CV), Galvanic Charge- Discharge (GCD), and Electron Impedance Spectroscopy (EIS) showed an excellent specific capacitance with 1M H<sub>3</sub>PO<sub>4</sub> as the electrolyte. This innovative approach will surely act as the valuable tools in dealing with universal plastic pollution.

**Keywords:** Graphene sheets, Cyclic Voltammetry, supercapacitors, pyrolysis, concrete materials, compressive



**Figure 1. The compression strength of WGS concrete blocks at different curing period**

**Acknowledgement:** Author acknowledges NMHS Kosi Katarmal, Almora for the financial assistance.

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P-3-05

## Design and synthesis of polyaniline/MWCNT composite hydrogel as binder-free flexible supercapacitor electrodes

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### ABSTRACT

Supercapacitors have drawn significant attention as flexible energy storage devices, owing to its fascinating properties such as high power density, fast charge-discharge characteristics, long cycle life and desirable safety [1]. In order to further improve the energy storage properties of supercapacitors, there is a need to develop suitable electrode materials having high conductivity, large specific surface area, light weight, good mechanical strength, high flexibility and low cost. Thus, the recent research is mainly aiming to develop advanced nanostructured electrode materials to achieve high performance supercapacitors [2]. Herein, the novel polyaniline/MWCNT composite hydrogel has been fabricated on carbon cloth using a facile synthesis method. The composite hydrogel has been synthesized via in-situ chemical polymerization of aniline in the presence of phytic acid which acts as dopant and gelatine medium both and thus used as a binder-free electrode for supercapacitor.

**Keywords:** supercapacitors, flexible, hydrogel

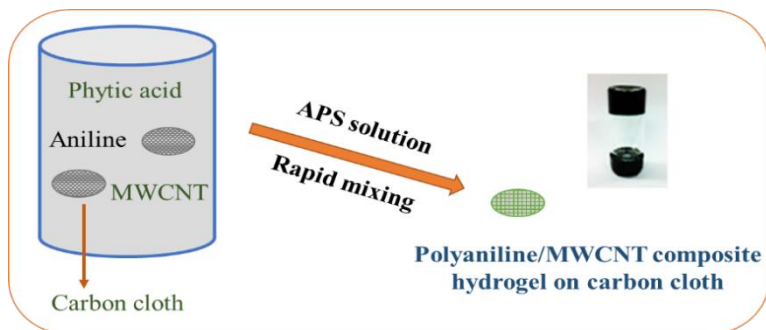


Figure 1. Schematic illustration of synthesis of polyaniline/ MWCNT composite hydrogel on carbon cloth.

The electrochemical performance of supercapacitor electrodes was investigated using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD) and electrochemical impedance spectroscopy (EIS) measurements. The electrochemical results show that the composite hydrogel possesses high specific capacitance of 276.56 F/g at a current density of 0.25 A/g in 1 M H<sub>2</sub>SO<sub>4</sub> solution which is higher as compared to polyaniline hydrogel. The supercapacitor electrode exhibits excellent cyclic stability up to 5000 successive cycles. Thus, it has been concluded that as prepared composite hydrogel can be considered as a promising electrode material for high performance flexible energy storage system.

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P-4-01

## Waste Generated 2D Carbon Nanomaterial for Water Purification and Bio-Imaging Application

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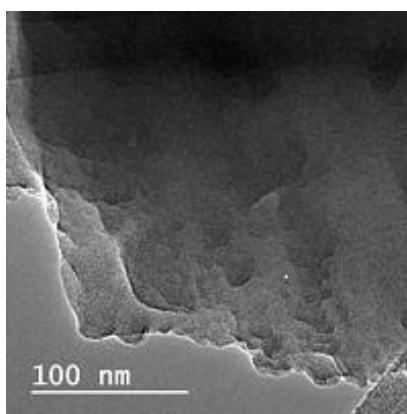
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### ABSTRACT

2D carbon nanomaterial such as graphene has gained attention of many scientists due to its exceptional large surface area, high electrical conductivity, good mechanical properties etc. Graphene oxide (GO), prepared by the chemical oxidization of graphite, has honey comb like structure decorated with several oxygenated functional groups i.e. carboxylic, hydroxyl, and epoxy groups which improve its dispersion in water and physiological environments.

In present time, the synthesis of graphene oxide in lab scale is done by hummer method in which use of concentrate acids and strong oxidizing agents are required. These chemicals are very toxic in nature and handling these chemicals need extra precaution for safety point of view. Here, we report a ecofriendly and greener technique to synthesis potassium doped graphene oxide (K-doped GO) using agricultural waste (*Quercus ilex* Fruit) as a precursor in which we totally avoided the use of harmful chemicals keeping principal of green chemistry in our mind. The elemental analysis and XPS studies showed the natural doping of potassium with high percentage (6.81%) in the synthesized material i.e. K-doped GO. The K-doped GO was specific and demonstrated bright blue photoluminescence (PL) under UV-light ( $\lambda_{\text{ex}}=365$  nm). This synthesized K-doped GO was an excellent bioimaging agent as well as act as visual heavy metal detection probe for iron. This 2D nanomaterial was also capable to remove the dyes from the water very quickly. So, synthesized K-doped GO can be used in the field of water purification, bio-imaging, heavy metal sensing.

**Keywords:** Agricultural waste, graphene oxide, heavy metal detection, waste plastic, water purification.



**Figure 1:** TEM image of synthesized K-doped graphene oxide from agricultural waste i.e. *Quercus ilex* Fruit.

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P-4-02

## Rice husk derived silica nano doped on calcium peroxide for fluoride removal from ground water

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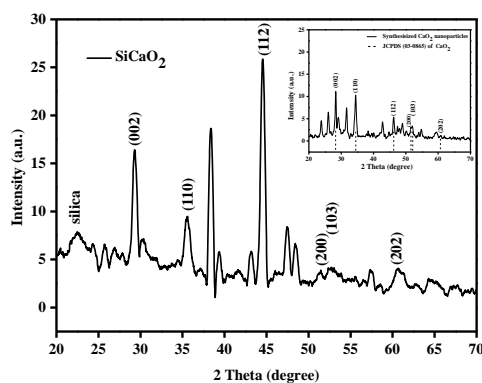
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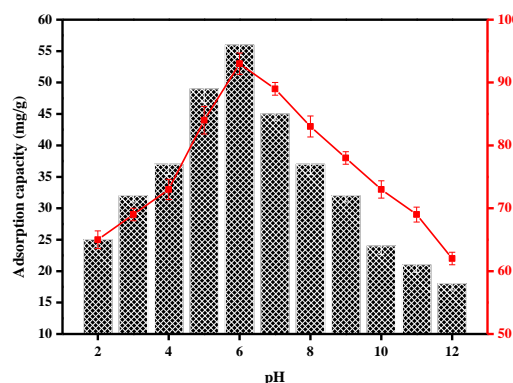
### ABSTRACT

Removal of fluoride is an essential for the human beings and animals. According to the WHO limit the fluoride should not be greater than 1.5 mg/L because it causes dental and bone deficiency to living entities. This problem arises day by day due to lack of defluoridation technique and expensive nanoparticles. Moreover, the cost effective and easy to use technology is not available. Likewise, many researchers has also used adsorbent which is expensive and less effective in removing fluoride. In the present work synthesis of Silica nano derived from rice husk doped on calcium peroxide ( $\text{SiCaO}_2$ ) nanoparticle was synthesized and determined the various factors affecting fluoride removal. The characterization of nanoparticle identified from Fourier-transform infrared spectroscopy, Scanning electron microscope, and X-ray powder diffraction. Experiments were performed to investigate the influence of nanoparticles with fluoride concentration, pH of solution, contact time, temperature, and adsorbent dose. Kinetic study and thermodynamic study was estimated. Recyclability experiment was also performed for fluoride removal. These results suggest that  $\text{SiCaO}_2$  nanoparticle may be used to develop a simple and efficient fluoride removal from ground water.

Keywords: adsorption, fluoride, Silica Nano, rice husk, calcium peroxide,



1. XRD of  $\text{SiCaO}_2$



2. Effect of pH of  $\text{SiCaO}_2$

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## Carbon based Nanomaterials as Electrochemical Sensor for Toxic Metal Ions in Environmental Applications

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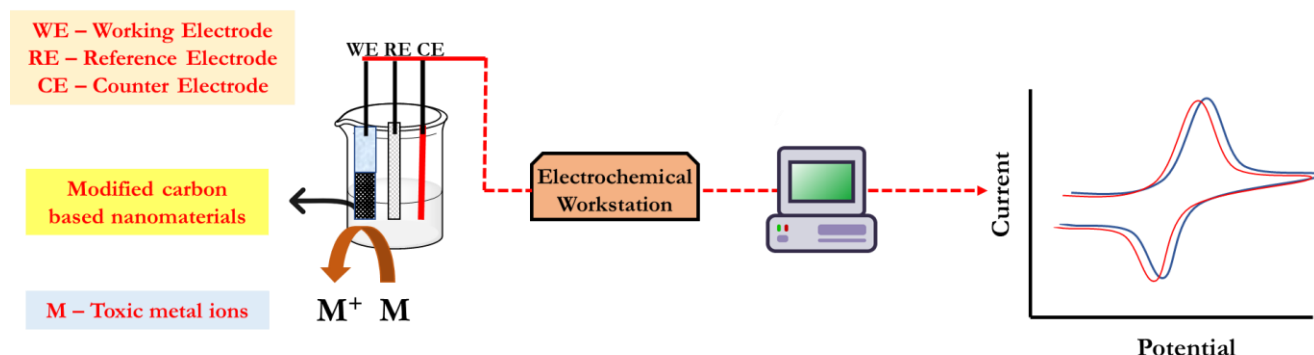
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### ABSTRACT

Toxic metal ions are one of micropollutants that are non-biodegradable and hazardous to human health even at trace levels. Excessive mining and production activities have resulted in release of toxic metal ions that ends up in our food chain causing serious health problems. Permissible limit for various toxic heavy metal ions in water that is suitable for drinking purpose has been set by World Health Organization (WHO). This leads to requirement of user friendly, fast, low cost, accurate, reliable, on-site and real-time monitoring techniques for detection of toxic metal ions. Various spectroscopic techniques are already in practice to sense toxic metal ions such as X-ray Photoelectron Spectroscopy (XPS), Flame Atomic Absorption Spectroscopy (FAAS) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS) etc. which are costly cumbersome, time consuming and lack speciation. Electrochemical sensor on the other hand are compact and less time consuming, hence a good alternative [1]. The sensitivity and selectivity of the electrochemical sensors can be improved multifold by modifying with numerous nanomaterials (NMs) such as metals, metal oxides and NMs based on Carbon etc. [2]. Carbon based nanomaterials (CBNMs) have received enormous attention in the development of electrochemical sensors by promoting electron transfer reactions, decreasing work potential within great surface areas, easy modification procedures, high mechanical strength and excellent conductivity. The present work, provides a review of recent advances of the use of electrochemical sensors fabricated with CBNMs for detection of various toxic metal ions. The electrochemical sensors fabricated with CBNMs have shown good performance with limit of detection (LOD) lower than WHO guidelines [3]. The various electrochemical techniques, along with their linear range and different sensing platform have been summarized. The future aspects, application and challenges are also commented.

**Keywords:** carbon, nanomaterials, electrochemical sensor, heavy metals, limit of detection



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P-4-04

## Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>): synthesis, characterization and its coupling with MoSe<sub>2</sub> for photocatalysts in water remediation under visible light irradiation

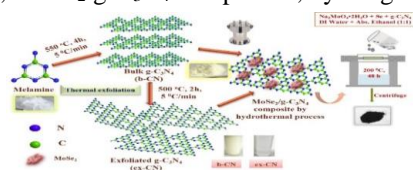
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### ABSTRACT

Exploring an effective method to mitigate environmental issues remains a challenge all over the world. Semiconductor photocatalysts has gained immense attention as a frontline solution for many applications. One such application is the destruction of many refractory pollutants to alleviate worsening situation of the environment. By employing an abundant solar energy as a source, semiconductor based photocatalysis are considered as a promising method for the remediation of environmental pollution and hence, it is vital to search for an appropriate visible-light driven semiconductor that can serve as a photocatalyst for reduction of environmental pollution.[1] Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) is one such photocatalysts that was developed in 2009[2] and achieved global eminence due to its visible light responsiveness, environmental benignity [3], cost effectiveness, high physiochemical stability and facile synthesis. It is a stable, metal-free  $\pi$ -conjugated system that have the capability to remove various pollutants under visible light irradiation. However, the photocatalytic activity is limited by high recombination rate of photogenerated charge carriers, low utilization of visible light and small surface area.[4] In order to eliminate such situation, constructing a cost-effective and efficient g-C<sub>3</sub>N<sub>4</sub> based systems with the combination of transition metal dichalcogenides (TMDs) can be opted. MoSe<sub>2</sub> is one such TMDs exhibiting metallic nature, provides higher electrical conductivity that can act as a promising candidate for photocatalysis.[5] In the present work, bulk g-C<sub>3</sub>N<sub>4</sub> was synthesized by thermal polymerization of nitrogen rich precursor, melamine. Further, exfoliation of g-C<sub>3</sub>N<sub>4</sub> was performed by two different methods, first one is a two-step liquid exfoliation process while the second one is thermal exfoliation method. The MoSe<sub>2</sub>/g-C<sub>3</sub>N<sub>4</sub> composites were prepared by simple hydrothermal process. To study and understand the photocatalytic activity towards degradation of Rhodamine B (RhB) along with the effect of both bulk g-C<sub>3</sub>N<sub>4</sub> and exfoliated g-C<sub>3</sub>N<sub>4</sub> on MoSe<sub>2</sub>, coupling of MoSe<sub>2</sub> was employed with bulk-g-C<sub>3</sub>N<sub>4</sub> as well as with exfoliated-g-C<sub>3</sub>N<sub>4</sub>. The results confirm that the MoSe<sub>2</sub>/g-C<sub>3</sub>N<sub>4</sub> composites shows a better photocatalytic performance compared to that of bulk-g-C<sub>3</sub>N<sub>4</sub> or exfoliated g-C<sub>3</sub>N<sub>4</sub> and can degrade 98% of Rhodamine-B (RhB) in about 50 min. The enhanced photocatalytic activity was due to better harvesting ability of visible light and improved separation of photogenerated electrons and holes. All the samples were well characterized by different characterization techniques.

**Keywords:** Graphitic carbon nitride, photocatalysis, MoSe<sub>2</sub>/g-C<sub>3</sub>N<sub>4</sub> composites, dye degradation,



Scheme 1: Schematic illustration of the synthesis of bulk, exfoliated g-C<sub>3</sub>N<sub>4</sub> and MoSe<sub>2</sub>/g-C<sub>3</sub>N<sub>4</sub> composites

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## Green Synthesized Nanomaterial based Colorimetric Sensors for Toxic Pollutants

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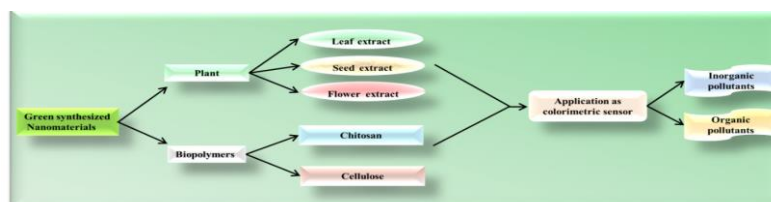
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### ABSTRACT

Nanotechnology has emerged as a significant tool in various fields of science. However, the synthesis of metal nanoparticles using physical and chemical methods are based on the use of toxic chemicals or reagents as stabilizing or capping agent and production of hazardous by-products have deleterious effect on environment. To avoid such consequences, green synthesis provides an eco-friendly and inexpensive alternative path for the synthesis of metal and metal oxide nanoparticles. Since nature provides variety of marvelous products in the form of plants, bacteria, fungi and biopolymers which serves the purpose of stabilizing and capping agent in a safer way. The major advantages of using these natural resources for the synthesis of nanoparticles are their presence in high abundance, non-toxicity, low cost and biocompatibility. This enhances their applications and acceptability. Recently, many researchers have successfully used different green resources like plant's leaf, seed, flower extracts, certain bacteria, fungus and biopolymers like chitosan, cellulose etc., to synthesize metal nanoparticles and therefore replaced the hazardous chemicals used in conventional route of synthesis. The size, shape and properties of nanoparticles synthesized using green materials were controlled by varying the reaction parameters such as concentration of the extract, pH, temperature and time [1]. The successful synthesis of nanoparticles using green approach was confirmed using various characterization tools like FTIR, SEM, TEM, UV-visible spectroscopy etc. The green synthesized nanoparticles due to their biocompatible nature and other magnificent intrinsic properties, like non-toxicity have various applications in biomedical, electronic and environmental remediation fields [2]. Recently, colorimetric sensors gained much attention due to its sensitive and selective color change which is visible by naked eye. Colorimetric sensors produced so far are based on noble metals like silver, gold and some metal oxide nanoparticles [3]. The highlight of this review is the green synthesis of metal and metal oxide nanoparticles using plant extracts and biopolymers, their characterization, factors affecting green synthesis and mechanism. Their specific application as colorimetric sensor for detection of toxic pollutants such as inorganic (metal ions), organic (pesticides, pharmaceutical drugs) and deadly chemicals in different samples are discussed in this work. Also, the advantages, drawbacks and future challenges of green synthesized metal and metal oxide nanoparticles will be evaluated thoroughly in this study.

**Keywords:** green nanomaterial, chitosan, colorimetric sensor, metal ions, organic pollutants



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P-5-01

## **Ethanol Bi-Reforming for Hydrogen Generation on Nickel Based Catalyst**

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### **ABSTRACT**

Hydrogen Gas is used for various applications in Refineries and also for synthesis of chemicals like Methanol, Ammonia, Dimethyl ether etc. Steam Reforming of Ethanol is an effective route for production of hydrogen gas. Use of CO<sub>2</sub> as additional component to steam is also more attractive as it reduces the overall carbon footprint for producing synthesis gas i.e. CO + H<sub>2</sub>.

In the present endeavour series of Nickel (Ni) catalysts using combination of Binary, Tertiary and Quaternary support were synthesized by using wet impregnation method and precipitation-deposition techniques. Combination of following elements, e.g. Aluminium (Al), Zirconia (Zr), Magnesium (Mg), Lanthanum (La) and Cerium (Ce) have been used as support [1,2]. Supports were synthesized by using Co-precipitation technique and analysed for physico-chemical properties. The catalysts were characterised for Temperature Programmed Reduction (TPR), BET-Surface Area, Nitrogen Pore Volume (N<sub>2</sub>-PV), Ammonia based Temperature Programme Desorption (NH<sub>3</sub>-TPD), X-Ray Diffraction (XRD) and Model reaction for Acidity/Basicity measurement. Nickel content was varied between 5% to 10% in the prepared catalyst and were analysed by Inductively Coupled Plasma (ICP) for metal analysis. These catalysts were used in the Ethanol Bi-Reforming Reaction in the Fixed-Bed Reactor [3]. The temperature of reaction was varied between 550-750°C and various other reaction parameters were also studied. Complete conversion of Ethanol was observed and around 60% yield of hydrogen was observed as compared to theoretical values. These catalysts were stable for 80 hours' Time on stream and no coking was observed. Best Catalysts having higher Hydrogen yield and higher stability observed were based on Alumina and Zirconia support with combination of Lanthanum and Ceria. The performance was attributed to Lower Acidity, Higher Surface Area with Optimum Nickel Content of 7.5 and 10.0 wt% in these catalysts.

**Keyword:** Ethanol, Bi-Reforming, Hydrogen Gas, Nickel Based Catalyst.

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P-5-02

## Sulphuric acid supported silica gel (H<sub>2</sub>SO<sub>4</sub>-SiO<sub>2</sub>) as an Efficient Catalyst for One-pot Multicomponent Synthesis of pyrano[2,3-*d*]pyrazol-amines under Ultrasonication

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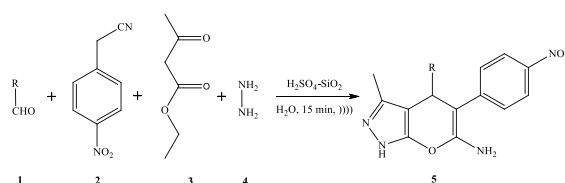
### ABSTRACT

The catalytic potential of Sulphuric acid supported silica gel (H<sub>2</sub>SO<sub>4</sub>-SiO<sub>2</sub>) as a catalyst has been assessed for the one-pot cyclo condensation reaction involving an aromatic aldehyde, 4-nitrophenylacetonitrile, ethyl acetoacetate and hydrazine to form poly functionalized pyrano[2,3-*d*]pyrazol-amines under ultrasonication. The strategy successively tolerates a variety of functional groups both electron-donating/electron-withdrawing and shows higher synthetic efficiency, product structural diversity. Moreover, the blend of Sulphuric acid supported silica gel and ultrasonication process is eco-compatible, environment-friendly, and the products are obtained in excellent yields without column chromatography. The feasibility of a gram scale reaction and catalyst recycling/reuse is demonstrated. By reaching a higher level of complexity in the products, this research explores a new direction in the field of construction of heterocycles *via* multicomponent approach.

**Keywords:** H<sub>2</sub>SO<sub>4</sub>-SiO<sub>2</sub>, Pyrano[2,3-*d*]pyrazol-amines, Four-component synthesis, Multicomponent reaction, Ultrasonication

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Scheme 1: Synthesis of pyrano[2,3-*d*]pyrazol-amines



P-5-03

## Synthesis of a novel bifunctional mesoporous Ti-SBA-15-SO<sub>3</sub>H catalyst and studies on their enhanced performance and kinetic modelling of lactic acid esterification reaction with n-butanol

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### ABSTRACT

In the present study, the mesoporous Ti-SBA-15-SO<sub>3</sub>H catalyst is synthesized by using the sol-gel method. Further, these materials have been characterized by different advanced analytical techniques such as Low angle X-ray diffraction (XRD), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Thermogravimetry/Differential thermal analysis (TG/DTA), N<sub>2</sub> adsorption/desorption studies, Fourier transform infrared spectroscopy (FT-IR), UV-Vis diffuse reflectance spectroscopy (DRS), X-ray photoelectron spectroscopy (XPS), Temperature-programmed desorption of ammonia (NH<sub>3</sub>-TPD) and Lactic acid esterification catalytic activity studies. The Ti-SBA-15-SO<sub>3</sub>H catalyst is found to have the surface area of 457 m<sup>2</sup>/g, the pore volume 0.12 cm<sup>3</sup>/g, the pore diameter of 3.16 nm, and high acid density of 1.72 mmol/g. The optimum reaction conditions for lactic acid esterification with n-butanol is found to be 1: 4 molar ratio, 3 wt-% catalysts, 115 °C temperature, and 120 min reaction time to obtain 72 % conversion. Further, the reusability tests reveal that the spent catalyst can be used for five successive runs without the loss of considerable activity. The pseudo-homogeneous model was able to describe the kinetics of this esterification with negligible error. The activation energy and equilibrium rate constant for Ti-SBA-15-SO<sub>3</sub>H is found to be E<sub>a</sub>=0.063 kJ/mol and K=5.019 lit/mol min, respectively, to catalyze the esterification of lactic acid with n-butanol. A plausible mechanism on the catalytic activity is proposed.

**Keywords:** Mesoporous Ti-SBA-15-SO<sub>3</sub>H, synthesis, characterization, lactic acid, n-butanol esterification, kinetic modelling.

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P-5-04

## Nano ZnO@PEG Catalyzed One-pot green synthesis of Pyrano[2,3-e]pyrimidines in Ethanol via One-Pot Multicomponent Approach

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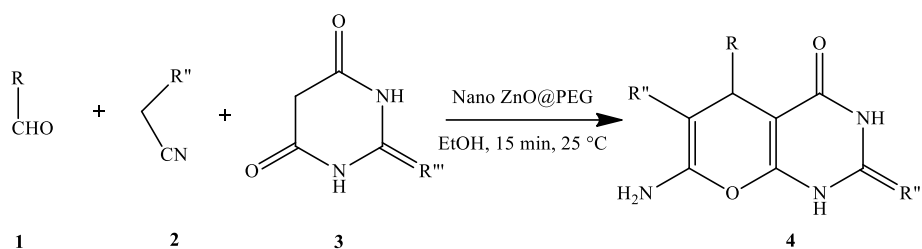
### ABSTRACT

Multicomponent reactions (MCRs) belong to an exciting class of organic reactions which has proven beneficial in all fields of synthetic organic chemistry. These reactions are performed in a one-pot, thus incorporating three or more reactants into a final product, giving rise to high levels of complexity and diversity. The most prominent applications of MCRs are observed in the synthesis of various N- and O- heterocycles, natural products, and peptides. We, herein report nano ZnO@PEG as an efficient catalyst, compatible with different variations of aldehydes (aryl/heteroaryl), active methyl compounds, and barbiturates affording the desired pyrano[2,3-e]pyrimidines in 91-97% yields. The electronic and the steric factors associated with the aldehydes did not influence the rate of the reaction in the presence of the nano ZnO@PEG catalyst. In comparison with the reported methods, our approach is eco-friendly, expedient, and environmentally benign. We have herein successfully demonstrated the application of ultrasonication in a multicomponent reaction (MCR), as the reaction is benign and convenient.

**Keywords:** Nano ZnO@PEG, Pyrano[2,3-e]pyrimidines, Three-component synthesis, Multicomponent reaction

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Scheme 1: Synthesis of pyrano[2,3-e]pyrimidines

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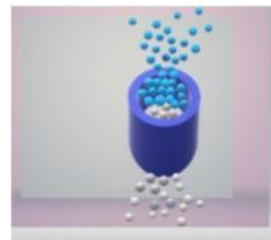


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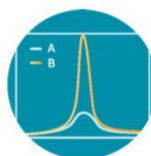
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