# National Conference on Advanced Materials for Photovoltaic and Supercapacitors (NCAMPS '17)

November 23th, 2017

# SOUVENIR

Convener

**Dr. R. Sathiyapriya**

Organized By

**Department of Physics**

## MAHENDRA ENGINEERING COLLEGE

(Autonomous)

Approved by AICTE, Affiliated to Anna University

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Salem-Tiruchengode Highway Mahendhirapuri, Mallasamudram-637 503,

Namakkal (Dt), Tamilnadu, India.

# MAHENDRA ENGINEERING COLLEGE

**(Autonomous)**

**Mahendhirapuri, Mallasamudram, Namakkal Dt -637 503.**

**Thirumigu. M. G. BharathKumar,**
**Chairman, Mahendra Educational Trust**

**23rd November 2017**

# MESSAGE

It gives me pleasure to note that the Department of Physics organizing a National Conference on Advanced Materials for Photovoltaic and Supercapacitors (NCAMPS), to be held on 23rd November, 2017, where a large number of eminent faculty members including Professors, Research scholars and students would deliberate on various important themes of the Conference.

The Institute also proposes to bring out a Souvenir on the occasion of the Conference containing the programme, special articles and write-ups on the theme of the conference. I wish all the success to the Department of Physics and the Organizer of the National Conference.

**[Thirumigu. M. G. BharathKumar]**
**Chairman, Mahendra Educational Trust**

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# Tentative Time Table

**National Conference on Advanced Materials for Photovoltaic and Supercapacitors-(NCAMPS '17), November 23, 2017**

**Date: 23rd November 2017** **Venue: Avvaiyar Arangam**

| Time | Schedule |
|---|---|
| 8.30 a.m. | Registration |
| 10.00 a.m. | Lighting Kuthuvilakku |
| 10.05 a.m. | Tamil thaivazthu<br>Honouring the Dignitories<br>Releasing the Souvenir |
| 10.10 a.m. | Welcome Address &<br>Introduction of guests |
| 10.20 a.m. | Felicitation |
| 11.00 a.m. | **Tea** |
| 11.20 a.m. | Keynote Address – Dr. P.M. Anbarasan |
| 12.10 p.m. | Keynote Address – Dr. M. Sathish |
| 1.00 p.m. | **Lunch** |
| 1.50 p.m. | Oral Presentation [Op01-Op12]<br>**[Avvaiyar Arangam]** |
| | Oral Presentation [Op13-Op21]<br>**[Dr. A.P.J Abdul Kalam Arangam]** |
| | Poster Presentation [Pp01-Pp33]<br>**[Department of R&D]** |
| 3.50 p.m. | **Tea** |
| 4.00 p.m. | Distribution of Certificates |
| 4.30 p.m. | Vote of Thanks |
| 4.35 p.m. | National Anthem |

**[Dr. R.Sathiyapriya]**
**Convener**

## About Mahendra Educational Trust

The Mahendra Educational Trust was established in the year 1978 by ***Shri. M. G. Bharath Kumar***, a renowned educationist with an object of imparting a high standard of education to rural children. The trust is located at Kalippatty - midway between Salem and Tiruchengode. Thiru. M.G. Bharath Kumar, the Chairman of the Trust is assisted by the Governing and Advisory Council in matters of Policy, Planning and Development of the Institutions. Tmt. Valliyammal Bharath Kumar, a best teacher awardee, is the Secretary of the Trust. Thiru Ba. Mahendhiran, a young and dynamic engineer, is the Managing Director. The Trust lays stress on providing quality education and maintaining high degree of discipline. To meet the demands of the people of Tiruchengode, Namakkal and Salem, the Trust broadened its educational service and started Schools and Colleges in those areas.

## About Mahendra Engineering College

Mahendra Engineering College was started in 1995 by Shri.M.G.Bharathkumar, a renowned educationist and a philanthropist with noble intent of educating the underprivileged in the Salem and Namakkal districts. The college is an Autonomous Institution and an ISO 9001:2008 certified institution. The College is offering 10 Undergraduate and 7 Postgraduate courses in Engineering. Here the students are offered unparalleled state of infrastructure, extremely committed and dedicated faculty that employs innovative learning techniques to create highly conductive environment. The technical knowledge gained by the students is compliment by imbibing interpersonal skills and spirit of entrepreneurship that makes them competitive enough to face the global challenges and emerge as achievers. The IE (I) chapter was inaugurated during the year 2008 and organized various Technical and Non-Technical Events.

## Programmes Offered:

**B.E. / B.Tech. Degree Programmes**

1. Mechanical Engineering
2. Electronics and Communication Engineering
3. Computer Science and Engineering
4. Information Technology
5. Electrical and Electronics Engineering
6. Civil Engineering
7. Electronics and Instrumentation Engineering
8. Aeronautical Engineering
9. Mechanical and Automation Engineering
10. Mechatronics Engineering
11. Agriculture engineering

**M.E / M.Tech Degree Programmes**

1. Computer Aided Design
2. Communication System Engineering
3. Computer Science and Engineering
4. Communication & Networking (Computer and Communication Engineering)
5. VLSI Design (Digital Communication and Networking)
6. Structural Engineering
7. Control Systems
8. Manufacturing Engineering
9. Environmental Engineering

**MBA**-Master of Business Administration

**MCA**-Master of Computer Application

## Location:

The College is situated in a sprawling campus of 130 acres in rural sylvan surroundings and is free from pollution. The College stands as colossus at Mahendhirapuri on Salem - Tiruchengode - Erode state highway, 27 Km from Salem and 33 Km from Erode and is well connected to all major cities, Industrial centres across the country through railway and road network. The area is characterized by educational promotion and economic transformation.

## About Department of Physics

The Department of Physics was established in the year 1995. The Department of Physics is one of the vibrant departments of the college. A team well experienced, highly motivated faculty with proven excellence in teaching and research carrying forward the motto of the institution. The Department aims to disseminate knowledge and skill based understanding of the concepts of science especially in areas relevant to Engineering and Technology. The department is equipped with modern lab and research facilities to improve the student's science knowledge and skills in order to make them to face the challenges in their professional career.

**Vision**

The Department functions with a vision to bring out innovative and high caliber scientific and technological manpower with a world class understanding of Physics.

**Mission**

The department has been working towards fulfilling its mission through a synergic combination of teaching and research. To promote excellence in technical education and scientific research through effective use of Physics in real-time engineering problems.

# CONTENTS

# Abstracts for Oral Presentation

## Volumetric and Viscosity Properties for the Binary Mixtures of 1-hexyle-3-methylimidazolium Tetrafluoroborate with butyl acetate

**A. Ayyasamy*** and Thanapathy. G

*Department of Physics, Poombukar College, Sirkali, Nagapattinam - 609107, Tamil Nadu, India*.

**Abstract:** In this work, densities and viscosities for the binary mixtures of 1- hexyle - 3-methylimidazolium tetrafluoroborate, [$C_6$mim] [$BF_4$], with butyl acetate, have been determined at 298.15 K. These data were used to calculate the excess molar volumes $V^E_m$ for the mixtures. It is shown that values of $V^E_m$ are negative, in the whole concentration range. The $V^E_m$ values show their minimum at the composition of $\chi_{IL} \sim 0.3$, exhibit a maximum at the same mole fraction. For the binary systems, the absolute values of $V^E_m$ decrease in the butyl acetate. The results are discussed in terms of the ion–dipole interactions between cations of the ionic liquid and the organic molecules and hydrogen bonding interactions between anions of the ionic liquid and the organic compounds.

**Keywords**: 1-hexyle-3-methylimidazolium tetrafluoroborate, Density, Viscosity, Excess molar volume, Viscosity deviation ,butyl acetate, Ionic liquids.

# Abstracts for Oral Presentation

## Topological, Morphalogical, Structural and Optical Properties of CdS Thin Film with Complex Agents TEA /Ammonia Mixer

**P. Settu[1]*,** G. Gopi[2], P.Baskaran[3], K. Manikandan[4]

*[1]*Department of Physics, Govt Polytechnic College, Sankarapuram-606401,Tamil nadu.*

[2]*Assistant Professor, Govt Arts College(Autonomus)-Salem-636007,Tamil nadu.*

[3]*Assistant Professor, Govt Arts College -Aiyalur-621713, Tamil nadu.*

[4]*Assistant Professor, Bharathidasan University Constituent Model College (Women), Veppur-621717, Tamil nadu.*

**Abstract:** This paper deals with the novel synthesis of CdS thin films with complexing agents TEA and Ammonia using the chemical bath deposition technique at room temperature UVis, FTIR, XRD, SEM and AFM characterisations were done. The influence of deposition and varying sulphur concentration on the optical absorption, transmittance, structural, surface morphological and topographical studies were examined. Band gap was observed for various sulphur concentrations structural studies revealed that, all the deposited films were nano-sized and crystalline in nature. Surface morphology showed that all the grains were spherical in nature and uniform. According to the properties observed it may be useful for solar cell and optoelectronics applications.

**Keywords:** CdS thin film, optical, structural, morphology, topography, complex agents, deposition duration and sulphur concentration.

# Abstracts for Oral Presentation

## ZnO-Reduced Graphene Oxide Nanocomposite for Supercapacitor Applications

**M. Iniya Pratheepa,** M. Lawrence*

*Department of Physics, St. Joseph's College (Autonomous), Tiruchirappalli, Tamilnadu.*

**Abstract:** A modified Hummers method has been proposed for preparing reduced graphene oxide (rGO) and the coprecipitation for zinc oxide (ZnO) nanocomposites. The obtained nanocomposites were characterized by scanning electron microscope (SEM), X-ray powder diffraction (XRD), Fourier transform infrared (FT-IR), Ultra violet visible spectrum(UV). The optical bandgap was observed to be 3.3 eV which estimated from Tauc's plot. It has been found that the morphology of the obtained structures can be modified by adjusting the synthesis conditions including the molar ratio of the starting materials. The charge storage ability, cycle stability and ion transport of the obtained rGO/ZnO nanocomposite were investigated by methods for cyclic voltammetry (CV), galvanostatic charge-discharge (GCD) cycling and electrochemical impedance spectroscopy (EIS). It has been demonstrated that the charge storage ability of the product is firmly influenced by its morphology while the cycle stability is affected by crystallinity. The highest specific capacitance for nanocomposite was found to be 371.36 F/g for nanoparticles at the scan rate of 10 mV/s.

**Keywords:** Modified hummers method, rGO/ZnO, XRD, Electrochemical property, Supercapacitor.

# Abstracts for Oral Presentation

## Study of the Optical Characteristics of Natural Sensitizers with Various Ph Values

**M. Nirmal Kumar***

*Department of Physics, Thiruvalluvar Government Arts College, Rasipuram.*

**Abstract:** Dye-sensitized solar cells (DSSCs) are new inventions in thin-film solar cells. DSSCs have a good depth in their nanostructure and hence absorb well the photons in the sunlight. Furthermore the dyes used in the cells are efficient in converting the absorbed photons into electrons. These solar cells have numerous advantages over their counterparts and are therefore commonly used in low-density applications and portable gadgets. In the present work, DSSC were prepared by using the plant materials BASELLA ALBA FRUITS UV- Visible absorption spectra of natural dye in solvent medium ethanol were carried out at various pH values. As the pH value increases from 2 to 5, absorption peak shows only negligible variation in their peak values and absorbance. But while using NaOH for pH variation, the absorption decreases for the values from 6 to 9. UV –Visible Spectroscopic study of natural sensitizes Effect of variation in pH value of Natural sensitizers in their optical characteristics for variation in their pH values (using HCL) shows small red shift. Therefore, the natural dye may be used as sensitizer with pH values between 2 and 5.

**Keywords**: DSSC, Natural Sensitizers, pH

# Abstracts for Oral Presentation

## Review of Perovskite Solar cells

T.S.Senthil and **C.R.Kalaiselvi ***

*Department of Physics, Erode Sengunthar Engineering College, Thudupathi, Erode, India.*

**Abstract:** Perovskite solar cells have recently emerged as a promising material for low cost, high efficiency and they have significant impact on the photovoltaic devices. Dye sensitized solar cells are the forerunners of perovskite solar cells. In liquid based dye sensitized solar cell structure the power conversion efficiency is low and also it had some stability issues. In 2012, a long term stable and high efficiency perovskite solar cell emerged by replacing the liquid electrolyte with solid hole conductor in organic metal halide perovskite materials. As perovskite has unique crystal make up it has some interesting properties such as superconductivity, giant magnetoresistance and ferroelectricity and these properties paves a way to the application of clean energy. This review summarizes the basic concepts of perovskite, their fabrication and its eminent properties which revolutionized the field of photovoltaic industry and also provides a platform for the solution of future energy crisis.

**Keywords:** Perovskite solar cells**,** superconductivity, giant magnetoresistance and ferroelectricity

# Abstracts for Oral Presentation

## Effect of Molarity on Sol-gel Routed Nano TiO2 Thin Films

**S.Lourduraj**[1] and R. Victor Williams*

*PG and Research Department of Physics, St.Joseph's College (Autonomous0*

*Bharathidasan University, Tiruchirapalli*

**Abstract:** This study presents the effect of molarity on the structural, optical and electrical properties of the $TiO_2$ films. The nanostructured titanium dioxide ($TiO_2$) thin films have been prepared for the molar concentrations of Titanium tetra isopropoxide (TTIP) 0.05M, 0.1M, 0.15M and 0.2 M by sol-gel routed spin coating technique with calcination at 450˚C. The processing parameters such as, pH value (8), catalyst HCl (0.1ml), spin speed (3000 rpm) and calcination temperature (450˚C) are optimized. The crystalline nature and surface morphology were analyzed by XRD, SEM, and AFM analysis. The XRD results confirm the films are crystalline with anatase phase and are nanostructured. The SEM micrographs of the $TiO_2$ film reveals the spherical nature of the particle. AFM analysis establishes that the uniformity of the $TiO_2$ thin film was optimized at 0.2 M. The optical measurements show that the transmittance depends on the molarity and the optical band gap energy of $TiO_2$ films found to be inversely proportional to molarity. The I-V characteristics exhibits that the molarity strongly influences the electrical conductivity of the film. The results indicate that the significant effect of molarity on structural, optical and electrical properties of nanostructured $TiO_2$ thin films will be useful to photovoltaic application.

**Keywords**: $TiO_2$ thin film; Titanium tetra isopropoxide; Sol-Gel; Precursor concentration; calcination temperature.

# Abstracts for Oral Presentation

## Enhancement in Photocatalytic and Antibacterial Performance of rGO based ternary nanocomposite

**S. Shanavas[1],** A. Priyadarsan[1] and P. M. Anbarasan1[*]

[1]*Department of Physics, Periyar University, Salem- 636 011, India.*

**Abstract:** A facetious approach for the production of novel hybrid nanocomposite was demonstrated via hydrothermal supported typical precipitation method. Absorption range and band gap energy were investigated by UV–Vis DRS. The surface morphology, elemental configuration, phase and crystal structure of as-synthesized nanocomposite was characterized by field emission scanning electron microscopy, High resolution transmission electron microscopy, energy dispersive X-ray spectroscopy and X-ray diffraction. The photocatalytic examination to degrade Reactive Blue 160 and inactivation of both positive and negative bacterial strains in aqueous solution were investigated under the visible light illumination. The combination of rGO with $La_2CuO_4/CeO_2$ nanocomposites leads to a better photocatalytic activity than other bare synthesized materials. The efficiency of RB160 decomposition increased with increasing pH (5–11) and catalyst dosage (0.01–0.03 g/l), but it gets decreased with increasing initial RB160 concentration (10–30 mg/l) and from that the optimum condition for the better photocatalytic performance was identified. The combination of rGO with binary nanocomposites leads to a better photocatalytic performance than other bare synthesized materials. The antibacterial activity of ternary hybrid nanocomposite showed visible light driven photocatalytic antibacterial activity with highly efficient performance. The enhanced photocatalytic and antibacterial activity of $La_2CuO_4/CeO_2$/rGO is promising for the further application of visible light driven photocatalyst in polluted water treatment.

**Keywords**:Photocatalytic, rGO, binary nanocomposites

## Synthesis & Characterisation of Perovskite Type Zn Doped Srtio$_3$ Solar Cells

**C. Indira Priyadharsini[1, 3],** A. Prakasam2, P. M. Anbarasan1,*

[1]*Department of Physics, Periyar University, Salem, India.*

[2]*Thiruvalluvar Govt. Arts College, Rasipuram, India.*

[3]*Muthayammal College of Arts & Science for Women, Rasipuram, India.*

**Abstract:** Zinc doped strontium titanate with rod-shaped morphology and different Zinc contents have been synthesized by a hydrothermal process. The obtained Zinc doped strontium titanate has been characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and ultraviolet (UV) diffuse reflectance spectra and photoluminescence analysis. The phase of the Zinc doped strontium titanate depends on the Zinc content. SEM observations show that the Zinc doped strontium titanate is composed of rod-shaped morphology with the diameter and length of nanoscale, microscale size in 10μm, respectively. The band gap of the Zn doped $SrTiO_3$ depends on the Zn content and decreases obviously from 4.8 eV to 3.6 eV with the vanadium content increasing from 1 mole ratio to 3 mole ratio. Zn doped $SrTiO_3$ shows highly efficient photoluminescence activity at the absorption range of 680nm. The results show that Zn doped strontium titanate is very promising for solar cell application.

**Keywords:** Perovskite, Band gap, Rod shaped morphology

# Abstracts for Oral Presentation

## Physico-Chemical and Structural investigation of $Bi_2O_3$-$SiO_2$-$Na_2O$ glasses through Ultrasonic and FTIR studies

**S. Anandhi** * and T.Sumathi

**Department of Physics, Bharath University, Chennai -600073*

*Department of Physics, Annamalai University, Annamalai Nagar 608002*

**Abstract:** Ternary bismuth silicate glasses with chemical formula $50Bi_2O_3$-$(50-x)SiO_2$-$xNa_2O$ (x=3,6,9,12 and 15mol%) have been prepared by conventional melt quenching method. Elastic and Structural properties of the glasses were investigated by measuring both longitudinal and shear velocities using the pulso-echo overlap method at 5 MHz and Fourier transform infrared (FTIR) spectroscopy respectively. The amorphous nature of the glass samples was ascertained using X-ray diffractometry (XRD). Interestingly, elastic constants and other parameters such as molar volume, Poisson's ratio, acoustic impedance, microhardness, Debye temperature and thermal expansion coefficient have been calculated using ultrasonic velocities and density measurements. The functional groups present in the glass samples have been confirmed by FTIR spectral analysis. Compositional dependence of ultrasonic velocities and related parameters are discussed to understand the rigidity and compactness of the glass system studied.

**Key words**: Ultrasonic velocity, FT-IR, XRD, Debye temperature, Elastic Moduli, Microhardness.

## Optical and electrical properties of glycine manganese chloride crystal

**G.Venkatesan[1],** S.Rajesh[2], S.Pari[1]*

[1] *Department of Physics, National College (Autonomous), Tiruchirappalli-620 001, India.*

[2] *Department of Physics, Pachayappa's College, Kanchipuram.*

**Abstract:** The organo-metal material of Glycine Manganese Chloride has been grown by solvent evaporation solution growth method. Single crystal XRD study has been carried out to confirm the grown crystal. FT-IR was recorded to identify the functional groups present in the crystal. The linear optical property of the grown crystal was analyzed by UV□Vis spectrum. Third order nonlinear optical properties was measured by Z-scan technique using Nd:YAG laser at 532 nm. Fluorescence emission revealed that can serve as a photo active material. Impedance and dielectric studies were also carried out for the material. Thermal property of the sample was analyzed by TG and DTA studies. The predicted NLO properties, UV-Vis absorbance and Z-scan studies indicate that the attractive material for optical applications.

**Keywords:** Optical materials and properties, Luminescence, Susceptibility, Electrical properties, Thermal properties

# Abstracts for Oral Presentation

## Synthesis and Characterization of Nanocrystalline Nickel Oxide Using Naoh and Oxalic Acid

[a]**M. Anbuvannan*,** [b]R.Rammohan, [c] P. Dhatshanamurthi

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[b]*Department of Physics, Annamalai University, Annamalainagar-608002*

[c]*Department of Chemistry, Sun Arts and Science College, keeranoor-606755*

**Abstract:** Precursors of Nickel oxide (NiO) nanoparticles were synthesized through a simple chemical precipitation method by changing the oxide source used for the synthesis. The synthesized precursors were subjected to thermo gravimetric analysis (TGA) to determine the temperature at which the precursors decompose into Nickel oxide. The obtained results of TGA suggest that precursor NiO prepared using sodium hydroxide (NaOH) showed NiO formation at 400°C, whereas, when oxalic acid was used as oxide source the formation of NiO takes place at 500°C. After calcinations of the precursors at respective temperatures NiO nanocrystals have been harvested. The synthesized NiO powders were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), photoluminescence (PL) spectroscopy, field emission scanning electron microscopy (FE-SEM) and energy dispersive X- ray analysis (EDX).

**Keywords**:Nanocrystalline, Nickel Oxide, Oxalic acid

# Abstracts for Oral Presentation

## Thermal, Physical and Structural Properties of Mixed Alkali and Transition Metal Ions in Sodium Borate Glass

**S. Rajesh[1]*** and R. Palani[2]

[1]*Department of Physics, Pachaiyappas College for men, Kanchipuram, Tamilnadu.*

[2]*Department of Physics, Annamalai University, Tamilnadu.*

**Abstract:** Glasses with composition $20Na_2O$-$(80-x)B_2O_3$-$xLi_2O$ and $20Na_2O$-$(80-x)B_2O_3$-$xWO_3$ (where x = 0 to 10 in steps 2 mole%) were characterized by the amorphous nature of the samples were ascertained using X-ray diffractometry (XRD), thermo gravimetric analysis (TGA), differential thermal analysis (DTA), microhardness and Fourier transform infrared spectroscopy (FTIR). The amorphous phase of the prepared glass samples was confirmed from their TGA, and DTA profiles. DTA profile yielded data of transition temperature ($T_g$), crystallization temperature ($T_p$) and the thermal stability ($\Delta T$) range of glasses. Microhardness studies exposed that the hardness of the sodium borate glass increases with an increase in applied load as well as with the doping of alkali and transition metal ions. Meyer's index number/work hardening exponent 'n' was calculated and it was found that the material belongs to a hard material category. FTIR spectra of the glasses were interpreted in terms of the structural transformations on the glass network by the changing composition. The FTIR spectral study reveals the existence of $BO_3$ and $BO_4$ groups with Li-O-Li and W-O-W vibrations in the present glasses. The presence of varied types like di, tetra, penta, and ortho borate groups are confirmed in the glass matrix.

**Keywords:** Sodium borate glasses, X-ray diffractometry (XRD), Thermo gravimetric analysis (TGA), Differential thermal analysis (DTA), Microhardness and Fourier transform infrared spectroscopy (FTIR).

# Abstracts for Oral Presentation

## Synthesis and characterization of magnetic nanoparticles and its applications of cellulase immobilization

**Kandasamy Selvam[1],** Thangaswamy Selvankumar[1*], Muthusamy Govarthanan[1 & 2], Arumugam Sengottaiyan[1], Chinnappan Sudhakar[1]

*[1] PG & Research Department of Biotechnology, Mahendra Arts and Science College (Autonomous), Kalippatti, Namakkal 637501, Tamil Nadu, India*

*[2]Division of Biotechnology, Advanced Institute of Environment and Bioscience, College of Environmental and Bioresource Sciences, Chonbuk National University, Iksan 570752, South Korea*

**Abstract:** Magnetic nanoparticles ($Fe_3O_4$) were synthesized by co-precipitating $Fe^{+2}$ and $Fe^{+3}$ ions in an ammonia solution and treating under hydrothermal conditions. Cellulase was immobilized onto $Fe_3O_4$ magnetic nanoparticles via glutaraldehyde activation. Response surface methodology based Box–Behnken design (BBD) was used to optimize the variables such as magnetic nanopartcles concentration, glutaraldehyde concentration, enzyme concentration, time course of cross linking. The BBD design analysis showed a reasonable adjustment of the quadratic model with the experimental data. Statistics based contour plots were generated to evaluate the changes in the response surface and to understand the relationship between the nanoparticles and the enzyme activity recovery. The Scanning electron microscopy (SEM), X-ray diffraction (XRD) analysis and Fourier transform infrared (FTIR) spectroscopy, Magnetic measurements (VSM) were studied to characterize size, structure, morphology and binding of enzyme onto the nanoparticles. The stability and activity of the bound cellulase was analyzed using various parameters like pH, temperature, reusability, and storage ability. The same was compared with the free cellulase for showing its enhanced stability and activity.

**Keywords**: Magnetic nanoparticles, Cellulase, Response surface methodology.

# Abstracts for Oral Presentation

## Eco-friendly synthesis and characterization of silver nanoparticles from *Piper betel* and their antidiabetic activity against alloxan induced albino rats

**Arumugam Sengottaiyan[1]*,** Thangaswamy Selvankumar[1], Muthusamy Govarthanan[1 & 2], Kandasamy Selvam[1&3], Chinnappan Sudhakar[1]

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*[3]Centre for Biotechnology, Muthayammal College of Arts and Science, Rasipuram, Namakkal 637 408, Tamil Nadu, India*

**Abstract:** *Piper betel*, a medicinal plant, traditionally used in treating diabetes mellitus. In this study, we used the leaf extract of the plant to synthesize silver nanoparticles (AgNPs), as a proposition to treat alloxan induced diabetic rats. The eco-friendly synthesised AgNPs were analyzed using UV–visible spectroscopy at 420nm and Fourier transform infra-red spectroscopy for their functional groups. Transmission electron microscopy revealed that, the synthesized particles are found to be 10-25 nm in size. Monodispersed and spherical nature of synthesized AgNPs were shown by scanning electron microscope and the presence of Ag in the AgNPs was confirmed by energy dispersive spectrum. The eco-friendly synthesised AgNPs were evaluated for its antidiabetic activity in alloxan-induced diabetic rats. AgNPs-treated diabetic rats found to be significantly improved the dyslipidemic condition as seen in the diabetic control. Furthermore, it also reduced the blood glucose level over the period of treatment. The improvement in body weight was also found to be evidence for *P. betel* extract-mediated synthesised AgNPs as a potential anti-diabetic agent against alloxan induced diabetic rats.

**Keywords**: Diabetes mellitus, *Piper betel,* Silver Nanoparticles, Alloxan

**Extraction optimization and characterization of bio-pigments from *Delonix regia* by using Box–Behnken design**

**P. Srinivasan**, C. Sudhakar[1], T. Selvankumar[1*], M. Govarthanan[1 & 2], K. Selvam[1], A. Sengottaiyan[1]

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*[2]Division of Biotechnology, Advanced Institute of Environment and Bioscience, College of Environmental and Bioresource Sciences, Chonbuk National University, Iksan 570752, South Korea*

**Abstract:** Currently, natural dyes and pigments gain more importance in food, textile industries and sensitized solar cells because of their non toxic and eco friendly characteristics. The aim of this study was to optimize the pigment extraction from the *Delonix regia* by Box–Behnken design (BBD). Response surface methodology (RSM) was applied to evaluate the optimal conditions of three process variables namely *D. regia* (g), extraction time (h) and temperature (□C). Statistics based contour and 3-D plots were generated to evaluate the changes in the response surface and to understand the relationship between the extraction and the pigment yield. The optimum process conditions were found to be mass of *D. regia*: 3 g, contact time: 3 h and extraction temperature: 30 □C. Response surface methodology was performed well to identify the optimal levels of extraction process variables and the validation of predicted model was fitted 99.76% with the experimental results conducted at the optimum conditions. Fourier transform infrared spectroscopy (FT-IR) was also confirmed the presence of Quercitin pigment by identifying the major functional groups.

**Keywords:** Bio-Pigment, Response surface methodology, FT-IR

# Abstracts for Oral Presentation

## Extraction of bio-pigments from *Lawsonia inermis* L. as a photosensitizer in Dye-sensitized solar cells

**Chinnappan Sudhakar[1],** Thangaswamy Selvankumar[1*], Muthusamy Govarthanan[1 & 2], Kandasamy Selvam[1], Arumugam Sengottaiyan[1]

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**Abstract:** Dye-sensitized solar cells (DSSC) are expected to be used for future clean energy. Currently, most of the researchers in this field use Ruthenium complex as dye in the dye-sensitized solar cells. However, Ruthenium is a rare metal and high cost. The present study was investigating the use of natural dye extract of *Lawsonia inermis* L. was used as sensitizer to fabricate titanium dioxide nanoparticles ($TiO_2$NPs) based dye sensitized solar cells. The dyes have shown absorption in broad range of the visible region (400-700 nm) of the solar spectrum and appreciable adsorption onto the semiconductor ($TiO_2$) surface. DSSC fabricated using the pre dye treated and pure $TiO_2$ NPs sensitized by natural dye extract of *L. inermis* showed a promising solar light to electron conversion efficiency of 1.01%. Natural pigments offer advantages of natural abundance, simplicity of preparation, low cost and environmental friendliness.

**Keywords**: Dye-sensitized solar cells, Natural dye, $TiO_2$, Photovoltaic

# Abstracts for Oral Presentation

## Synthesis of Multiwalled Carbon Nanotubes for the Removal of Industrial Textile Dyes

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**Abstract:** Textile dyes are chemicals with complex aromatic structure designed to resist the effects of laundering and sunshine. A great number of dyes and other chemicals are used in textile wet processing. There are more than 105 commercially available dyes with over $1X10^6$ ton of dye stuff produced annually worldwide. Among these available dyes, azodyes constitute about 70% of all known dyestuffs in the world and represent 70% of total dyes produced per year, thus making them the largest and most important group of synthetic colorants released into the environment. Azo dyes are difficult to treat by convententional wastewater treatment method. Compared with physical and chemical and biological techniques are preferable because of economical advantages and low possibility of by products production. At present, a number of studied focused on MWCNTs, which are able to decolorize azo dyes and efficient application. Multi-walled carbon nanotubes (MWCNTs were prepared by CVD method and further characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared (FT-IR), and UV-vis absorption spectra. The performances of the MWCNTs were evaluated for the decomposition of Reactive light yellow K-6G (K-6G) and Mordant black 7 (MB 7) azo dyes solution. The results showed that the addition of MWCNTs has the adsorption activity for the degradation of azo dyes K-6G and MB 7. The effect of MWCNTs content, catalyst dosage, pH, and initial dye concentration were examined as operational parameters. The kinetics of photocatalytic degradation of two dyes was found, the degradation efficiency still higher than 70%.

**Keywords:** Multi Walled Carbon nanotubes (MWCNT), CVD, Azo dyes. Textile Dye.

# Abstracts for Oral Presentation

## Analysis on cobalt doped tungsten oxides ($WO_3$) for superconducting applications

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**Abstract:** Nanodimensional pristine $WO_3.H_2O$ and with cobalt as dopant have been synthesized by using $CoCl_2.6H_2O$ and $Na_2WO_4.2H_2O$ with the ratios 2 and 5 wt.% using facile household microwave irradiation process. The resultant process were annealed at 600°C in air for 6 h in order to improve their crystalanity and to remove excess of by products and impurities. The samples were characterized with powder X-ray diffraction, field emission scanning electron microscopy, UV-VIS diffusion reflectance spectroscopy, photoluminescence spectroscopy along with, the corresponding magnetic behaviors of the products were analyzed through and vibrational sample magnetometer. X-ray diffraction patterns showed $WO_3.H_2O$ crystallized with orthorhombic phase. The annealing effect showed that doped $WO_3$ (Co ≈ 2 wt.%) formed with orthorhombic phase and the remaining products were found to be monoclinic phase (pure and Co ≈ 5 wt.%) indicating the role of dopant in determining the crystalline phase of the end products. The effect of doping on crystalline perfection of the samples was also monitored using power X-ray analysis. FE-SEM micrographs suggested that the dopants are able to influence the growth rate and morphology of the prepared nanopowders. UV-VIS-DRS spectroscopy was employed to determine the optical band gap of these samples and the results revealed the incorporation of dopant (Co ion) in the intermediate energy level in determining the optical band gap. Blue emissions were verified using PL at room temperature for the annealed samples when exited with 390 nm wavelength. The difference in peak intensity observed through PL spectra attributed to the possible distortions in $WO_4^{2-}$ tetrahedron group during microwave irradiation process. The unexpected results from hysteresis loops from

vibrational sample magnetometer on the annealed samples suggest that the cobalt doped samples try to persist well into the superconducting or diamagnetic state, namely the coexistence of dia and ferromagnetism.

**Keywords:** Tungsten oxide, Microwave irradiation, Cobalt doping, Nanoparticles.

## Green Synthesis of Zno Nanoparticles Using Abrus Precatorius Seeds Extract and their Characterization

**N.Subathra[1],** P.Duraisamy[2], Pradeepkumar[3]

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**Abstract:** In modern science Nanotechnology is a ablaze field for the researchers.Nanoparticles having a size of 1-100 nm in one dimension, is used significantly concerning medical chemistry, atomic physics, and all other known fields. Nanoparticles are used immensely due to its small size,orientation, physical properties,which are reportedly shown to change the performance of any other material which is in contact with these tiny particles. These particles can be prepared easily by different chemical, physical, and biological approaches. But the biological approach is the most emerging approach of preparation, because, this method is easier than the other methods, ecofriendly and less time consuming. The semiconductor ZnO has gained substantial interest in the research community in part because of its large exciton binding energy 60 meV which couldc lead to lasing action based on excitation recombination even above room temperature. The Green synthesis was done by using the aqueous solution of *Abrus precatorius* seeds extract and zinc acetate. A fixed ratio of plant extract to metal ion was prepared and the color change was observed which proved the formation of nanoparticles. The nanoparticles were characterized by UV-vis Spectrophotometer, FTIR, DLS, Zeta Analysis, XRD, and SEM. The particlessynthesized were of the size ranging from 40-50 nm.

# Abstracts for Oral Presentation

## Role of microwave on structural, optical and photocatalytic activity of tin oxide nanoparticles

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**Abstract:** A facile and rapid microwave irradiation method was used to synthesis of nanocrystalline tin oxide (SnO & $SnO_2$) powders with different microwave power (360 W, 600 W and 900 W) and the effect of microwave power on the structural, surface morphology, optical and photocatalytic activity has been systematically investigated. Powder X-ray diffraction (PXRD) results suggest the samples were tetragonal Romarchite and tetragonal rutile type structure of SnO and $SnO_2$ respectively. Transmission electron microscope (TEM) images illustrates that both SnO and $SnO_2$ consists of spherical shaped morphology with an average diameter of around 25-40 nm, which is in good agreement with the grain size calculated from XRD results. Raman, Photoluminescence and Energy dispersive spectra (EDS) analysis spectra results indicate that the as-synthesized samples were oxygen deficient with the increase of microwave power up to 900 W. A considerable red-shift in the absorption edge and decreasing the band-gap (3.67-3.57 eV) of $SnO_2$ was observed with the increase of microwave power. The photocatalytic activity was monitored via the degradation of Methylene blue (MB) and Rhodamine B (RhB) dyes under visible light irradiation and $SnO_2$-900 W sample shows better photocatalytic activity than SnO-300 W and $SnO_2$-600 W. The possible photocatalytic mechanism was also discussed in detail.

**Keywords:** Tin oxides, Microwave, Optical properties, Transmission electron microscope, Catalyst, Visible light.

## Study of Silver Nano Dots and Their Related Characteristics and Applications

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**Abstract:** Today, Silver nano dots have a variety of potential applications in the field of modern medicine and industrial electronics. Their electronic structures can be tailor made and their properties differ depending on their sizes and shapes. They can be created at lab following any of these procedures either top to bottom or bottom to top approach. And at the nano scale dimensions with varying optical and electronic, mechanical properties, many new and novel applications from infrared detectors, laser and photoluminescence to solar cells are created. Silver nano dots emit light at a characteristic wavelength when excited, this wavelength emitted depends on the size of the nano dot therefore it is easier to control the size of the silver nano dots harvested in the lab. This unique property finds potential applications in the field of medicine and industrial electronics.

**Keywords:** Silver nano dots, electronic properties, Applications.

# Abstract for Poster Presentation

## Green and Environmentally Sustainable Synthesis of Sn and F Doped ZnO Nanoparticles via an Aqueous Solution Route for Antibacterial Applications

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**Abstract:** To date, zinc oxide (ZnO) with various morphology and structures such as nanoparticles, nanorods, nanoplates, nanocubes, nanoflowers and so on, have been prepared through diverse approaches. ZnO presents several interesting properties in various fields such as piezoelectricity, electronics, optics, thermal and medicine. However, in this present investigation, we have synthesized ZnO nanoparticles simultaneously doped with tin (Sn) and fluorine (F) by an aqueous solution route. The structural, optical, morphological, compositional and antibacterial activities of the synthesized products were characterized by X-ray diffraction (XRD), UV-Vis spectroscopy, scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS) and well diffusion method. The XRD results indicate that ZnO nanoparticles are solid solutions crystallizing in pure hexagonal würtzite structure and consisted of a mixture of nanoparticles with grain size between 19 and 27 nm. The UV-Vis absorption spectra show that the Sn and F doped ZnO nanoparticles exhibits a blue shift in the absorption edge. The SEM image of the samples varies from hexagonal rods to spherical shape structure and the EDS spectra confirm the substitution of Sn and F into ZnO lattice. The zone of inhibition for the *E.Coli* bacteria is found to be increased with increase in the dopant concentration.

**Keywords:** ZnO:Sn:F Nanoparticles, Aqueous solution route, Doping effect.

# Abstract for Poster Presentation

## Design and Testing of Solar Distillation

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**Abstract:** The purpose of this project is to fabricate a solar water distillation system that can purify the water, which is impure by using a systematic arrangement must have low cost for manufacturing and works based on renewable energy of solar. There is less amount of water only left on earth that is safe to drink without purification after 20-25 years from today. 99% of Earth's water is in a solid state and other impure form and the remaining is in liquid form. Due to this reason, water purification is necessary. Because of this, purposes the solar still is constructed which will convert the impure water into pure water using the renewable solar energy. The incoming solar radiation from the sun is heating the water, which placed in the basin in impure form, and this water gets evaporated and condensed into pure drinkable water.

**Keywords**: Solar Distillation, Solar Water Purification, Solar Still, Renewable Energy.

## Abstract for Poster Presentation

### First Principle Study of Highly Efficient Organic Dye Sensitized Solar Cell Based on D-π-A Architecture with Different Spacer Units

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**Abstract:** A series of novel organic dyes (ICS1, ICS2, ICS3, ICS4 and ICS5) with D-π-A structural configuration incorporating indolocarbazole moiety as donor (D) unit, thiophene as π-linker and 2-cyanoacrylic acid as acceptor unit were investigated. Indolocarbazole based D-π-A dyes composed of different spacer groups were designed. By modulating spacer unit, the efficiency of D-π-A dyes based dye-sensitized solar cells (DSSCs) can be further improved. Density Functional Theory (DFT) and Time-dependent DFT (TD-DFT) methods reveal that the physical properties of dyes. In the present work, five novel push-pull organic dyes only differing in spacer have been designed based on experimental literature value of IC-2. In order to further improve the light-harvesting capability of indolocarbazole dye and to examine the spacer influence on dye performance were discussed. Furthermore, the designed organic dyes could exhibit good photovoltaic performance of charge transfer characteristics, driving force of electron injection, dye regeneration and light harvesting efficiency (LHE). Finally, ICS5 dyes can serve as an excellent spacer groups than ICS2 for future DSSCs applications.

**Keywords:** D-π-A, DSSCs, DFT and TD-DFT, LHE.

## Abstract for Poster Presentation

# Crystal structure analysis of 4-((2(2-bromophenoxy) Phenyl) ethynyl)-N, N-diethylaniline

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**Abstract:** Single crystals of 4-((2(2-bromophenoxy) phenyl) ethynyl)-N, N-diethylaniline were grown by slow evaporation method and X-ray diffraction analysis reveals monoclinic P21/c space group with unit cell dimensions of a = 9.0761 (9) Å, b= 7.5220(7) Å, c= 30.468 (3) Å and β= 97.921(3)°. Crystal data were collected using BRUKER SMART APEX II CCD X-ray diffractometer. The structure was solved by direct method and refined on $F^2$ by full-matrix least-squares procedure to the final $R_1$ of 0.051 using SHELXL programs.

**Key Words:** Bromophenoxy, Diethylaniline, Crystal packing and Crystal structure.

# Abstract for Poster Presentation

## Study of Structural, Geometrical and NLO Properties of Pterostilbene for DSSC Applications

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**Abstract:** The geometries, electronic structures, polarizabilities, and hyperpolarizabilities of organic dye sensitizer Pterostilbene studied based on ab initio Hartee Fock (HF) and Density Functional Theory (DFT) using the hybrid functional B3LYP. UV-Visible (UV-Vis) spectrum was investigated by Time Dependent- DFT (TD-DFT). Features of the electronic absorption spectrum in the visible and near-UV regions were assigned based on TD-DFT calculations. The absorption bands are assigned to $\pi \rightarrow \pi^*$ transitions. Calculated results suggest that the three excited states with the lowest excited energies in *Pterostilbene dye* are due to photo induced electron transfer processes. The interfacial electron transfer between semiconductor $TiO_2$ electrode and dye sensitizer *Pterostilbene dye* is due to an electron injection process from excited dye to the semiconductor's conduction band. The role of cyanine and methyl group in *Pterostilbene dye* in geometries, electronic structures, and spectral properties were analyzed.

**Keywords:** Pterostilbene, TD-DFT, UV-Vis and NLO

# Abstract for Poster Presentation

## Crystallization and Characterization of Piperidinium 4-Nitrophenolate Using Quantum Chemical Calculations for Optoelectronic Applications

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**Abstract:** Large size and high quality single crystals of organic nonlinear optical material Piperidinium 4-Nitrophenolate (P4NP) have been grown by solution growth method. This crystal belongs to monoclinic system with non-centrosymmetric space group of $P2_1$. To confirm its structure and compositions, this material was subjected to powder X-ray diffraction and microanalysis studies. Fourier transform infrared (FTIR), UV–Vis and Photoluminescence spectra have been recorded and extensive spectroscopic investigations have been carried out. Static and dynamic hyperpolarizability were calculated to confirm the suitability of the crystal for nonlinear optical applications. In addition, Frontier Molecular Orbital (FMO), Mulliken charge and Molecular Electrostatic Potential (MEP) analyses were performed by Density Functional Theory (DFT) at the B3LYP/6-31G basis set.

**Keywords:** Piperidinium 4-Nitrophenolate crystal, spectral analyses, hyperpolarizability, nonlinear optics (NLO) and Density Functional Theory (DFT)

# Abstract for Poster Presentation

## Effect of Mn Concentration on Structural, Thermal and Optical Properties in $Baso_4$ Nanoparticles

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**Abstract:** In the present investigation, pure and diverse moles of Mn doped $BaSO_4$ nanoparticles were synthesized through chemical precipitation method. The structural, functional groups, band gap energy, thermal property, morphology and elemental composition of the synthesized products were reported through X–Ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FT–IR), UV–Visible–Diffused Reflectance Spectroscopy (UV–VIS–DRS), Thermo Gravimetric and Differential Thermal Analysis (TG–DTA), Field Emission Scanning Electron Microscopy (FE–SEM), Transmission Electron Microscopy (TEM) and Energy Dispersive Spectroscopy (EDS). Increasing and decreasing tendency of lattice parameters have been observed with increase in Mn doping concentrations. From the FT–IR technique, presence of functional groups on the pure and Mn doped $BaSO_4$ nanoparticles were identified. Using UV–Vis–DRS study, band gap energies of as synthesized pure and Mn–$BaSO_4$ NPs were identified, and were found to be 4.05–3.74 eV and 4.10–3.78 eV, respectively. Both the Thermo Gravimetric Analysis (TGA) and Differential Thermal Analysis (DTA) curves of the $BaSO_4$ NPs showed no further weight loss and thermal effect at a temperature above 630 °C. Moreover, flaky like morphological structure of the pure and Mn–$BaSO_4$ nanoparticles have been observed from the images obtained from the microscopic techniques (FE–SEM and TEM). From EDS measurements, existence of $Mn^{2+}$ ion was confirmed.

**Keywords:** Mn doped $BaSO_4$, XRD, FT–IR, UV–VIS–DRS, FE–SEM and TEM.

# Abstract for Poster Presentation

## Synthesis and Characterization of Pure and Ni Doped Copper Oxide Nano Particles

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**Abstract:** Nano particles of metal oxides are manufactured in the large scale because of their industrial applications. Copper Oxide is an important p-type semiconductor, has drawn increasing attention in the application of gas sensors because of low cost, excellent reactivity, high stability and non-toxicity, and also the secondary architectures composed of nanostructured building blocks have attracted significant interest in material synthesis and device fabrications. In the present investigation pure and Ni doped CuO nano particles have been prepared by co-precipitation method. The crystalline natures of the sample were also confirmed by X-ray diffraction pattern. The crystalline size of the pure and Ni doped nano particle were determined as 13 nm, 12 nm and 14 nm respectively. FT-IR spectra identify the functional group present in the molecular structure. There is a shift in the lower frequency region confirmed the presence of the dopants (Ni). The surface morphology of the prepared materials were also analysed by FE-SEM. It reveals the polycrystalline porous morphology with a nano flower structure. The small crystallites agglomerated to form nanoflowers and nano sheets. The energy gap values for pure and doped (Ni) CuO were also determined. An anti-bacterial study shows that the zone of inhibition is high for the CuO and doped (Ni) CuO nano particle. CuO nanoparticle exhibited strong antibacterial activity against bacterial species.

**Keywords:** Antibacterial activity, Co-precipitation, Copper Oxide, FT-IR, Nanoflower, SEM, XRD.

# Abstract for Poster Presentation

## Synthesis and characterization of Manganese (5, 10 wt%) doped tin oxide ($SnO_2$) nanoparticles

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**Abstract:** $SnO_2$ / Mn doped $SnO_2$ nano particles were synthesized by simple hydrothermal method. Pure Tinoxide and manganese doped Tinoxide were characterized by XRD, TEM, UV-Vis (DRS) spectra. XRD patterns revealed the formation of single phase rutile structure with particles are in nano dimensions.TEM image shows that $SnO_2$ nano particles are in spherical shaped structure and by the addition of Manganese (Mn) does not change the shape of the nano particles structure. The UV-Vis DRS studies were revealed the optical band gap energy was calculated from 3.67 eV to 3.25eV for $SnO_2$ and Mn doped $SnO_2$ nano particles. It shows that the doping of Mn decreasing the bandgap energy of pure and doped $SnO_2$ nano particles. UV –Vis absorbance spectra shows a red shift from 368 nm to 600 nm,, further it was shifted to the higher wavelength with increasing the doping concentration.

**Keywords:** Nanoparticle, Hydrothermal, Manganese, Tin oxide

# Abstract for Poster Presentation

## Optical properties of 2-Hydroxy-1-Naphthaldehyde Phenylhydrazone on Silver Nanoparticles

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**Abstract:** Water - soluble silver nanoparticles of different sizes have been prepared by chemical reduction method and characterized using optical absorption spectroscopy. The interaction between silver nanoparticles and 2-hydroxy-1-naphthaldehyde phenylhydrazone (HNPH) has been investigated using optical absorption and fluorescence emission techniques. The increases in size of the silver nanoparticles cause a decrease in the quenching of fluorescence of HNPH. The concentration of the particle material dependent on the fluorophore intensity has been studied. The Stern – Volmer quenching constants and the association constants have also been calculated.

**Keywords:** Silver Nanoparticles, 2-Hydroxy-1-Naphthaldehyde Phenylhydrazone, Optical properties

# Abstract for Poster Presentation

## Growth and characterization of Organic NLO Crystal Triphenyl methane 4 nitroaniline aniline

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**Abstract:** Single crystals of Triphenyl methane 4 nitroaniline an organic NLO material have been grown slow evaporation method at room temperature. The grown crystals were characterized by UV-Vis spectroscopy, FTIR spectroscopy, Powder XRD, Dielectric studies,TGDTA Analysis,Flurescence and NLO studies. In these studies elaborately gives the properties of the grown crystal. The experimental results suggest the suitability of the grown crystal for opto electronic application.

**Keywords**: crystal growth UV-Vis spectroscopy, FTIR, Powder XRD studies, SHG test.

# Abstract for Poster Presentation

## Hydrothermally synthesis of Bismuth vanadates with different shapes for high-performance supercapacitors

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**Abstract:** A facile and low-cost stratagem has been established for the synthesis of Bismuth Vanadate with different shapes via one-step hydrothermal method. Various $BiVO_4$ Nps were synthesized through changing the operation temperatures. Further they were analytically characterized by XRD, FTIR, SEM and Electrochemical Studies. In Fig.1. XRD pattern has showed the different types of the crystal structures due to their operating temperatures. FTIR was used to investigate V-O groups and also removal of organic impurities in the as-prepared BiVO4. Different morphologies were obtained for all BiVO4 samples. The electrochemical studies were carried out for all the samples.

**Keywords:** Bismuth Vanadate, Hydrothermal method, XRD, SEM, Supercapacitor

# Abstract for Poster Presentation

## Molecular Structure, Molecular Docking, Vibrational Spectra, Nbo and Uv-Vis Analysis of Acetaminophen

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**Abstract:** The molecular structural parameters and vibrational frequencies of the fundamental modes of Acetaminophen have been obtained using Density functional theory (DFT) technique in the B3LYP approximation with 6-31G(d,p) basis sets. Detailed vibrational assignments of the observed FT-IR and FT-Raman bands have been proposed on the basis of potential energy distribution (PED). The difference between the observed and the calculated wavenumbers values are very small. The theoretically predicted FT-IR and FT-Raman spectra of the title molecule have been constructed. The molecular electrostatic potential has been mapped primarily for predicting sites and relative reactivities toward electrophilic and nucleophilic attack. The intramolecular contacts have been interpreted using Natural Bond Orbital (NBO). The absorption wavelength, energy and oscillator's strength are calculated by TD-DFT and Acetaminophen is approach complement with the experimental findings. The molecular modelings are drawn and showed the bond length, bond angle, chemical reactivity, energy components (kcal/mol) and binding energy (kcal/mol) for all the title compounds and also protein for the ligand is shown. The study suggests further investigation on Acetaminophen for their biological activity importance.

**Keywords:** Acetaminophen, UV-Visible, TED, Molecular Docking.

# Abstract for Poster Presentation

## Green synthesis of silver nanoparticles using different volume of *Trichodesma indicum* leaf extract and their antibacterial and photocatalytic activities.

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**Abstract:** By the green synthesis process, silver nanoparticles (Ag NPs) were prepared using *Trichodesma indicum* (*T. indicum*) leaf extract at different (5, 10 and 15 mL) concentrations. The formation of Ag NPs was confirmed by UV–vis spectrophotometer with Surface Plasmon Resonance (SPR) at 443 nm. After this confirmation, influence of leaf extract concentrations on the structural and surface morphological properties was studied. Along with their physical properties, antibacterial activity against pathogenic (*B. cereus* and *E. coli*) bacteria and photocatalytic de-colorization of methylene blue were examined. The XRD studies revealed that all the nanopatricles exhibited preferential orientation along the (111) plane of silver. The crystallite size decreases as the extract concentration is increased. From SEM images, it is found that the particles are spherical in shape and the size of the particles decreased drastically when the leaf extracts concentration is greater than 10 mL. The TEM images strongly support the result observed from the SEM studies. FT-IR analysis showed the plant compounds are involved in reduction of $Ag^{+}$ ions to $Ag^{\circ}$. Ag NPs synthesized at 15 mL leaf extract greatly resist the growth of both species and were decomposed 82 % of MB within 210 min. This ability of Ag NPs can be due to the small spherical shape particles and larger $Ag^{+}$ ion release.

**Keywords:** Green synthesis, *Trichodesma indicum,* Ag NPs, structural studies, antibacterial and photocatalysis.

# Abstract for Poster Presentation

## Reduced Particles Size Enhances The Catalytic And Antibacterial Activities Of Green Synthesized Silver Nanoparticles Using Trichodesmaindicum Leaf Extract

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**Abstract:** By the green synthesis process, silver nanoparticles were prepared using *Trichodesmaindicum* (*T.indicum*) leaf extract at different (5, 10 and 15 mL) concentrations. The formation of Ag NPs was confirmed by UV–vis spectrophotometer withsurface plasmonresonance at 443 nm. After this confirmation, influence of leaf extract concentrations on the structural and surface morphological properties was studied. Along with their physical properties, antibacterial activity against pathogenic (*B.cereus*and *E. coli*) bacteria and photocatalytic de-colorization of methylene blue were examined. The XRD studies revealed that all the nanopatricles exhibited preferential orientation along the (111) plane of silver. The crystallite size decreases with larger dislocation density as the extract concentration is increased. From SEM images it is found that the particles are spherical in shape and the size of the particles decreased drastically when the leaf extracts concentration is greater than 10 mL. The TEM image strongly support the result observed from the SEM studies. FTIR analysis showed the plant compoundsare involved in reduction of $Ag^{+}$ ions to $Ag^{0}$. Ag NPs synthesized at 15 mL leaf extract greatly resist the growth of both species and were decomposed 82 % of MB within 210 min. This ability of Ag NPs can be due to the small spherical shapeparticles and larger $Ag^{+}$ ion release caused by higher dislocation density.

**Keywords:** green synthesis, Ag NPs, structural studies, antibacterial and photocatalysis

# Abstract for Poster Presentation

## STUDIES ON GROWTH, VIBRATIONAL, OPTICAL, MECHANICAL, DIELECTRICAL PROPERTIES OF GZAS SINGLE CRYSTAL

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**Abstract:** Single crystals of Glycine Zinc Chloride Ammonium sulphate (GZAS), a semi organic material has been grown from solution by slow evaporation method at temperature of 303 K. The crystalline nature and its various planes of reflections were observed by the powder XRD. FTIR confirms the presence of functional groups in the grown crystal. The UV-Vis-NIR spectral analysis was recorded to study the optical behavior of GZAS single crystal. Its mechanical hardness was estimated by Vickers microhardness tester. The grown crystal comes under soft material category. The dielectric constant and dielectric loss was measured as a function of frequency for varying temperature. Cole-Cole plot was drawn to characterize the electrical property.

**Keywords:** Crystal growth, Powder XRD, FTIR, Vickers microhardness tester, Cole-Cole plot.

# Abstract for Poster Presentation

## Study of Dc Glow Discharge Plasma on Various Metal Oxide Nano Particles Doped Semiconductor Films

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**Abstract:** The metal oxide Nano particles doped semiconductor films were prepared by sol-gel technique, Dip-coating method. Copper oxide doped with silicon, nickel oxide doped with silicon and tin oxide doped with silicon are the three kinds of nano particles are prepared .The metal oxide nano particles doped with semiconductor film was exposed to DC glow discharge plasma and its optical analysis Ultra Violet visible band gap study, X Ray diffraction method and Weight loss analysis of the plasma treated and untreated films were analysed. Ultra Violet absorption of these films was changed due to the plasma treatment. At the same time, the film had a similar wave length in the visible region (>250 nm) and the absorption value of the plasma treated film was increased when compared to the untreated film. In UV visible band gap study, the optical band gaps were calculated from the absorption spectrum. The band gap energy of the film decreases due to the plasma treatment. In X Ray diffraction method, full width half maximum progressively increased in the treated films when compared to untreated films. From weight loss analysis the rapid removal of low molecular contaminants such as additive processing acids and absorbed species resulting in etching of the surface.

**Keywords:** Dc glow discharge plasma, semiconducting nano particles.

# Abstract for Poster Presentation

## Phase Evaluation, Microscopy, Band Gap and Efficiency of Fe-Doped Nanocrystalline SrMno3 by Microwave Method

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**Abstract:** Pure and Iron (Fe) doped strontium manganate ($Fe_xSr_{1-x}MnO_3$) with x= 0.3 mole ratio were prepared by microwave method and calcinated at 500°C for 2 hours. X-ray analysis (XRD) of the synthesized sample confirmed the major phases to be cubic perovskite structure, crystallite size by Scherrer's formula and planes of orientation of the peaks along directions having minimum energy leading to thermodynamic stability of the phases developed. Absorption due to symmetric and asymmetric stretching of inorganic bond formation for the required coordination was determined by Fourier transform infrared spectroscopy (FTIR). Band gap analyses of the sintered samples were studied by UV-VIS spectroscopy using Tauc plot. Morphological studies were carried out by SEM analysis. Efficiency of the Solar cells was studied and exhibit power conversion efficiency of 11%.

**Keywords:** microwave method, morphology, efficiency

# Abstract for Poster Presentation

## Crystal growth and characterization of potash alum single crystal for optoelectronic devices

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**Abstract:** Single crystal of pure potash alum is grown by slow evaporation technique at room temperature. The crystal structure of grown crystal was confirmed by X-ray diffraction technique. The functional groups present in the crystal were analyzed by FT-IR spectrum. The optical transmittance of the crystals was found in the visible region from 380 nm-1100 nm revealing suitability of potash alum single crystal for opto-electronic devices. Dielectric loss and constant of the grown crystal are also evaluated for different frequencies.

**Keywords:** Single crystal, Potash alum, Optoelectronic

# Abstract for Poster Presentation

## Green Synthesis and Antibacterial Activity of Silver Nanoparticles Using Allium Cepa Extract

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**Abstract:** Green synthesis of silver nanoparticles(AgNPs) using aqueous extract of Allium Cepa by waterbath at 60$^{o}$C. AgNPs size were found by powder X-ray diffraction technique. The various modes of vibrations were identified to confirm the functional groups present in theAgNPs. The optical properties of AgNPs were analysed using UV-Vis and fluresence spectra. The supercapacitance behaviour of the AgNPs were determined from cyclic voltametry method. Antibacterial activity of silvernanoparticles were tested with Gram +ve and Gram -ve bacterium.

**Keywords:** Silver Nanoparticles, XRD, FT-IR,UV-Vis, ANTIBACTERIAL ACTIVITY.

# Abstract for Poster Presentation

## Effect of Picric Acid on Growth, Spectral, Optical and Mechanical Studies of Bisthiourea Lithium Chloride (Btlc) Crystals by Slow Evaporation Method

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**Abstract:** Single crystals of Organometallic Bisthiourea Lithium Chloride (BTLC) have been grown in the presence of picric acid, by adopting slow evaporation method and purity of the crystals have been increased by repeated recrystallization process. Good quality crystals were harvested in a span of 10 days. Different characterization studies have been carried out to find the suitability of the crystal for fabrication of devices. The FTIR study confirms the incorporation of aromatic ring with metal ions through thiourea. From UV-Vis spectral analysis, the transparency window of the crystal observed from 480 nm to1100 nmand the optical band gap was calculated using transmittance data. The mechanical properties of Picric acid doped BTLC crystals were evaluated by Vickers microhardness tester. The Meyer index 'n' is calculated as more than 1.6 which confirms the crystal belongs to the soft material category. The results are discussed in detail.

**Keywords:** Organometallic material, Aromatic ring, FTIR, UV-Vis spectral analysis, Mechanical study.

# Abstract for Poster Presentation

## Studies on the effect of Sodium Chloride on Ammonium Dihydrogen Phosphate Single Crystals

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**Abstract:** Single crystals of pure and 0.5 mol% sodium chloride (NaCl) doped ammonium dihydrogen phosphate (ADP) were grown from aqueous solution by slow evaporation technique at room temperature. The grown crystals were characterized by powder X-ray diffraction (PXRD) and the lattice parameters were calculated. The functional groups present in the grown crystals were confirmed by FTIR studies. The optical transparency of the grown crystals was determined using UV-vis-NIR spectroscopic studies. The mechanical property of the crystals was found out by microhardness measurement.

**Key words**: ADP crystal, slow evaporation technique, PXRD, FTIR, UV-vis-NIR

# Abstract for Poster Presentation

## Synthesis, Characterization and Photocatalytic Activities of Fluorine Doped $TiO_2$ Nanoparticles

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**Abstract:** Titanium dioxide ($TiO_2$) nanoparticles and fluorine doped titanium dioxide (F-$TiO_2$) nanoparticles were successfully synthesized by sol-gel method. The as-synthesized $TiO_2$ and F-$TiO_2$ nanoparticles were calcinated at 500°C for 5 hours. The as-synthesized $TiO_2$ and F-$TiO_2$ nanoparticles were subjected to X-Ray Diffraction spectroscopy (XRD), UV-Visible spectroscopy (UV) studies, Fourier Transform Infrared Spectroscopy (FTIR), Energy Dispersive X-ray Analysis (EDS) and Scanning Electron Microscopy (SEM) studies. The crystallite size of as-synthesized $TiO_2$ and F-$TiO_2$ nanoparticle calculated from the broadening of diffraction peaks using Scherer formula were approximately 19.72 nm and 8.33 nm respectively. FTIR confirms the presence of O-Ti-O stretching vibration in the synthesized samples. UV-Vis study reveals that the band gap of fluorine doped $TiO_2$ is increased and hence it was concluded that the particle size of fluorine doped $TiO_2$ is reduced compared with as-synthesized $TiO_2$. PL studies showed the decrease in PL intensity for fluorine doped $TiO_2$ attributed to the lower recombination rate of electron-hole pair under light irradiation. Thus Fluorine doped $TiO_2$ could be considered as a good candidate for photocatalytic activity. Fluorine doped $TiO_2$ nanoparticles shows higher photocatalytic activity than pure $TiO_2$ nanoparticles which could be attributed to smaller crystalline size, well crystalline phase narrow band gap and intense absorption in the visible light region.

**Key words**: Nanoparticles, Fluorine Doped $TiO_2$, Photocatalytic

# Abstract for Poster Presentation

## Spectral Energy Performance of Pure and Cu Doped Tungsten Oxides for Electro chromic Applications

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**Abstract**: The existence of electrochromic effects among various metal oxide films are as they change their optical transmittance upon charge insertion and extraction. The integration of these materials into multilayer devices suits for optical modulations which are being developed for the application of 'smart' windows that are at the forefront of emerging energy saving advances in civil technologies. Specifically, tungsten oxides are a kind of metal oxides with excellent electrical and optical properties which have been proved as a promising candidate for electrochromic applications. In this paper, we are presenting the better performance of pure and -Cu- doped tungsten oxide thin films on conducting glass plate (ITO) substrate. The structural properties of the prepared thin films are investigated by powder X-ray diffraction studies, annealed at different temperatures. This study reveals that the products are belong to orthorhombic and monoclinic phases, respectively. The optical properties of the thin films are discussed to the operated range. Results from the voltammetry measurements showed the better electrochemical performances at standard conditions and functional groups are analyzed by Raman spectroscopic technique. We also study optical energy performance of the present thin films in the fully bleached, fully colored states and intermediate states. We compare the performance of these thin films with the available low – E windows. All the results supports that the materials have good optical and electrochromic properties with long term durability.

**Keywords:** Tungsten oxide, Microwave irradiation, Cobalt doping, Nanoparticles

# Abstract for Poster Presentation

## Magnetic Behaviour of Chromium Doped Tungsten Oxide ($WO_3$) Nanomaterials

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**Abstract:** Nanocrystalline $WO_3.H_2O$ nanopowders, doped with Chromium (2 and 5 wt%) have been synthesized in a facile microwave irradiation process, followed by the annealing process. The samples were characterized with powder X-ray diffraction, field emission scanning electron microscopy, UV-VIS diffusion reflectance spectroscopy, photoluminescence spectroscopy and cyclic voltammetry (CV). X-ray diffraction patterns showed both undoped and doped $WO_3.H_2O$ crystallized with orthorhombic phase. Annealing h-$WO_3$ at 600˚C 6h in air resulted in the different products, $W_{17}O_{47}$ (monoclinic) for undoped, $WO_3$ orthorhombic for 2 wt% Cr doped and $WO_3$ (monoclinic) for 5 wt% Cr doped. FE-SEM micrographs suggested that the dopants are able to influence the growth rate and morphology of the prepared nanopowders. The difference in peak intensity observed through PL spectra attributed to the possible distortions in $WO_4^{2-}$ tetrahedron group during microwave irradiation process. Electrochemical studies showed the possible enhanced catalytic behavior of doped (5wt.%) as prepared samples than that of others. The temperature dependent magnetic susceptibility (300 K to 2 K) and isothermal magnetization measurements showed the enhancement in magnetic behaviour of the samples for diamagnetic to antiferromagnetic nature which is clearly shows the incorporation of dopants at tungsten lattice site and in determining the resultant magnetic behaviour of the samples.

**Keywords:** Tungsten oxide, Microwave irradiation, doping, Nanoparticles.

# Abstract for Poster Presentation

## Spectral Analysis, Quantum chemical modelling of Light Harvesting Efficiency (LHE) Enhancement on beta-Isosafrole for the Application of Dye Sensitized Solar Cells along with field Variation

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**Abstract:** The structural and several spectroscopic features along with non-linear optical properties of beta-Isosafrole(BIS) studied using experimental techniques and tools derived from the quantum chemical calculations. A complete vibrational and molecular structure analysis has been performed based on the quantum mechanical approach by DFT (B3LYP/B3PW91) calculations. The assignments made at DFT level of theory with only reasonably deviations from the experimental values seem to be correct. The MESP map shows the negative potential sites are on oxygen atoms as well as the positive potential sites are around the hydrogen atoms. The title compound consist of electron-donor and -acceptor/anchoring, connected by the pi-conjugated linker as an electron spacer. Particularly, both electron-donor and pi-conjugated linkers are significant and build impact on the performance of the BIS in the DSSCs. Computational analysis is showed that a BIS with stronger electron donating group enhances the HOMO energy as compared to a weaker electron-donating group. The time-dependent density functional theory (TD-DFT) method is also performed to observe the electronic absorption spectra of BIS. The Natural Bond Orbital (NBO) analysis is also revealed that the origin of charge transfer arises from electron-donating group to electron-withdrawing moiety. Finally the molecular and electronic properties, Fukui indices mulliken charges and thermodynamic properties have also been determined. The present quantum chemical study may lead to the understanding of properties and activity of BIS and may also help in its use for more advance applications with lesser environmental impairment. The computed results propose that the intermolecular charge-transfer mechanism is effective in this D- π -A compound when applied to DSSC.

**Keywords:** BIS, Interaction, DFT, Reactivity descriptors, DSSC

# Abstract for Poster Presentation

## A rapid one-pot synthesis of CuO rice-like nanostructure with enhanced electrochemical performance

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**Abstract:** We report the fabrication of high stable rice-like CuO nanostructures were synthesized by a facile and one step hydrothermal method using urea as a fuel agent. The thermo gravimetric nature, phase purity, morphology, and structure of rice-like CuO nanostructures are characterized by Thermo gravimetric-Differential Thermal Analyzer (TG-DTA), powder X-ray diffraction (PXRD), field emission scanning electron microscopy (FESEM), energy dispersive X-ray spectroscopy (EDS). XRD reveals that formation of monoclinic CuO with an average crystallite size of around 20 nm. FESEM showed the rice-like morphology with an average size of 40-50 and 100-120 nm along the shorter axle and longer axle, respectively. X-ray photoelectron spectroscopy (XPS) and Electron paramagnetic resonance (EPR) spectra confirms that the presence of copper in $Cu^{2+}$ state. Further we have have to use these electrodes for electrochemical supercapacitive properties, like cyclicvoltammetry (CV), galvanostatic charge/discharge (GCD), and electrochemical impedance spectroscopy (EIS).

***Keywords:*** CuO, hydrothermal, optical properties, electrochemical energy storage, pseudocapacitors

# Abstract for Poster Presentation

## Photo Catalytic Properties of Tio2 Nanoparticles for Decorated Multiwall Carbon Nanotubes

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**Abstract:** Titanium oxide ($TiO_2$) nanoparticles were prepared by pyrolysis method. The crystalline size of the nanoparticles have been analysed by x-ray diffraction technique .The arrangement of atoms under different magnification are carries out using FE Scanning Electron Microscopy and Transmission Electron Microscopy method.SEM Image inferred that the nanoparticles are nearly uniform size. This application in the field of decorated multiwall carbon nanotubes are also discussed

**Keywords**: Titanium oxide, Pyrolysis method, decorated multiwall carbon Nano tubes.

# Abstract for Poster Presentation

## $Li^+$ ions doping effect on structural, absorption, emission behavior of ZnO nanoparticles

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**Abstract:** Pure and Li doped ZnO nanoparticles (NPs) ($Zn_{1-X}Li_XO$) were prepared by co-precipitation method. The crystalline phase and incorporations of Li in ZnO host were confirmed from XRD data. The morphological image of prepared NPs was recorded from SEM technique. The absorption behavior of pure and Li doped ZnO was analyzed by UV-Drs spectroscopy measurements. The incorporation effect of Li ions on emission behavior was characterized from PL emission spectroscopy. The presence of lattice defects and dopant ions enhanced PL emissions are observed, the correlations are presented.

**Keywords:** Nanoparticles, ZnO, $Li^+$ ions.

# Abstract for Poster Presentation

## Microstructural Alalysis of ZnO Thin Film by Spray Deposition Method

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**Abstract:** Zinc oxide (ZnO) is one of the most functional oxides with direct band gap. ZnO is a II-IV wide bandgap (3.37 ev) material that exhibits semiconduction, piezoelectric and pyroelectric multiple properties. ZnO thin film is an interesting TCO material due to its high optical transmission and electrical conduction. ZnO thin films were prepared by the spray Pyrolysis method. X-RAY DIFFRACTION studies revealed that the ZnO thin films were crystalline in nature with highly oriented along (O O 2) plane. X-ray line broadening technique is adopted by referring with silicon sample to correct instrumental broadening effect. It is found that grain size for the preferential orientation is about 27nm. SEM analysis revealed formation of particles with different shapes and sizes .the particles have enough activation energy to occupy the sites on the crystal lattice and hence lead to growth in preferential orientation.

**Keywords:** Zinc oxide, XRD, SEM.

# Abstract for Poster Presentation

## Rhodamine B base In Different Solvents Containing β-Cyclodextrin

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**Abstract:** Addition of β-Cyclodextrin to aqueous solutions of rhodamine B base results in the deaggregation of the dye to its monomer form. This is due to the association of monomeric rhodamine B base to the cyclodextrin. The absorption and emission spectra of the aqueous dye solution have been described. This has also been proved by UV-Vis, FTIR and Scanning Eelectron Microscope (SEM). Ground state (Kg ) and excited state (Ke) formation contants have been calculated and reported.

**Keywords:** Rhodamine B base, β-Cyclodextrin, Fluorescence, FTIR.

# Abstract for Poster Presentation

## Enhanced Visible Light Photocatalytic Activity of Pure and Palladium (Pd) doped $SnO_2$ Nanoparticles by a Microwave Route

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**Abstract:** In this paper, we report palladium (Pd) doping induced modifications in the structural, optical and photocatalytic behavior of $SnO_2$ nanoparticles. Powder X-ray diffraction (XRD) and Transmission electron microscope (TEM) studies confirmed that both the pure and Pd doped $SnO_2$ (Pd: 0, 5, 10 wt%) crystallized in tetragonal rutile-type structure with spherical morphology. Furthermore crystallinity is reduced upon Pd doping. The crystallite size decreased from 42 nm to 35 nm and 31 for pure, 5 and 10 wt% Pd doped $SnO_2$ respectively. A noticeable red shift in the absorption edge was found and band gap narrowing in the range of 3.67 – 3.25 eV after doping by Pd. The photoluminescence (PL) emissions observed in the visible region are attributed to the defect levels rising due to oxygen vacancies. The photocatalytic activities of the pure and Pd doped $SnO_2$ samples were evaluated by the degradation of Methylene Blue (MB) Rhodamine B (RHB) in an aqueous solution under visible light irradiation. The photocatalytic activity and reusability of Pd (10 wt%) doped $SnO_2$ was much higher than that of the pure $SnO_2$. The improvement mechanism by Pd doping was also discussed.

**Keywords:** $SnO_2$, Pd doping, Microwave irradiation, Catalyst, Methylene blue, visible light