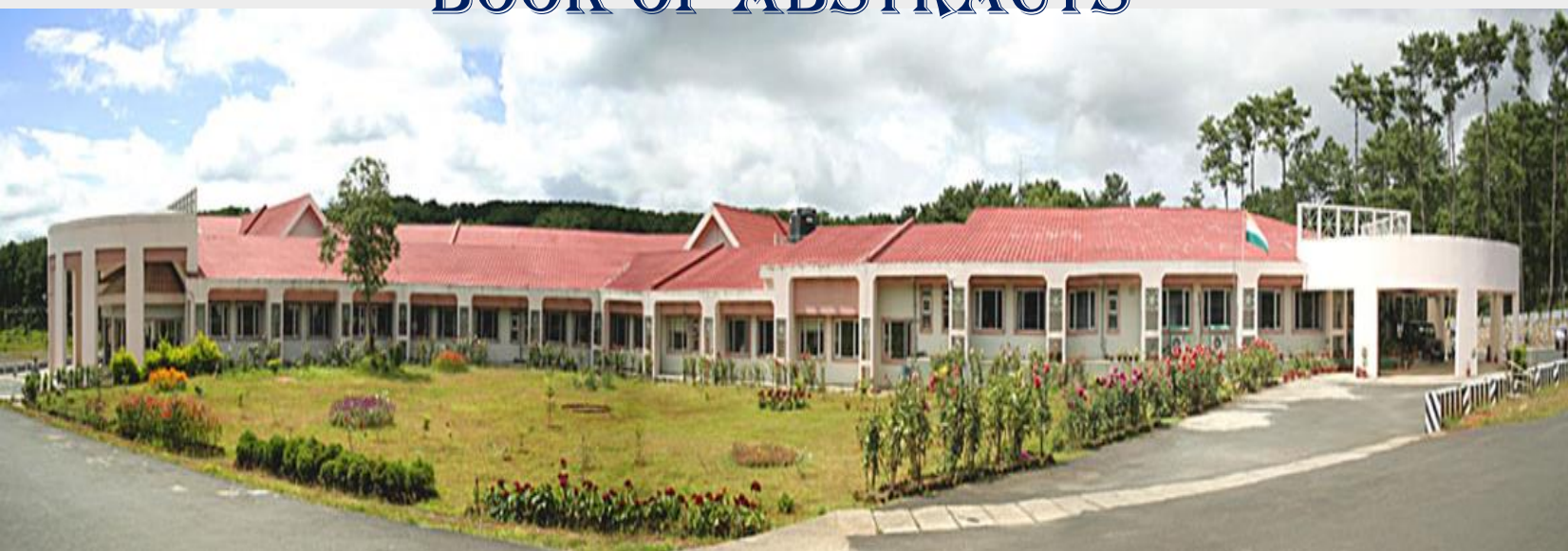




**National Seminar**  
on  
**Contemporary Challenges in Chemistry**  
**(NSC3-2018)**



**BOOK OF ABSTRACTS**



**Organized by:**

**Department of Chemistry, NEHU, Shillong**

*In association with*

**SNBNCBS, Kolkata**

**20-21 November, 2018**  
**NEHU, Shillong**



## BOOK OF ABSTRACTS

**National Seminar**

**on**

***Contemporary Challenges in Chemistry***

***(NSC3-2018)***

*Celebrating 125<sup>th</sup> birth anniversary of  
Prof. S. N. Bose*

***Organized by:***

**Department of Chemistry, NEHU, Shillong**

*In association with*

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**20-21 November, 2018**

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(Jointly organized by the Department of Chemistry, NEHU, Shillong and S N Bose National Center for Basic Sciences, Kolkata)

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**PROGRAMME**

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**November 20, 2018**

**Inauguration: 10:00 – 10.30**

*Tea Break: 10.30 – 11.00 am*

**Session – I**

**11.00 – 11.40 Prof. S. Ghosh (IACS)**

**11.40 – 12.20 Prof. G. Das (IITG)**

**12.20 – 13.00 Prof. S. Adhikari (IACS)**

*Lunch Break: 13.00 – 14.00*

**Session – II**

**14.00 – 14.40 Prof. T. Punniyamurthy (IITG)**

**14.40 – 15.20 Prof. R. Das (WBSU)**

**Outreach program**

**15.30 – 16.30 Life & Work of Prof. S. N. Bose**

*by*

**Prof. Samit Kr. Ray, Director, SNBNCBS**

*Tea Break: 16.30 – 17.00*

**November 21, 2018**

**Session – III**

**9.30 – 10.10 Prof. M. Qureshi (IITG)**

**10.10 – 10.50 Prof. S. Ghosh (JU)**

*Tea Break: 10.50 – 11.15*

**Session – IV**

**11.15 – 11.55 Prof. T. K. Paine (IACS)**

**11.55 – 12.35 Prof. P. Phukan (GU)**

**12.35 – 13.15 Dr. A. Singha Roy (NITM)**

*Lunch Break: 13.15 – 14.00*

**Session – V**

**14.00 – 14.30 Dr. M. Velusamy (NEHU)**

**14.30 – 14.45 Dr. B. Dam (NEHU)**

**14.45 – 15.00 Dr. T. Wagay (NEHU)**

**15.00 – 15.15 Ms. P. Baruah (NEHU)**

**15.15 – 15.30 Mr. B. Sen (NEHU)**

**Poster Session: 15.30 – 16.30**

*Tea Break: 16.30 – 16.45*

**16.45 – 17.00 Valedictory Function**

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**Organizing Committee:** Prof. S. K. Srivastava, Vice-Chancellor, NEHU (Patron);  
Prof. A. K. Chandra (Chairman); Prof. S. Mitra (Convener);  
Prof. G. Bez; Prof. H. Askari; Dr. S. Khatua



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*Invited talks*

- T01 H-bonding Regulated Supramolecular Nanostructures and Impact on Multivalent Binding: **Suhrit Ghosh (IACS)**
- T02 A Multi-Functional Aggregation-Induced Emission (AIE) Active Luminogens Renders Al(III) Sensing and Subsequent Tracking of Interaction with DNA: **Gopal Das (IITG)**
- T03 Beyond Born-Oppenheimer Theories on Molecular Processes and Phase Transitions in Solids: **Satrajit Adhikari (IACS)**
- T04 Regioselective Carbon-Carbon and Carbon-Heteroatom Bond Formation via C-H Functionalization: **Tharmalingam Punniyamurthy (IITG)**
- T05 Photophysics of Molecular Probes: From Supramolecular Assemblies to Interfaces: **Ranjan Das (WBSU)**
- T06 Synthesis and characterization of Gemini surfactant and its interaction with conventional surfactant and polymer: **Soumen Ghosh (JU)**
- T07 Ligand-Field Effects on the Reactivity of Mononuclear Nonheme Iron (IV)-Oxo Complexes: **Tapan Kanti Paine (IACS)**
- T08 Rational design of Nano Functional Materials for Renewable Energy Conversion: **Mohammad Qureshi (IITG)**
- T09 Strategies for the synthesis heterocycles as bioactive targets: **Prodeep Phukan (GU)**
- T10 Study of interactions between bioactive dietary flavonoids and lysozyme: **Atanu Singha Roy (NITM)**
- T11 Dye Sensitized Solar Cells (DSSC) – an overview: **Marappan Velusamy (NEHU)**





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*Oral presentations*

- T12 Graphite oxide: An efficient and reusable carbocatalyst for the syntheses of dihydropyrimidine derivatives: **Binoyargha Dam**, Ramen Jamatia, Ajay Gupta, Amarta Kumar Pal
- T13 Aggregation and adsorption behavior of cis-[Co(dap)<sub>2</sub>(C<sub>12</sub>H<sub>25</sub>NH<sub>2</sub>)<sub>2</sub>](NO<sub>3</sub>)<sub>3</sub> in aqueous sodium nitrate: **Tariq Ahmad Wagay**, Kochi Ismail, Hassan Askari
- T14 Quantifying acetylcholinesterase activity using fluorimetric methods: Dual therapeutic effect of anti-diabetic drugs: **Prayasee Baruah**, Sivaprasad Mitra
- T15 Remarkable Selectivity towards Hypochlorous Acid (HOCl) by a Ru(II) Complex through the C(sp<sup>2</sup>)-H Hydroxylation in a Triazole Pyridine Ligand: Imaging of Endogenous Hypochlorous Acid in Living Cells: **Bhaskar Sen**, Snehadrinarayan Khatua

*Poster presentations*

- P01 Exhibition of various bonding modes of pyrazine azine based ligands towards arene rhodium and iridium complexes: synthesis and biological studies: **Agreedda Lapasam**, Emma Pinder, Roger M Phillips, Mohan Rao Kollipara
- P02 Green approach towards the Synthesis of pyrazoloquinolinones and triazoloquinazolinone derivatives using Nickel nanoparticles as a regioselective catalyst: **Aiborlang Thongni**, Nongthombam Geetmani Singh, Rishanlang Nongkhlaw
- P03 Aggregation and surface properties of cobalt based metallosurfactant in different electrolyte media: **Anushmita Charingia**, Tariq Ahmad Wagay, Hassan Askari
- P04 A novel, efficient and green iron based organo-nanocatalyst in synthesis of spirooxindole derivatives: **Arup Dutta**, Rishanlang Nongkhlaw
- P05 Synthesis of 1,8-dioxo-octahydroxanthenes using CTAB as a catalyst: **Balamphrang Kharrngi**



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**CONTENTS**

- P06 Nickel-Nickel Bonds in Paddlewheel-related Binuclear Nickel Complexes: Some Computational Perspectives: **D. R. Langstieh**, R. H. Duncan Lyngdoh
- P07 Metal-Metal Bond Lengths and Bond Orders (including Quadruple and Quintuple) in Dimanganese Paddlewheel-Type Complexes: A Computational Study: **Fitzerald Hujon**, R. H. Duncan Lyngdoh
- P08 Green and efficient protocol for the synthesis of pyrimido[4,5-b] quinoline-2,4-diones under irradiation of UV365 light: **George Kupar Kharmawlong**, Rishanlang Nongkhlaw
- P09 Ethyl acetate as an acetyl surrogate for the iodine catalyzed acetylation of alcohols : **Grace Basumatary**, Ghanashyam Bez
- P10 COD Removal Studies of Binary Mixture of Dyes in Aqueous solution by Heterogeneous Fenton and Photo-Fenton Processes: **J.E. Kumar**, M.K. Sahoo
- P11 Synthesis and structural studies of arene Ru(II), Cp\*Rh(III) and Cp\*Ir(III) complexes containing benzhydrazone derivative ligands: **Lathewdeipor Shadap**, Kollipara Mohan Rao
- P12 Versatile coordination modes of benzothiazole hydrazone derivatives towards Ru(II), Rh(III) and Ir(III) complexes and their reactivity studies with azides and activated alkynes: **Lincoln Dkhar**, Mohan Rao Kollipara
- P13 Active Tin Mediated Selective Propargylation of Aldehyde in Water at Ambient Temperature: **Micky Lanster Sawkmie**, Dipankar Paul, Paresh Nath Chatterjee
- P14 A New Cyclometalated Iridium(III) Complex of PyridinylimidazoPyridine Ligand with Aggregation Induced Emission (AIE) Characteristics: **Monosh Rabha**, T.Khamrang, M.Velusamy, Snehadrinarayan Khatua
- P15 Graphite Oxide as a Potent Metal-free Carbocatalyst for Synthesis of biologically active 5-Arylidene Rhodanines: **Noimur Rahman**, Rishanlang Nongkhlaw
- P16 Assymmetric synthesis of  $\beta$ -nitroalcohol using N'-Phenyl-N-benzyl Lprolinamide in the presence of copper acetate: **Rahul Mohanta**, Ghanashyam Bez
- P17 Reduced Graphene oxide supported copper oxide nanocomposite: An efficient heterogeneous catalyst for the synthesis of Ynones and 1, 5- diazepines: **Rajib Sarkar**, A. K. Pal



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**CONTENTS**

- P18 Vitamin B1 immobilized on silane-functionalized magnetic nanoparticles as an eco-friendly and efficient catalyst in synthesis of benzo[b]pyran derivatives under ultrasonic irradiation: **Ridaphun Nongrum**, Rishanlang Nongkhlaw
- P19 Intercalation of Ag-Mn(III)Oxyhydroxide in the course of Seed Mediated Growth of Bi<sub>2</sub>Se<sub>3</sub> Disks for High-Rate Capable Symmetric Supercapacitors: **Rishika Chakraborty**, Mukul Pradhan
- P20 G-Quadruplex Selective Ru(II) Complex Based Photoluminescent ‘off-on’ Probe for RNase H Activity Detection: **Sanjoy Kumar Sheet**, Snehadrinarayan Khatua
- P21 Synthesis of Chemically Stable Au-Fe<sub>2</sub>O<sub>3</sub>-Mn<sub>3</sub>O<sub>4</sub> Composite Nanorod through Redox Guided Shape-transformation of Fe<sub>3</sub>O<sub>4</sub> Nanoflake for Highly Efficient Solid-State Symmetric Supercapacitor Device: **Siddheswar Rudra**, Mukul Pradhan
- P22 Mixed Micellar System of Cationic Gemini Surfactant and Conventional Cationic Surfactants: Effects of Chain Length: **Smarling Suting**, Tariq Ahmad Wagay, Hassan Askari
- P23 Biophysical and Computational Explorations of Hemoglobin– Flavonoid Complexes: **Sourav Das**, Atanu Singha Roy
- P24 Thio-Urea based Single Molecular Dual Analyte Probes for Colorimetric Hg<sup>2+</sup> and Fluorometric AcO<sup>-</sup> Detection and Bioimaging: **Sumit Kumar Patra**, Snehadrinarayan Khatua
- P25 Degradation and COD removal studies of Acid Orange 8 in aqueous medium by Fenton process: **Tsungom M**, Mihir Kumar Sahoo
- P26 Photocatalytic Oxidation of L- 3, 4 -dihydroxyphenylalanine using Cadmium Sulfide Nanoparticles: A Case of Catechol Oxidase Mimetic Behaviour: **Wandibahun Warjri**, Dipika Saha, Siewdor Diamai, Devendra P.S. Negi
- P27 Fluorescence modulation and anti-cholinergic activity of substituted chromones in presence of human serum albumin: **Anindita Bhatta**, Mostofa Aatur Rohman, Prayasee Baruah and Sivaprasad Mitra



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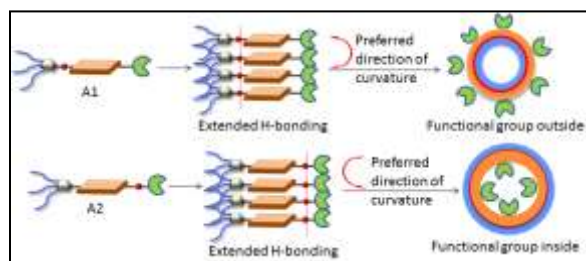
INVITED TALK

**H-bonding Regulated Supramolecular Nanostructures and Impact on Multivalent Binding**

*Suhrit Ghosh*

Professor, School of Applied and Interdisciplinary Sciences, Indian Association for the Cultivation of Science, Kolkata-700032, India, Email: [psusg2@iacs.res.in](mailto:psusg2@iacs.res.in)

It remains a challenging task to control the functional group display at the inner or outer surface of a vesicle at will. Even though it has been attempted using unsymmetric bolaamphiphiles, lack of control in their lateral orientation results in random distribution of the two different hydrophilic head groups in the exo- and endo- wall. We have recently solved this classical problem by H-bonding functional group attached  $\pi$ -Amphiphiles (Scheme 1). Basically, driven by the motivation to form extended H-bonding, both A-1 and A-2 undergo uni-directional orientation and furthermore the propensity of the H-bonded chain to remain at the inner wall implicates display of the functional group attached to the H-bonded arm to converge at the inner wall while the functional group attached with the other arm are displayed at the outer surface. This has been tested with series of unsymmetric bolaamphiphiles having different anionic head groups. Subsequent studies demonstrate the possibilities of precisely tuning the size and surface charge density of such vesicles by systematic variation of the structure of the ionic head groups which was reflected in their ability to inhibit the enzymatic activity of ChT. Most recently, H-bonding regulated functional group display has also been verified by the glycol-cluster effect exhibited by sugar-functionalized similar  $\pi$ -amphiphiles. Hydrazide containing bolaamphiphile produces unsymmetric membrane leading to effective display of the sugar moieties at the vesicular surface which enables much efficient binding with ConA compared to control molecule lacking any H-



bonding group. Interestingly when the hydrazide group was replaced by amide, the amphiphile revealed cylindrical micellar structure which appears to endow even better multivalent effect for interaction with biological targets owing to more adaptable nature of cylindrical structure than vesicle. Highlights of these results will be described in the presentation.

**References :** (1) Sikder, A.; Das, A.; Ghosh, S. *Angew. Chem. Int. Ed.* **2015**, *54*, 6755-6760; (2) Sikder, A.; Ray, D.; Aswal, V. K.; Ghosh, S. *Langmuir* **2018**, *34*, 868-875; (3) Sikder, A.; Sarkar, J.; Sakurai, T.; Seki, S.; Ghosh, S. *Nanoscale* **2018**, *10*, 3272-3280; (4) Sikder, A.; Ray, D.; Aswal, V. K.; Ghosh, S. *Angew. Chem. Int. Ed.* **2018**, DOI: 10.1002/anie.201812217.





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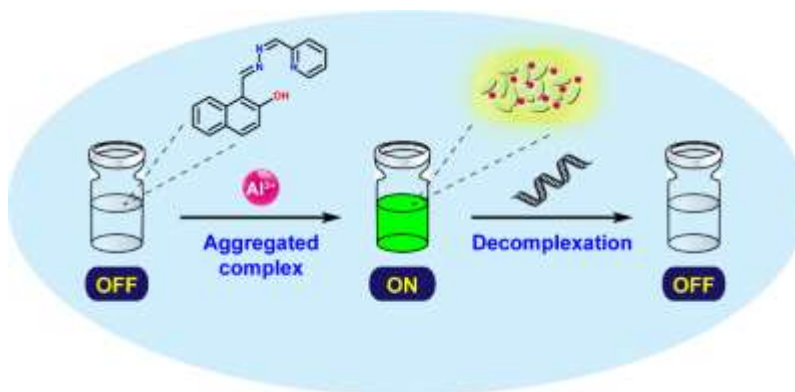
INVITED TALK

**A Multi-Functional Aggregation-Induced Emission (AIE) Active Luminogens Renders Al(III) Sensing and Subsequent Tracking of Interaction with DNA**

*Dr. Gopal Das*

Department of Chemistry, Indian Institute of Technology Guwahati, Assam – 781 039,  
India, E-mail: [gdas@iitg.ac.in](mailto:gdas@iitg.ac.in)

A Multi-Functional Aggregation-Induced Emission (AIE) Active luminogens can selectively sense Al(III) ions in physiological conditions. The sensing behavior of Al(III) is manifested by strong fluorescence and UV/Vis responses. The probe exhibits an aggregation-induced emission (AIE) in presence of excesses Al(III), which is an added advantage for the ion sensing properties. The Probe-Al(III) ensemble could subsequently facilitate tracking of interaction with DNA in solution. The switch ON/OFF behavior of the ligand is also checked inside live human cancer cells (HeLa). Cytotoxic studies of the probe and its complex are also examined towards Human cancer cell lines.



**Reference:** [1] An aggregation-induced emission (AIE) active probe renders Al(III) sensing and tracking of subsequent interaction with DNA. Soham Samanta, Sudeep Goswami, Md. Najbul Hoque, Aiyagari Ramesh and Gopal Das, Chem. Commun., 2014, 50, 11833.



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INVITED TALK

**Beyond Born-Oppenheimer Theories on Molecular Processes and Phase Transitions in Solids**

**Satrajit Adhikari**

Senior Professor of Theoretical Chemistry

School of Chemical Science, Indian Association for the Cultivation of Science, Kolkata-700032,  
India, Email: [pcsa@iacs.res.in](mailto:pcsa@iacs.res.in)

The formulation of beyond Born-Oppenheimer (BBO) methodology is briefly presented from first principle for the construction of diabatic potential energy surfaces (PESs) both for spectroscopic [1-3] ( $\text{Na}_3$ ,  $\text{K}_3$ ,  $\text{NO}_2$ ,  $\text{NO}_3$ ,  $\text{C}_6\text{H}_6^+$  and  $\text{C}_6\text{H}_3\text{F}_3^+$ ) and scattering [4] processes ( $\text{D}^+ + \text{H}_2$ ). Jahn-Teller (JT) and Renner-Teller (RT) types of conical intersections (CIs) along with Pseudo Jahn-Teller (PJT) interactions in those systems and semi-circular CI seam (rather than a CI point) between the ground and first excited states of  $\text{H}_3^+$  system are the new interesting observations. The nuclear dynamics is performed on the diabatic PESs of  $\text{Na}_3$ ,  $\text{NO}_2$  and  $\text{NO}_3$  to calculate the photoelectron spectrum, which matches quite well with the experimentally measured ones. Moreover, we carry out reactive scattering dynamics [4,5] on the diabatic surfaces for  $\text{H}_3^+$  system in hyperspherical coordinates for total angular momentum zero and non-zero situation to reproduce experimental cross sections and rate coefficients for reactive non-charge and charge transfer processes. Optical spectra of  $\text{REMnO}_3$  ( $\text{RE} = \text{La}, \text{Pr}, \text{Nd}, \text{Sm}, \text{Eu}, \text{Gd}, \text{Tb}, \text{Dy}$ ) shows anomalous temperature dependence around the Neel temperature [6]. This behavior could be due to Jahn-Teller effect both in ground and excited state. Such observations have been investigated [7] theoretically to explain the experimental spectra due to the excitations of the quantum rotors.

**References:** [1] S. Mukherjee, S. Bandopadhyay, A. K. Paul, and S. Adhikari, *J. Phys. Chem. A*, **117**, 3475 (2013); [2] S. Mukherjee, B. Mukherjee, S. Sardar, and S. Adhikari, *J. Chem. Phys.*, **143**, 244307 (2015); [3] B. Mukherjee, S. Mukherjee, S. Sardar, K. R. Shamasundar, and S. Adhikari, *Mol. Phys.*, **115**, 2833 (2017); [4] S. Ghosh, S. Mukherjee, B. Mukherjee, S. Mandal, R. Sharma, P. Chaudhury, and S. Adhikari, *J. Chem. Phys.*, **147**, 074105 (2017); [5] S. Ghosh, T. Sahoo, S. Adhikari, R. Sharma, and A. J. C. Varandas, *J. Phys. Chem. A*, **119**, 12392 (2015). [6] N. N. Kovaleva, et. al., *JETP*, **122**, 890 (2016); [7] J. Dutta, N. N. Kovaleva, and S. Adhikari, *J. Chem. Phys.*, (submitted, 2018).



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INVITED TALK

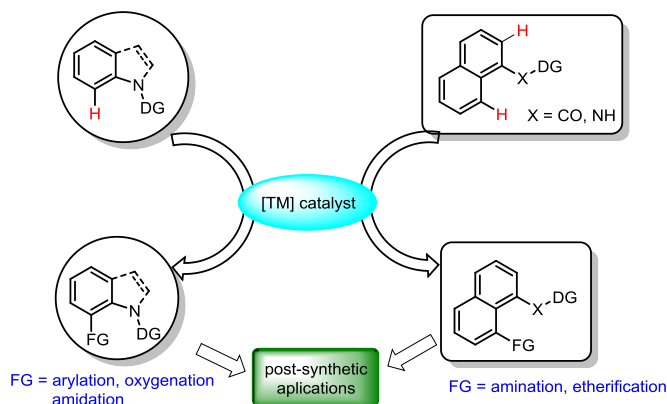
**Regioselective Carbon-Carbon and Carbon-Heteroatom Bond Formation via C-H Functionalization**

**Tharmalingam Punniyamurthy**

Department of Chemistry, Indian Institute of Technology Guwahati

Guwahati 781039 Email: [tpunni@iitg.ac.in](mailto:tpunni@iitg.ac.in)

C-H activation is an important process to transform the simple substrates into complex molecules with structural diversity. However, the selectivity is the major issue in this fundamental transformation when the substrate has more than one C-H bond with similar reactivity. One of the solutions to this problem is try to have functional group five or six bonds away from the C-H that is to be functionalized and use the functional group to chelate with metal catalyst and activate the C-H bond through cyclometation. This concept has attracted considerable attention in the past 10-15 years and considerable progress has been made. In this talk, I shall present our group recent contribution on the directed  $sp^2$  C-H activation and their application of regioselective carbon-carbon and carbon-heteroatom bond formation. The synthetic and mechanistic aspects will be covered.



**References**

1. T. Sarkar, S. Pradhan and T. Punniyamurthy, *J. Org. Chem.* **2018**, 83, 0000.
2. S. Roy, S. Pradhan and T. Punniyamurthy, *Chem. Commun.* **2018**, 54, 3899.
3. P. B. De, S. Pradhan, S. Banerjee and T. Punniyamurthy, *Chem. Commun.* **2018**, 54, 2494.
4. D. Mahesh, V. Satheesh, S. V. Kumar and T. Punniyamurthy, *Org. Lett.* **2017**, 19, 6554.
5. S. Pradhan, P. B. De and T. Punniyamurthy, *J. Org. Chem.* **2017**, 82, 4883.



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**INVITED TALK**

**Photophysics of Molecular Probes: From Supramolecular Assemblies to Interfaces**

***Professor Ranjan Das***

Department of Chemistry, West Bengal State University

Different classes of novel, and common molecular probes have been used to probe organized assemblies, molecular hosts, biomolecular systems and different interfaces. The work unravels (i) modulation of proton transfer dynamics of a 3-hydroxychromone (3HC) based fluorescent dye, and its subsequent application in probing biomolecular interactions (ii) application of a novel fluorescent nucleoside in monitoring nucleic acid structure and dynamics (iii) application of selective oxazole based dyes in probing relaxation dynamics in organized assemblies, molecular hosts and biomolecular recognition (iv) application of novel charge transfer dyes in probing protein-surfactant and lipid-water interfaces, and application of a few well known dyes in probing solvation and molecular recognition of a lipid bilayer under phase transition.





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INVITED TALK

**Synthesis and characterization of Gemini surfactant and its interaction with conventional surfactant and polymer**

*Soumen Ghosh*

Centre for Surface Science, Physical Chemistry Section, Department of Chemistry, Jadavpur University, Kolkata – 700032, India, E-mail: [gsoumen70@hotmail.com](mailto:gsoumen70@hotmail.com)

Gemini surfactants are a special class of surfactants where two monomeric surfactants (two hydrophilic and two hydrophobic groups) are coupled together via a spacer. Gemini surfactants have attracted considerable interest for their various surface-active properties superior to those of corresponding conventional surfactants. Due to the enhanced surface activity, emulsifying property, enzyme inhibiting activity and mildness to skin, this surfactant finds manifold applications in detergent and cosmetic industries. Here, the detailed study of mixed micellization of gemini surfactant with conventional one has been attempted. Regarding this, investigation of interaction of gemini with polymer and protein molecules has also been performed.

**References:**

- 1. S. Ghosh, and T. Chakraborty *J. Phys. Chem. B*, **2007**, *111*, 8080-8088.
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**INVITED TALK**

**Ligand-Field Effects on the Reactivity of Mononuclear  
Nonheme Iron (IV)-Oxo Complexes**

*Tapan Kanti Paine*

School of Chemical Sciences, Indian Association for the Cultivation of Science, 2A & 2B Raja S.  
C. Mullick Road, Jadavpur, Kolkata 700032. E-mail: [ictkp@iacs.res.in](mailto:ictkp@iacs.res.in)

A large variety of iron enzymes activates  $O_2$  to catalyze biologically important oxidation reactions.<sup>[1]</sup> For many of these oxidation reactions, the reductive activation of dioxygen at the reduced iron center leads to the generation of high-valent iron-oxo species as the active oxidant. The characterization of high-spin nonheme iron(IV)-oxo intermediates in taurine  $\alpha$ -ketoglutarate dioxygenase (TauD) and in other nonheme iron oxygenases<sup>[2]</sup> has fueled interest in synthesis and reactivity studies of nonheme iron-oxo complexes. Consequently, many mononuclear nonheme iron(IV)-oxo complexes supported by polydentate ligands have been reported over the last several years.<sup>[3-5]</sup> These complexes display varying degrees of stability and exhibit versatile reactivity such as C-H bond activation and oxo atom transfer reactions. While enzymatic systems involve high-spin ( $S = 2$ ) iron(IV)-oxo oxidants, the majority of the well-characterized synthetic iron(IV)-oxo complexes possess an  $S = 1$  ground spin state. Recently, the isolation and reactivity studies of a few high-spin iron(IV)-oxo complexes have been reported.<sup>[6]</sup> Theoretical calculations suggest that  $S = 2$  iron(IV)-oxo species are more reactive toward C-H bond activation than the  $S = 1$  species;<sup>[7]</sup> which would be an obvious reason for the presence of  $S = 2$  spin state in intermediates for both mononuclear and dinuclear nonheme enzyme sites in contrast to the low-spin form that is found in heme enzymes. To stabilize high-spin iron(IV)-oxo complexes, weak-field supporting ligands are required. Therefore, appropriate design of the supporting ligand is required to tune the stability and reactivity of the resulting iron-oxo complexes.

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**INVITED TALK**

*Continued from the previous page.....*

In that direction, we have been exploring the effect of ligand fields through electronic and structural tuning of polydentate ligands on the reactivity and stability of the corresponding iron(IV)-oxo complexes. As a result of our investigation, we have isolated an iron(II) complex supported by a substituted pentadentate ligand, bis(6-methylpyridin-2-yl)-*N,N*-bis((pyridin-2-yl)methyl)methanamine (N4Py<sup>Me2</sup>).<sup>[8]</sup> While the iron(II)-triflate complex is high-spin in the solid state, it displays temperature-dependent spin crossover in solution. The iron(II) complex reacts with *m*-CPBA in acetonitrile to generate an *S* = 1 metastable iron-oxo species, [Fe<sup>IV</sup>(O)(N4Py<sup>Me2</sup>)]<sup>2+</sup> with a half-life (*t*<sub>1/2</sub>) of 14 min at 298 K. The iron(IV)-oxo is one of the most reactive oxo transfer agents and is capable of oxygenating the relatively strong C-H bonds of aliphatic substrates including that of cyclohexane. The electronic and/or structural factors governing the stability and reactivity of the high-valent iron-oxo oxidant will be presented in the talk.

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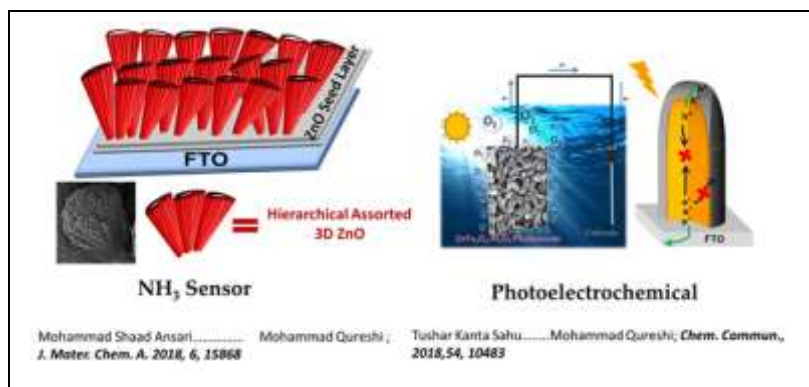
**Rational design of Nano Functional Materials for Renewable Energy Conversion**

**Mohammad Qureshi**

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Email:mq@iitg.ac.in

Major contributors for enhancing the efficacy of the devices involving energy conversion has been explored based on semiconductors which are designed to serve specific purpose. Surface area, carrier transport and electrolyte diffusion are three major issues being addressed through rational design. Better Ohmic contact between the active materials and the collecting electrodes, which are generally transparent conducting oxides plays important role in the devices, where in charge collection is critical in expressing the efficacy of a device. We report the growth of three-dimensional/ one dimensional oxide semiconductors under a controlled hydrothermal route for low Ohmic contact, allowing efficient charge injection. We have successfully demonstrated the applications of the as-characterized multifunctional structures in photovoltaic, photo electrochemical and selective chemical vapor sensing. Improved performance of the device mainly attributed to the larger surface to volume ratio for sensitizer loading; better light-scattering effect, better charge separation and collection at the electrode.



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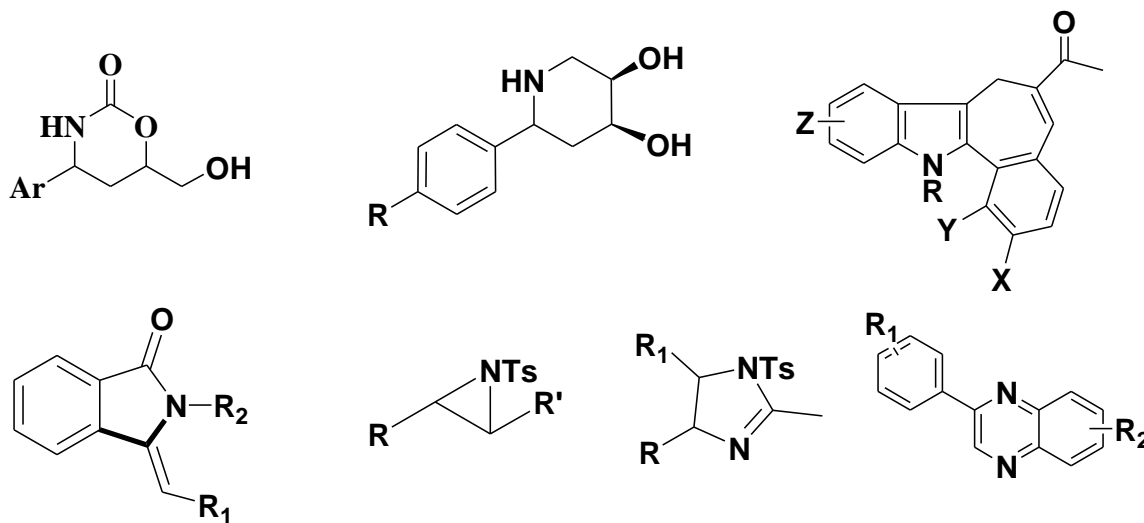
**Strategies for the synthesis heterocycles as bioactive targets**

*Professor Prodeep Phukan*

Department of Chemistry, Gauhati University, Guwahati-781014, Assam

E-mail: [pphukan@yahoo.com](mailto:pphukan@yahoo.com)

Heterocycles are present in a wide variety of natural products, biomolecules, drugs, vitamins and other important compounds of commercial value. Property of such structures can be conveniently tuned further by attaching appropriate functionality. Therefore, considerable attention has been received in recent years to design and develop efficient methods to synthesize new heterocyclic structures. In this presentation we would like to address different synthetic pathways that we have developed for construction of heterocyclic building blocks to achieve bioactive targets.



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**INVITED TALK**

**Study of interactions between bioactive dietary flavonoids and lysozyme**

**Atanu Singha Roy**

Department of Chemistry, NIT Meghalaya, Shillong 793 003

The understanding of protein-ligand interactions (PLI) at molecular level is of fundamental importance in the field of life sciences, clinical biology and pharmaceutical sciences. The information of drug transportation and distribution in correlation with binding mechanism and dynamics can also be elucidated on the basis of PLI. Binding of various ligands with the biological targets have imperative implications in the field of drug delivery and development. Again the specific modes of binding and the consequent removal at the target sites by the carrier protein is a requisite aspect in the field of drug targeting and drug delivery. The distribution and metabolism of many biologically beneficial molecules (e.g. steroids, heme, exogenous drugs, natural products etc.) in the body are directly related to their relative binding affinities toward the carrier proteins. Lysozyme is called the muramidase and has the capacity to bind with a variety of drug molecules. The anti-microbial protein is responsible for diverse physiological and pharmaceutical functions. Hence its interface with the biologically active dietary flavonoids has some significant understanding in the field of transportation and metabolism process of small drug like molecules. The binding of dietary polyphenols with lysozyme have been executed with the help of multi-spectroscopic and molecular docking studies. The intrinsic fluorescence of lysozyme has been quenched in the presences of the ligands (Figure 1) via static quenching mechanism. It has been observed that the binding affinities were moderate ( $10^4$ - $10^5$  M<sup>-1</sup>) in nature and several non-covalent forces are involved in the complexation processes. During binding with the ligands, the structural alteration of lysozyme has also been observed. The enzymatic activity of lysozyme is inhibited in the presences of the flavonoids. Molecular docking studies revealed that the flavonoids bind near to the active site of lysozyme [1-4].

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INVITED TALK

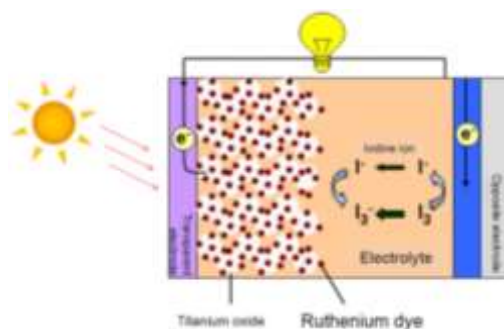
**Dye Sensitized Solar Cells (DSSC) – an overview**

**Marappan Velusamy**

Centre for Advanced Studies in Chemistry, North-Eastern Hill University, Shillong 793022

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Dye-sensitized solar cells (DSSCs), as a new type of photovoltaic technology, have been considered to be a credible alternative to conventional inorganic silicon based (p-n junction) solar cells because of their ease of fabrication, high efficiency, and cost effectiveness. To achieve high solar power conversion efficiency, great research efforts are focused on designing and synthesizing new photosensitizers, electrolytes and electrodes. The role of the dye is similar to the role of chlorophyll in plants; it harvests solar light and transfers the energy via electron transfer to a suitable material to produce electricity as opposed to chemical energy in plants. The highest conversion efficiencies were obtained with a ruthenium complexes of dyes,  $\eta = 13.1\%$  with a cobalt redox electrolyte and  $\eta = 7.5\%$  with a tri-iodide redox electrolyte. The basic principles of the operation of DSCs, factors affecting the efficiency and the state-of-the-art as well as the potentials for future development are described.



**Figure 1.** Working principle of a DSSC.

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**ORAL PRESENTATION**

**Graphite oxide: An efficient and reusable carbocatalyst for the syntheses of dihydropyrimidine derivatives**

*Binoyargha Dam, Ramen Jamatia, Ajay Gupta and Amarta Kumar Pal\**

Department of Chemistry, Centre for Advanced Studies, North-Eastern Hill University, Shillong-793022, Meghalaya

Green chemistry or sustainable chemistry is a philosophy of modern day chemical research and engineering which deals with the development of environment friendly procedures<sup>1</sup> for synthesizing biologically relevant compounds. Now a day, the field of catalysis has emerged as heart of many chemical transformations because it lowers the activation energy and makes the reaction viable. Application of clean and reusable catalytic material is one of the principles of green chemistry.<sup>2-5</sup> Due to high natural abundance of carbon, development of carbon materials as green catalysts is one of the hot topics in modern day research.<sup>6</sup> Significance of graphene in engineering, nanotechnology, and electrochemistry has been documented by the Nobel Prize in the year 2010.<sup>7,8</sup> Herein graphite oxide was synthesized by following modified Hummer's method,<sup>9</sup> characterized by various analytical techniques like FT-IR, PXRD, SEM, HR-TEM, EDX, XPS, TGA and Raman analyses. After characterization it was exploited for the greener metal free syntheses of dihydropyrimidine derivatives under solvent free reaction conditions. Diversity in the formation of these heterocyclic moieties has been exhibited with the tolerance of a large number of functional groups, establishing the generality of this protocol. Present metal free catalytic process abolishes the risk of metal contamination in product which is feasible for pharmaceutical industries. Graphite oxide catalyst is easy to handle, non-corrosive and retained its catalytic activities till nine consecutive runs. Present methodology showed good result under gram scale condition thereby indicating its applicability in academic as well as industries in near future.

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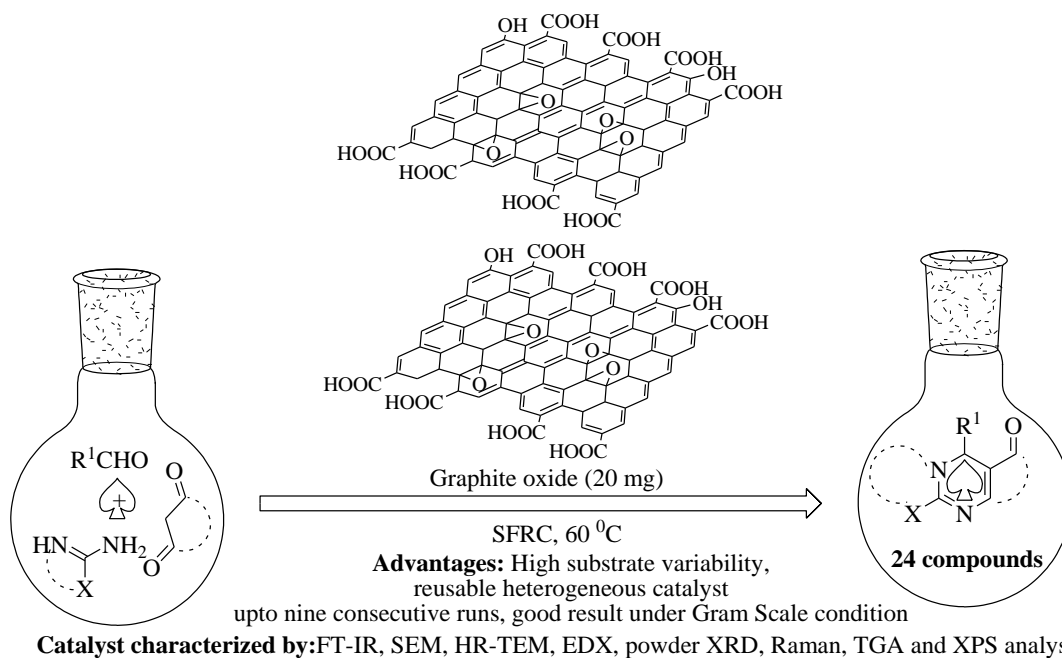
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**ORAL PRESENTATION**

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**ORAL PRESENTATION**

**Aggregation and adsorption behavior of  
*cis*-[Co(dap)<sub>2</sub>(C<sub>12</sub>H<sub>25</sub>NH<sub>2</sub>)<sub>2</sub>](NO<sub>3</sub>)<sub>3</sub> in aqueous sodium nitrate**

*Tariq Ahmad Wagay, Kochi Ismail and Hassan Askari*

Department of Chemistry, Centre for Advanced Studies, North-Eastern Hill University,  
Shillong-793022, Meghalaya

Metallosurfactants are emerging as a new class of materials with a range of properties inherent to both metal complexes and surfactants. Looking at the potential applications of these materials in diverse fields, studying the fundamental aspects of their adsorption and aggregation is necessary. *Cis*-bis(1,3-diaminopropane)bis(dodecylamine)cobalt(III) nitrate (DDCN), *cis*-[Co(dap)<sub>2</sub>(C<sub>12</sub>H<sub>25</sub>NH<sub>2</sub>)<sub>2</sub>](NO<sub>3</sub>)<sub>3</sub> was synthesized and its critical micelle concentration values were determined in aqueous medium as a function of sodium nitrate concentration by using surface tension, conductivity and UV-Visible spectrophotometric methods. Thermal gravimetric analysis showed stability of DDCN up to about 183 °C. DDCN has a salt dependent counterion binding constant, a low value equal to 0.16 becomes more than double (0.43) above 0.025 mol kg<sup>-1</sup> NaNO<sub>3</sub>. The counterion binding constant value of DDCN is however surprisingly low compared to other ionic surfactants. Dynamic light scattering measurements revealed large size aggregates (hydrodynamic diameter = 116 nm with polydispersity index = 0.23) of DDCN which grow even larger on adding NaNO<sub>3</sub>. Small angle neutron scattering measurements also showed presence of large size DDCN aggregates existing probably as micellar clusters. Adsorption behavior of DDCN was assessed by calculating surface excess and area per molecule at the air/water interface.

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ORAL PRESENTATION

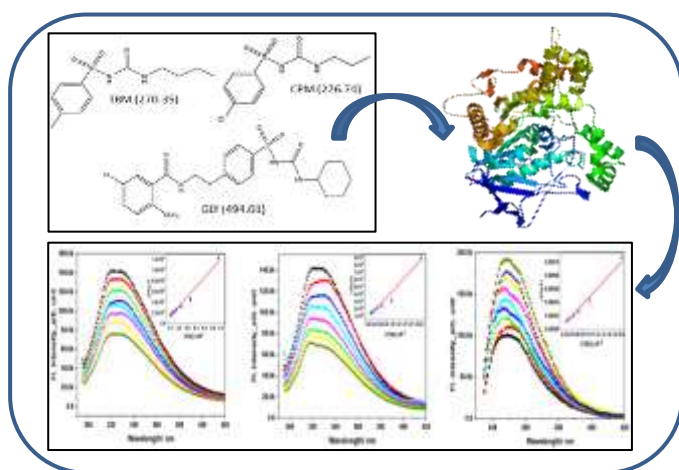
**Quantifying acetylcholinesterase activity using fluorimetric methods:  
Dual therapeutic effect of anti-diabetic drugs**

*Prayasee Baruah, Sivaprasad Mitra*

Centre for Advanced Studies in Chemistry, North-Eastern Hill University, Shillong 793022, India.

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Alzheimer's disease (AD), a chronic and common neurodegenerative disorder characterized by progressive cognitive and neuropsychiatric dysfunction, is the most prevalent form of dementia. The cholinergic hypothesis of Alzheimer's disease deems the deficiency of acetylcholine responsible for memory impairment in AD and places focus on the vital role of the enzyme Acetylcholinesterase (AChE) in the process. AChE hydrolyzes acetylcholine into acetate and choline which triggers the termination of neurotransmission in brain synapses resulting in the malfunction of cognition pattern. Many of the drugs used in the treatment of AD are based on enhancing cholinergic activity by suppressing the activity of AChE.<sup>1,2</sup> Along with the most commonly used Ellman method of enzyme analysis, fluorescence methods have gained an upsurge in recent times for the quantification of the strength, mode and site of binding during inhibition. Tolbutamide ( $IC_{50} = 28.9 \pm 1.60 \mu M$ ), Chlorpropamide ( $IC_{50} = 5.72 \pm 0.24 \mu M$ ) and Glyburide ( $IC_{50} = 0.74 \pm 0.02 \mu M$ ) were three anti-diabetic drugs which, in addition to their normal anti-diabetic activity, exhibited moderate to strong inhibitory effects on AChE. The results obtained from fluorescence studies were in good correlation with the findings from kinetic experiments and



the free energy change for drug-enzyme binding obtained from fluorescence experiments corroborated closely with the results of molecular docking calculations.

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**ORAL PRESENTATION**

**Remarkable Selectivity towards Hypochlorous Acid (HOCl) by a Ru(II) Complex through the C(sp<sup>2</sup>)-H Hydroxylation in a Triazole Pyridine Ligand: Imaging of Endogenous Hypochlorous Acid in Living Cells**

*Bhaskar Sen, Snehadrinarayan Khatua\**

Centre for Advanced Studies, Department of Chemistry, North Eastern Hill University, Shillong, Meghalaya – 793022, India. (snehadri@gmail.com)

The detection and quantification of reactive oxygen species (ROS) in living organism is of great concerned to the researchers because of an excess and abnormal hypochlorite production in living systems has been linked to various types of diseases, such as atherosclerosis, osteoarthritis, rheumatoid arthritis and even cancers.<sup>1</sup> Among the various ROS, hypochlorous acid/hypochlorite (HOCl/ClO<sup>-</sup>) is generated in a regular manner from hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) and chloride ions (Cl<sup>-</sup>) by a heme enzyme, myeloperoxidase (MPO)-catalyzed reaction and responsible to construct immune system in living organisms.<sup>2</sup> Till date, most of the reported HOCl/ClO<sup>-</sup> probes were constructed by introducing signalling unit such as, rhodamine, fluorescein, BODIPY, tetraphenylethylene, pyrene, cyanine, coumarin, fluorescent polymers, MOFs, lanthanide complexes with traditional reacting group such as, spirolactam ring, p-methoxyphenol, phenothiazines, imidazoline-2-thione, sulphur/selenide and oxime moieties.<sup>3</sup> In this regards, luminescent Ru(II) complexes as chemosensors/probes have attracted because of its visible excitation wavelengths and large Stoke's shift, relatively long excited state lifetimes, suitable redox properties and high stability in aqueous media compared with those of pure organic luminophores.<sup>4</sup> Herein, we report a new method for HOCl/ClO<sup>-</sup> detection via C(sp<sup>2</sup>)-H hydroxylation in 1,2,3-triazole pyridine ligand activated by coordinated Ru(II) in **Ru-1** complex. The probe was used to image exogenous as well as endogenous HOCl/ClO<sup>-</sup>, stimulated by LPS and paraquat in HEK293T cells.

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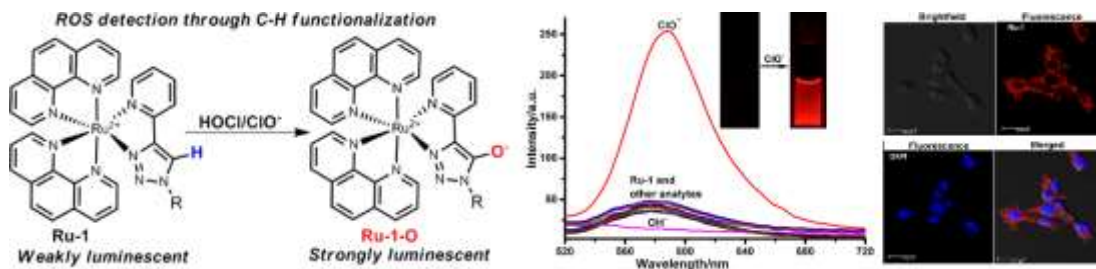
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**ORAL PRESENTATION**

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**Figure 1.** Luminescent detection of HOCl/OCl<sup>-</sup> via C-H functionalization

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POSTER PRESENTATION

**Exhibition of various bonding modes of pyrazine azine based ligands towards arene rhodium and iridium complexes: synthesis and biological studies**

*Agreeda Lapasam<sup>1</sup>, Emma Pinder<sup>2</sup>, Roger M Phillips<sup>2</sup>, Mohan Rao Kollipara<sup>\*1</sup>*

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<sup>2</sup>Department of Pharmacy, School of Applied Sciences, University of Huddersfield, Huddersfield HD1 3DH, UK

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The reaction of multidentate azine ligands was investigated towards Cp\*Rh and Cp\*Ir complexes. The reaction of [Cp\*MCl<sub>2</sub>]<sub>2</sub> (M = Rh and Ir) with azine Schiff-base ligands L1-L2 in different molar ratios led to the formation of mononuclear and dinuclear complexes. The ligands exhibited interesting coordination modes towards the metal atom in dinuclear complexes. In rhodium complexes the ligands behaved as uni-negative tetradentate bridging ligand coordinating both rhodium centers in a bidentate fashion; whereas, in iridium complexes the ligands acts as tridentate bridging manner in which one iridium center coordinate in a bidentate fashion and the other in monodentate fashion. In the mononuclear complexes, the ligands are coordinated to the metal atom in a bidentate N∩N fashion through pyridine nitrogen and azine nitrogen. All these complexes were isolated and characterized by various spectroscopic and analytical techniques. The molecular structures of the representative complexes have been determined by single crystal X-ray diffraction studies. Further the cytotoxicity studies of the ligands and its complexes evaluated against HT-29 (Human Colorectal Adenocarcinoma Cell Line), HCT-116 +/+, HCT-116 -/- (human colorectal cancer), MIA-Ca-P2 (human pancreatic cancer) and ARPE-19 (non-cancer retinal epithelium) cancer cell lines and it showed that the ligands displayed no activity.



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POSTER PRESENTATION

**Green approach towards the Synthesis of pyrazoloquinolinones and triazoloquinazolinone derivatives using Nickel nanoparticles as a regioselective catalyst**

*Aiborlang Thongni, Nongthombam Geetmani Singh and Rishanlang Nongkhlaw\**

Department of Chemistry, North-Eastern Hills University, Shillong, Meghalaya-793022, India.

\*Email: [rlnongkhlaw@nehu.ac.in](mailto:rlnongkhlaw@nehu.ac.in)

Here the synthesis of biologically important pyrazoloquinolinone and triazoloquinazolinone derivatives via the Hantzsch and Biginelli type condensation reaction of 3-amino-1H-1,2,4-triazole/ 3-amino-5-methyl-1H-pyrazole, dimedone and aryl aldehydes was explored. The condensation reaction was carried out under reflux condition using Nickel nanoparticles as a potent eco-friendly catalyst. Because of their unique recyclability, these nano-catalysts can be easily recovered with the help of an external magnet at the end of the reaction. In addition to its easy recovery, the catalyst can be reused for multiple times without losing a significant amount of its catalytic activity or without compromising the yield of the products. This protocol eliminates the usage of many toxic reagents and reduces the complexity of many work-up conditions, which are the main focus in our green approach [1].

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**POSTER PRESENTATION**

**Aggregation and surface properties of cobalt based metallosurfactant in different electrolyte media**

*Anushmita Charingia, Tariq Ahmad Wagay and Hassan Askari*

Department of Chemistry, North-Eastern Hill University, Shillong-793022

Micellization parameters of surfactants are significantly affected by the addition of electrolytes. The influence of added electrolyte on the micellization properties of ionic surfactants is ascribed entirely to the counter ion effect. Metallosurfactants are new class of surfactants that offer interesting alternatives to conventional surfactants because of the range of properties inherent to the metal complex. The study of metallosurfactants has been concentrated mainly on the synthesis aspects and fundamental aspects of adsorption and aggregation behavior of metallo-surfactants are scarce. In view of that point, we have synthesized cis-chlorobis(ethylenediamine)dodecylaminecobalt(III)chloride metallo-surfactants, (CDCC) and characterized by FT-NMR, FT-IR, UV-Vis, FESEM and EDS techniques. The cmc values of CDCC as a function of different electrolyte concentration of sodium chloride, sodium acetate, sodium propionate and sodium butyrate are determined by surface tension, conductivity and spectrophotometric methods. The thermal behavior of CDCC is also studied using TGA technique. The physicochemical parameters of CDCC have been estimated. The size of the metallo-aggregates was measured by Dynamic Light Scattering (DLS) measurements and TEM methods.

**References:**

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- [2] N. Sultana, K. Ismail, *Journal of Molecular Liquids* 213 (2016) 145–152
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National Seminar  
on  
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**POSTER PRESENTATION**

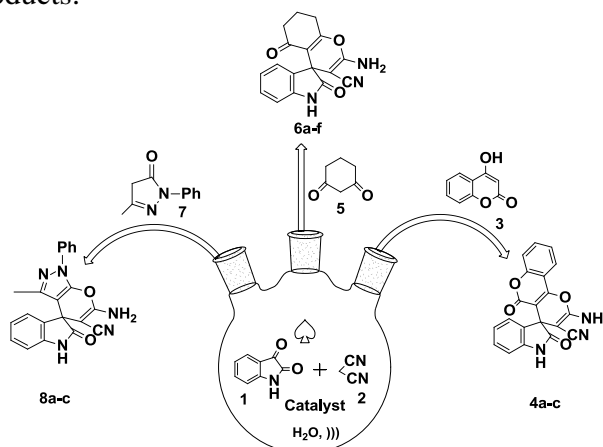
**A novel, efficient and green iron based organo-nanocatalyst in synthesis of spirooxindole derivatives**

*Arup Dutta and Rishanlang Nongkhlaw\**

Department of Chemistry, North-Eastern Hill University, Shillong, Meghalaya-793022, India

\*E-mail: rlnongkhlaw@nehu.ac.in

Of late, organo-nanocatalysis has emerged as a powerful tool in organic synthesis due to its various advantages, especially in terms of catalyst recyclability and reusability [1-2]. Modern synthetic chemists are always in a thirst of developing novel catalysts for improving the synthetic protocols of heterocyclic scaffolds which is a very challenging task. In our present work, *L*-glutamine functionalized iron based nanocatalyst was prepared by encapsulating Fe<sub>2</sub>O<sub>3</sub>@SiO<sub>2</sub> nanoparticles with *L*-glutamine. The catalytic efficiency of the environmentally benign organo-nanocatalyst was exploited for the synthesis of a library of spirooxindole derivatives. The catalyst proved to be highly efficient and was easily retrieved from the reaction mixture by using an external magnet. Also, the catalyst was reused upto six successive runs without compromising any appreciable yield of the products.



**Scheme 1:** Synthesis of spirooxindoles

**References:** [1]. N. Rahman, G. S. Nongthombam, J. W. S. Rani, R. Nongrum, G. K. Kharmawlong and R. Nongkhlaw; *Current Organocatalysis*, **2018**, *5*, 150 – 161; [2]. N. G. Singh, M. Lily, S. P. Devi, N. Rahman, A. Ahmed, A. K. Chandra and R. Nongkhlaw, *Green Chem.*, **2016**, *18*, 4216-4227.





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POSTER PRESENTATION

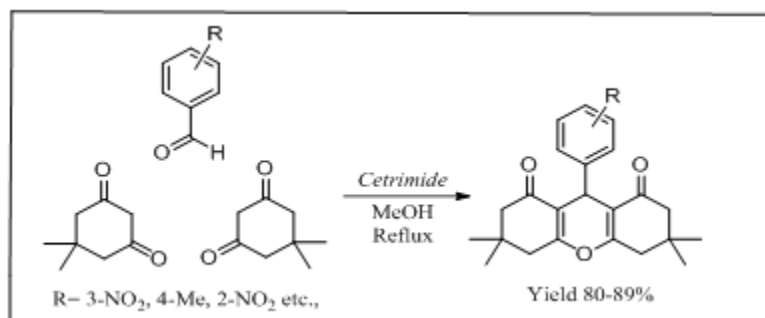
**Synthesis of 1,8-dioxo-octahydroxanthenes using CTAB as a catalyst**

*Balamphrang Kharrngi*

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Email- [b.kharrngi@gmail.com](mailto:b.kharrngi@gmail.com)

Xanthene derivatives have demonstrated anticancer, antiviral, antibacterial, and anti-inflammatory activities besides being used in laser technologies and as fluorescent materials for visualization of biomolecules.<sup>1</sup> Most of the reported methods have used Lewis and Bronsted acids catalysts including their heterogeneous counterpart to affect the synthesis of 1,8-dioxo-octahydroxanthenes starting from the reaction of aldehydes with dimedone. The fact that acid catalysed synthesis often suffers from functional group compatibility issues, low yield is one of the major concerns. In recent years, phase transfer catalyst (PTC) have shown tremendous efficacy to catalyse carbon-carbon bond forming reactions,<sup>2</sup> we planned to screen a series of PTC as catalyst for the synthesis of 1,8-dioxo-octahydroxanthenes. Our study led to development of an efficient method for the



synthesis of 1,8-dioxo-octahydroxanthenes and their derivatives using cetrinide or cetyltrimethylammonium bromide (CTAB), [(C<sub>16</sub>H<sub>33</sub>)N(CH<sub>3</sub>)<sub>3</sub>Br], as a catalyst from aromatic aldehydes and dimedone under reflux condition in methanol.

**Reference:**

1. N.Mulakayala, G. P. Kumar, D. Rambabu, M.Aeluri, M.V. Basaveswara Rao, M Pal. Tetrahedron Lett. 2012, 53, 6923.
2. Oluwayemisi A. Olorode<sup>1</sup>, Emmanuel A Bamigbol, Ofonime M Ogba, Int.J. Pharm. Pharm. Sci.2015, 7, 3.



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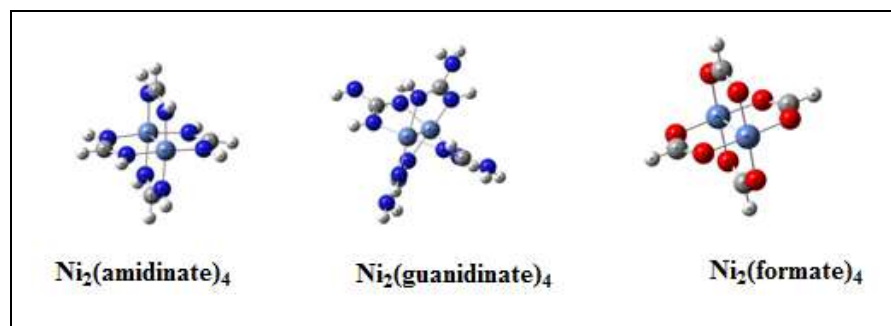
POSTER PRESENTATION

**Nickel-Nickel Bonds in Paddlewheel-related Binuclear Nickel Complexes: Some Computational Perspectives**

*D.R.Langstieh, R.H.DuncanLyngdoh\**

Department of Chemistry, North Eastern Hill University, Shillong 793 022, India

Many binuclear nickel complexes having bimetallic  $(Ni_2)^{+n}$  cores with Ni(0), Ni(I), Ni(II) and Ni(III) centres have been experimentally characterized. Some are of the paddlewheel-related type  $Ni_2L_x$  ( $x = 2, 3, 4$ ) containing monanionic bidentate ligands **L** of the  $(X-CR=Y)^-$  structure ( $X, Y = O, N$ ;  $R =$  carbon or nitrogen group). Experimental Ni-Ni bond lengths in these range from  $x.xxx$  to  $x.xxx$  Å. Unfortunately, binuclear complexes in general do not have formal Ni-Ni bond order values assigned to them, making categorization very challenging. This density functional theory (DFT) study is an attempt to address this issue. The M06-L DFT method with the 6-31G\*\* and LANL2DZ basis sets is used to study three series of dinickelamidinate, guanidinate and formate complexes with digonal, trigonal and tetragonal ligand arrays around the  $(Ni_2)^{+n}$  core, where the three lowest-lying spin states are considered for each case to predict the ground state structure and spin multiplicity. All the Ni-Ni bonds are assigned formal bond order (fBO) values by inspection on the basis of electron counting. These fBO values are compared with the equilibrium Ni-Ni bond distance  $R_{NiNi}$  and the Wiberg bond strength index  $W_{NiNi}$  in each case. It becomes possible to categorize the Ni-Ni bond lengths and  $W_{NiNi}$  index values into distinct ranges as per the Ni-Ni bond



order (fBO) values from 0.5 to 3. The computational results compare well with the limited experimental data available on Ni-Ni bond lengths.

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- [1] Cotton, F. A.; Murillo, C. A.; Walton, R. A. (Eds.). *Multiple Bonds Between Metal Atoms*, 3<sup>rd</sup> Edn. (Springer Science and Business Media, New York, 2005)..
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POSTER PRESENTATION

**Metal-Metal Bond Lengths and Bond Orders (including Quadruple and Quintuple) in Dimanganese Paddlewheel-Type Complexes: A Computational Study**

*Fitzerald Hujon, R. H. Duncan Lyngdoh*

Department of Chemistry, North Eastern Hill University, Shillong – 793 022, India

The metal-metal bonds in dimanganese complexes have been measured by experimental characterization of over 20 such complexes, where the covalent single and multiple Mn-Mn bond lengths range from 2.17 to 2.70 Å. No known dimanganese complexes are known so far of the binuclear paddlewheel type well-known for vanadium, chromium, iron and cobalt. This leads us to explore Mn-Mn bonds in various series of dimanganese paddlewheel complexes containing ligands of the monanionic bidentate (XH-CZ=YH)<sup>-</sup> structure (X, Y = N, O; Z = H, NH<sub>2</sub>) in an array around an (Mn<sub>2</sub>)<sup>+n</sup> core. These ligands include the amidinate, guanidinate, formate and carboxamidate ions. The array may have two, three or four such ligands, yielding, respectively, the digonal planar, trigonal lantern and tetragonal paddlewheel series of complexes. Using the M06-L DFT method with the 6-31+G\*\* and LANL2DZ basis sets, four series of complexes Mn<sub>2</sub>L<sub>x</sub> (L = amidinate, guanidinate, formate and carboxamidate; x = 2, 3, 4) are studied from the point of view of the Mn-Mn bond lengths and bond orders. A variety of spin states are also incorporated in order to predict the ground states for each complex. Mn-Mn bond lengths from 1.757 to 2.840 Å are found, with Mn-Mn bond orders from 1 to 5. Of special note are the super-short quadruple and quintuple Mn-Mn bonds found in some cases, unprecedented experimentally and very rarely predicted theoretically.

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POSTER PRESENTATION

**Green and efficient protocol for the synthesis of pyrimido[4,5-b]quinoline-2,4-diones under irradiation of UV365 light**

*George Kupar Kharmawlong, Rishanlang Nongkhlaw\**

Department of Chemistry, North-Eastern Hill University, Shillong, Meghalaya –  
793022, India

An efficient method have been developed for the synthesis of biologically important pyrimido [4,5 b]quinolinone-2,4-diones[1] from aromatic amines, aryl aldehyde and barbituric acid. The condition for this method was simple and operates at room temperature under direct irradiation of UV<sub>365</sub> in the absence of a photocatalyst [2]. The reaction mixture was made homogeneous by the supply of air bubble continuously for an appropriate time. The product formed was filtered and washed with warm water and then with ethyl acetate to ensure complete removal of impurities and starting material. The purity of the product was confirmed by <sup>1</sup>H-NMR and <sup>13</sup>C-NMR. The reported approach demonstrates several merits such as clean reaction condition, high yield, chromatography-free synthesis and use of cheap water-glycerol solvent system which is also an environment friendly solvent. The applicability of this protocol for large-scale synthesis of pyrimido[4,5-b]quinolinone-2,4-diones without wasting any expensive chemical is an added advantage.

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POSTER PRESENTATION

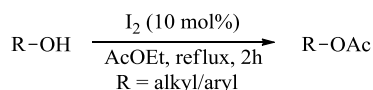
**Ethyl acetate as an acetyl surrogate for the iodine catalyzed acetylation of alcohols**

*Grace Basumatary and Ghanashyam Bez\**

Department of Chemistry, North Eastern Hill University, Shillong-793022, India

Email: [Gracebasu12@gmail.com](mailto:Gracebasu12@gmail.com)

Acetylation of alcohols was carried out by refluxing a solution of alcohol in ethyl acetate in the presence of a catalytic amount of molecular iodine. Amines and phenols hardly undergoes acetylation under our reaction conditions to make the method highly chemoselective. The use of ethyl acetate as acetylating agent in the place of commonly used acetic anhydride,<sup>1</sup> iodine<sup>2</sup> as environmentally benign catalyst, and simple reaction protocol make the protocol very competitive.



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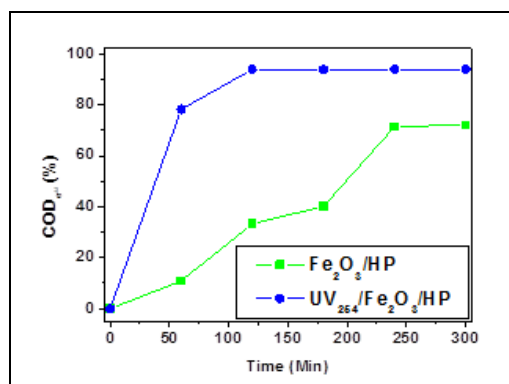
**POSTER PRESENTATION**

**COD Removal Studies of Binary Mixture of Dyes in Aqueous solution  
by Heterogeneous Fenton and Photo-Fenton Processes**

*J.E. Kumar and M.K. Sahoo\**

<sup>a</sup> Centre for Advanced Studies in Chemistry, Department of Chemistry, North-Eastern Hill University, Shillong, Meghalaya - 793022  
[john.elisa90@gmail.com](mailto:john.elisa90@gmail.com); [mksahoo@nehu.ac.in](mailto:mksahoo@nehu.ac.in)

Chemical Oxygen Demand (COD) removal studies of mixture of two azo dyes (PonceauXylidine, PX and Acid Blue 29, AB 29) were carried out by heterogeneous Fenton ( $\text{Fe}_2\text{O}_3/\text{HP}$ ) and Photo-Fenton processes ( $\text{UV}_{254}/\text{Fe}_2\text{O}_3/\text{HP}$ ) using  $\text{Fe}_2\text{O}_3$  and  $\text{H}_2\text{O}_2$  (HP) as heterogeneous catalyst and oxidant respectively for both the processes. The  $\text{Fe}_2\text{O}_3$  nano particles ( $n\text{-Fe}_2\text{O}_3$ ) were synthesized by chemical co-precipitation method [1] and were further characterized by TEM, SEM, VSM, powder XRD Raman spectroscopy and FT-IR. In the initial period the COD removal efficiency ( $\text{COD}_{\text{eff}}$ ) in  $\text{Fe}_2\text{O}_3/\text{HP}$  process was negligible, which reached to a mere 10.8% in 60 min. However, it reached to the value of 72.1% in 300 min at its optimum parameters ( $[\text{Fe}_2\text{O}_3] = 4.0 \text{ g/L}$ ;  $[\text{HP}] = 7.0 \text{ mM}$ ;  $[\text{AB}] = [\text{PX}] = 0.15 \text{ mM}$ ;  $\text{pH} = 3$ ) established in the first part of the experiment. To increase  $\text{COD}_{\text{eff}}$ , the experiment was performed in the presence of UV light ( $\lambda = 254 \text{ nm}$ ) with an intensity of  $0.46 \text{ mW/cm}^2$ , the so called heterogeneous Photo-Fenton process. The impact of UV light can be observed by comparing the  $\text{COD}_{\text{eff}}$  in both the process at 60 min: while it is 10.8% in the former, it is 78.3% in the later (Fig.1). On further increase in treatment period to 120 min,



$\text{COD}_{\text{eff}}$  was increased to 94.0%, which remains constant until 300 min of irradiation. The role played by  $\text{HO}^\bullet$  radicals in the COD removal process was established by using tert-butanol, a known scavenger of hydroxyl radical. The presence of tert-butanol was found to adversely affect the COD removal process.

**Figure1.** Effect of time on  $\text{COD}_{\text{eff}}$  of binary mixture dyes in the heterogeneous Fenton and Photo-Fenton processes:  $[\text{AB}] = [\text{PX}] = 0.15 \text{ mM}$ ;  $[\text{Fe}_2\text{O}_3] = 4.0 \text{ g/L}$ ;  $[\text{HP}] = 7.0 \text{ mM}$ ;  $\text{pH} = 3$ ; light intensity =  $0.46 \text{ mW/cm}^2$ .

**Reference**

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POSTER PRESENTATION

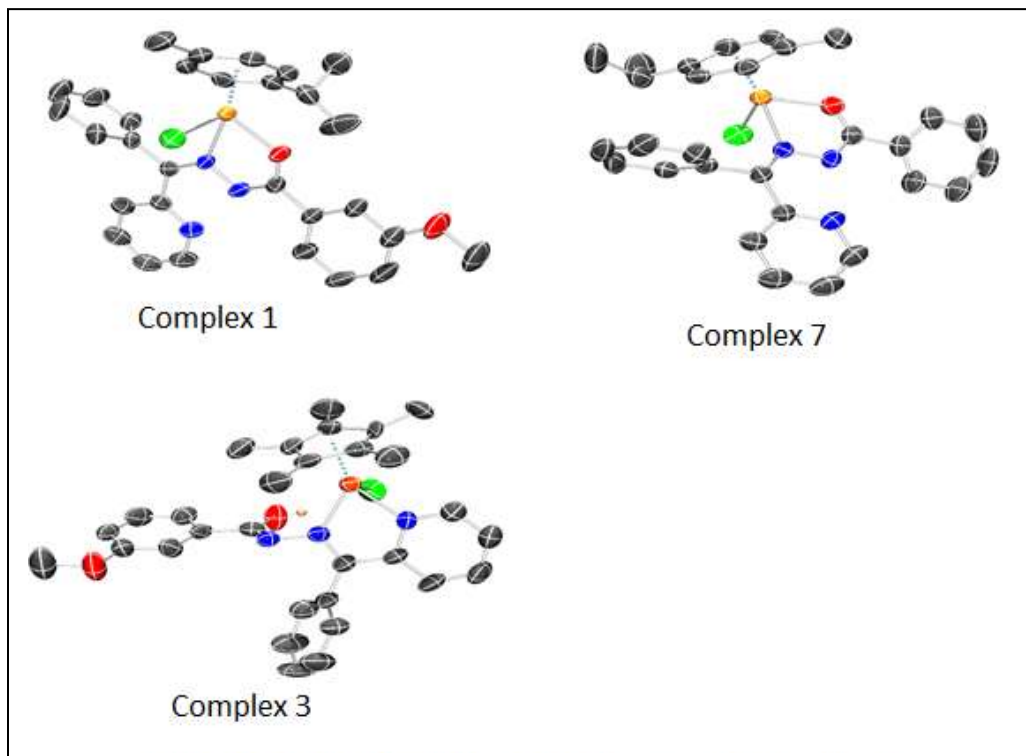
**Synthesis and structural studies of arene Ru(II), Cp\*Rh(III) and Cp\*Ir(III) complexes containing benzhydrazone derivative ligands**

*Lathewdeipor Shadap and Kollipara Mohan Rao\**

*Centre for Advanced Studies in Chemistry, North-Eastern Hill University, Shillong 793022*

E mail: [mohanrao59@gmail.com](mailto:mohanrao59@gmail.com)

Half-sandwich ruthenium, rhodium and iridium complexes were synthesized with benzhydrazone derivative ligands **L1**, **L2** and **L3** by the reaction of [(arene)MCl<sub>2</sub>]<sub>2</sub> (arene = *p*-cymene/Cp\* and M = Ru/Rh/Ir) in methanol in 1:2 (M: L) ratio yielding mononuclear cationic complexes. All these complexes were isolated as PF<sub>6</sub> salts where (arene)M = (*p*-cymene) Ru (**1,4,7**); Cp\*Rh (**2,5,8**) and Cp\*Ir (**3,6,9**) and were characterized by FT-IR, <sup>1</sup>H NMR, UV-Visible, mass spectral studies and X-ray crystallography. X-ray crystallographic studies revealed in the ruthenium complexes, the ligands bind to the metal centre through nitrogen and oxygen atom while in rhodium and iridium complexes the ligands bind through nitrogen atom of the pyridine ring and imine nitrogen.





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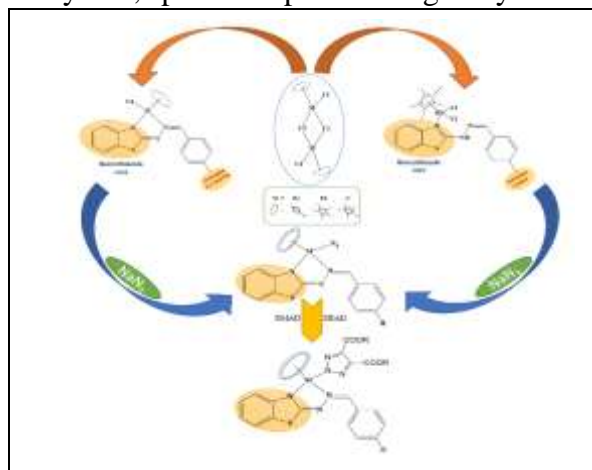
**POSTER PRESENTATION**

**Versatile coordination modes of benzothiazole hydrazone derivatives towards Ru(II), Rh(III) and Ir(III) complexes and their reactivity studies with azides and activated alkynes**

*Lincoln Dkhar, Mohan Rao Kollipara\**

Department of Chemistry North Eastern Hill University Shillong-793022

Metal precursors of the type  $[(p\text{-cymene})\text{RuCl}_2]_2$  and  $[\text{Cp}^*\text{MCl}_2]_2$  (M= Rh/Ir) on reacting with benzothiazole hydrazones ligands (L1, L2 & L3) in the ratio of 1:2 (M:L), leads to the formation of cationic complex  $[(p\text{-cymene})\text{Ru}\{\kappa^2_{(\text{NN}')} \text{L1}\} \text{Cl}] \text{Cl}$  (**1**) and a series of neutral complexes (**2-9**) having the chemical formula  $[\text{Cp}^*\text{Rh}\{\kappa^1_{(\text{N})} \text{L1/L2}\} \text{Cl}_2]$  (**2** and **5**),  $[(p\text{-cymene})\text{Ru}\{\kappa^2_{(\text{NN}')} \text{L2/L3}\} \text{Cl}_2]$  (**4** and **7**),  $[\text{Cp}^*\text{Rh}\{\kappa^1_{(\text{NN}')} \text{L3}\} \text{Cl}]$  (**8**) and  $[\text{Cp}^*\text{Ir}\{\kappa^2_{(\text{NN}')} \text{L}\} \text{Cl}]$  (**3**, **6** and **9**) where L= L1, L2 and L3 respectively. Ligand L1 exhibit different binding modes with metal precursors to yield cationic, neutral mono-dentate and neutral bidentate complexes **1**, **2** and **3** respectively. Ligand L2 binds to Ru and Ir in a bidentate fashion (N, N') where as in the case of Rh it binds only through the benzothiazole nitrogen forming mono-dentate complex. Ligand L3 binds to the metal centres through both the nitrogen atoms of the benzothiazole core and imine forming neutral bidentate (N, N') five membered metallocycle. Complexes of **1**, **2**, **4**, **6**, **7** and **8** were further treated with sodium azide to yield azido compounds. These azido complexes were then reacted with activated acetylenes of dimethyl and diethyl acetylene carboxylates which undergo [3+2] cycloadditions to formed arene ruthenium/rhodiumtriazolato complexes. All these complexes were characterized by analytical, spectroscopic and single crystal x-ray diffraction studies. The molecular structures of all



the complexes revealed the distinctive three-legged structure, resemblance to that of a piano stool having pseudo octahedral geometry around the metal centre. None of the compounds/ligands exhibited anti-bacterial activity towards gram-positive and gram-negative bacteria.

**Figure 1.** Figure showing the reactivity studies of complexes **1-9**.



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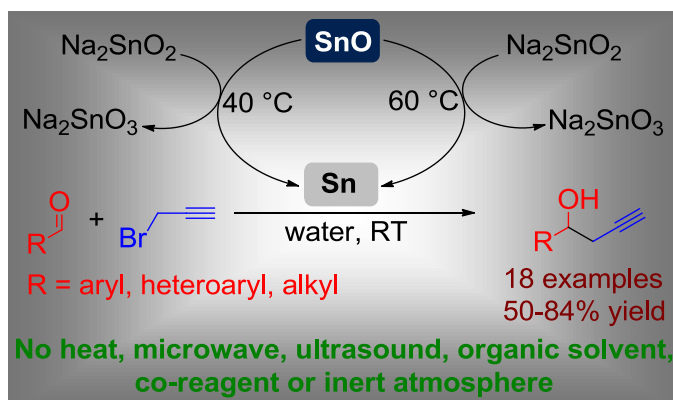
**Active Tin Mediated Selective Propargylation of Aldehyde in Water at Ambient Temperature**

*Micky Lanster Sawkmie, Dipankar Paul, Paresh Nath Chatterjee\**

Department of Chemistry, National Institute of Technology Meghalaya, Shillong-793003, India

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Active Sn(0) particles are synthesized in high yields by the chemical reduction of the blue-black stannous oxide using freshly prepared sodium stannite solution as reducing agent at 40 °C and 60 °C. The Sn(0) particles are characterized using powder XRD, SEM and DSC. The as-synthesized Sn(0) particles are applied as reagent for the regioselective synthesis of homopropargyl alcohols from propargyl bromide and aldehydes in distilled water at room temperature (in 50-84% yields). No assistance of heat, microwave, ultrasound, organic co-solvent, co-reagent or inert atmosphere is required for this reaction. The propargylation reaction is highly chemoselective towards aldehyde over other less electrophilic carbonyl functional groups such as ketone, amide and carboxylic acid. Our in-house synthesized homopropargyl alcohols can be used to synthesize conjugated 1,3-diynes.



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POSTER PRESENTATION

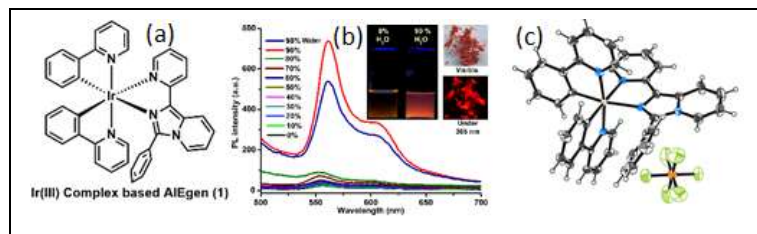
**A New Cyclometalated Iridium(III) Complex of PyridinylimidazoPyridine Ligand with Aggregation Induced-Emission (AIE) Characteristics**

*Monosh Rabha, T.Khamrang, M.Velusamy, Snehadrinarayan Khatua\**

Centre for Advance Studies, Department of Chemistry, North-Eastern Hill University, Shillong, Meghalaya-793022, India. [snehadri@gmail.com](mailto:snehadri@gmail.com)

Development of aggregation induced emission (AIE)-active photoluminescent ruthenium(II) and iridium(III) complexes have attracted increasing attention in inorganic photochemistry.<sup>[1]</sup> CyclometalatedIr(III) complexes with long luminescence lifetime, large Stokes shifts, high quantum yields and versatile colour tuning with simple modifications of the coordinating ligands have been utilised in the fields of organic light-emitting diodes, photoredox catalysis, luminescent probes for biological systems and solar energy harvesting.<sup>[2]</sup> Luminophores with strong emission in the aggregated and solid state have been widely studied as fluorescence “turn-on” or “light-up” molecular and bio-sensors. Therefore, development of well-organized luminescent materials possessing AIE property and solid-state emission is of a great interest not only from a technological perspective, but also in biological science.<sup>[3]</sup>

Herein, we present the synthesis and characterization of new AIE-active cyclometalatedIr(III) complex. The AIE property was supported by UV-vis and PL spectroscopic and DLS studies. The crystal packing clearly shows the anion assisted  $\pi$ - $\pi$  stacking interactions, which restricts the intramolecular motion leading to aggregate formation and inhibition of nonradiative decay from excited state resulting in luminescent enhancement.<sup>[4]</sup> This AIE-active Ir(III) complex can be used as biologically important cell marker or in organelle specific live cell imaging.



**Figure:** (a) Schematic representation of AIE-active Ir(III) complex; (b) AIE in PL spectroscopy of **1** (50  $\mu$ M) in THF-water (0–90%) ( $\lambda_{\text{ex}} = 380$  nm). (Inset) Digital photographs of **1** in 0% and 90% of water in THF under UV (365 nm) illumination and color of crystalline **1** under visible and UV

light (365 nm). (c) ORTEP diagram of complex **1** with 30% thermal ellipsoid probability.

**References:** [1] (a) S. K. Sheet, B. Sen, S. K. Patra, M. Rabha, K. Aguan, S. Khatua, *ACS Appl. Mater. Interfaces*, **2018**, *10*, 14356. (b) S. K. Sheet, B. Sen, K. Aguan, S. Khatua, *Dalton Trans.* **2018**, *47*, 11477. [2] (a) Q. Zhao, F. Li, C. Huang, *Chem. Soc. Rev.* **2010**, *39*, 3007. (b) Q. Zhao, C. Huang, F. Li, *Chem. Soc. Rev.* **2011**, *40*, 2508. [3] L. Ravotto and P. Ceroni, *Coord. Chem. Rev.* **2017**, *346*, 62. [4] J. Mei, N. L. C. Leung, R. T. K. Kwok, J. W. Y. Lam, B. Z. Tang, *Chem. Rev.* **2015**, *115*, 11718.





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POSTER PRESENTATION

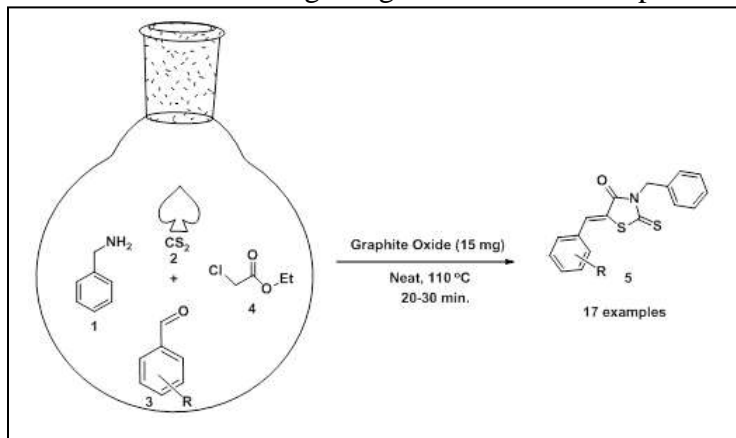
**Graphite Oxide as a Potent Metal-free Carbocatalyst for Synthesis of biologically active 5-Arylidene Rhodanines**

*Noimur Rahman and Rishanlang Nongkhlaw\**

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Development of non-noxious, environment-friendly, cost effective and simple work-up procedures which provide high productivity under mild reaction conditions has been always a matter of interest to synthetic chemists [1-2]. In the present work, we report an improved synthetic approach towards the synthesis of 5-arylidenerhodanines using graphite oxide (GO) as a green, highly efficient and metal free carbocatalyst [3-5]. The reaction was investigated at room temperature as well as at 80°C under solvent free condition. The present catalytic process eliminates the inconvenience of metal waste disposal, metal contamination in the product and metal toxicity which will be of high significance to the pharmaceutical industries. Further, the present



methodology addresses several issues of sustainability and environmental problems like catalyst reusability (six consecutive runs), solvent free reaction condition (SFRC) and also shows high substrate variability.

**Scheme1.** Synthesis of 5-arylidene rhodanines

**References:** [1] Rao, C. N.; Sood, A. K.; Subrahmanyam, K. S.; Govindaraj, A. *Angew. Chem., Int. Ed.*, 2009, **48**, 7752; [2] Hummers, W. S.; Offemann, R. E. *J. Am. Chem. Soc.*, 1958, **80**, 1339; [3] Brodie, C. B. *Ann. Chim. Phys.*, 1860, **59**, 466; [4] Wu, J.; Pisula, W.; Mullen, K. *Chem. Rev.*, 2007, **107**, 718; [5] Li, D.; Kaner, R. B. *Science*, 2008, **320**, 1170



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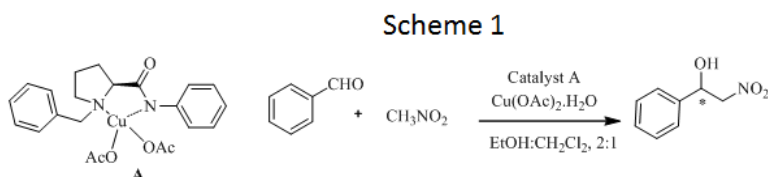
POSTER PRESENTATION

**Assymmetric synthesis of  $\beta$ -nitroalcohol using *N'*-Phenyl-*N*-benzyl L-prolinamide in the presence of copper acetate.**

*Rahul Mohanta and Ghanashyam Bez\**

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The Henry (nitroaldol) reaction is an important carbon–carbon bond forming reaction, which can produce a new stereogenic center at the  $\beta$ -position of the nitro functionality. Since the resulting  $\beta$ -nitro alcohol adducts are valuable synthetic intermediate and useful building blocks for many biological active compounds, much effort has been focused on the development of the asymmetric Henry reactions. A simple, yet highly effective catalyst for asymmetric Henry reaction is developed employing L-Phenyl-*N*-benzylprolinamide in the presence of  $\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$ . Although secondary amine is not ideal to catalyse Henry reaction, to explore the possibility of using secondary amine as a ligand in the presence of  $\text{Cu}(\text{OAc})_2$ , we planned to carry out a reaction of *p*-chlorobenzaldehyde with nitromethane with various ligands besides L-proline.<sup>1,2</sup> Interestingly, catalyst system (catalyst A) gave excellent yields with very good to excellent enantioselectivity (upto >99%) of  $\beta$ -nitroalcohols and requires no base additives unlike many other Cu(II)-complex catalysed Henry reaction.<sup>3</sup> The synthesized catalysts and  $\beta$ -nitroalcohol were characterized by FT-IR, NMR, XRD and Mass spectrometer.



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POSTER PRESENTATION

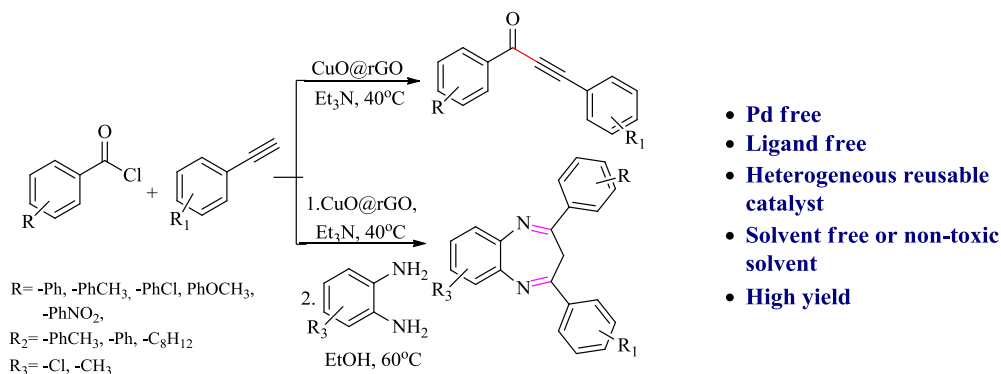
**Reduced Graphene oxide supported copper oxide nanocomposite: An efficient heterogeneous catalyst for the synthesis of Ynones and 1, 5-diazepines**

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An efficient heterogeneous reusable CuO@rGO nanocomposites has been synthesized successfully.<sup>1,2</sup> The formation of the catalyst was then investigated using various techniques such as TEM, SEM, PXRD, XPS, FT-IR, EDX and ICP-OES. The catalyst was then utilized for the synthesis of ynones and subsequently for biologically active 1,5-diazepines in one pot *via* sequential addition of acyl chlorides, terminal alkynes and *o*-phenylenediamines. The methodology initially involves the in situ formation of ynones which react with *o*-phenylenediamines in presence of ethanol to afford wide variety of benzodiazepines. The catalyst can be easily recoverable and reused for several times without much decrease in its catalytic activity.



**Scheme 1:** General scheme for the synthesis of various ynones and 1,5-benzodiazepines.

**References:**

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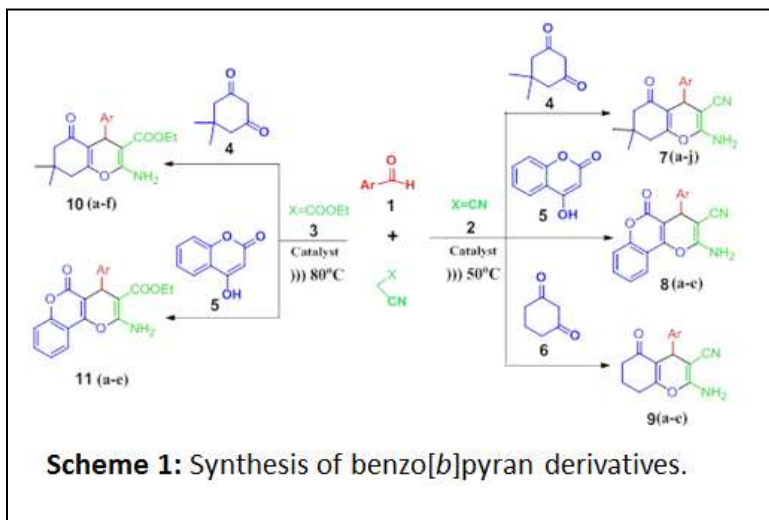
**Vitamin B<sub>1</sub> immobilized on silane-functionalized magnetic nanoparticles as an eco-friendly and efficient catalyst in synthesis of benzo[*b*]pyran derivatives under ultrasonic irradiation**

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In the recent years, organo-nanocatalysis [1-2] has emerged as a powerful synthetic paradigm to synthesize medicinally important organic molecules because of its biodegradability, commercial availability, low toxicity, operational simplicity *etc.* Herein, we report an eco-friendly and efficient multicomponent synthesis of benzo[*b*]pyrans catalyzed by vitamin B<sub>1</sub> immobilized on silane-functionalized magnetic nanoparticles under ultrasonic conditions. The synthesized organo-nanocatalyst was characterized by various analytical techniques and it was exploited in the



synthesis of several classes of benzo[*b*]pyran derivatives with satisfactory yields. The nanocatalyst was magnetically retrievable and could be easily recycled. The notable highlights of this synthetic protocol include simple work-up procedure, mild reaction conditions, easy catalyst recovery and recyclability, shorter reaction times and use of green catalyst and solvents.

**References:** [1]. N. Rahman, G. S. Nongthombam, J. W. S. Rani, R. Nongrum, G. K. Kharmawlong and R. Nongkhlaw; *Current Organocatalysis*, **2018**, 5, 150 – 161.

[2]. N. G. Singh, M. Lily, S. P. Devi, N. Rahman, A. Ahmed, A. K. Chandra and R. Nongkhlaw, *Green Chem.*, **2016**, 18, 4216-4227.



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POSTER PRESENTATION

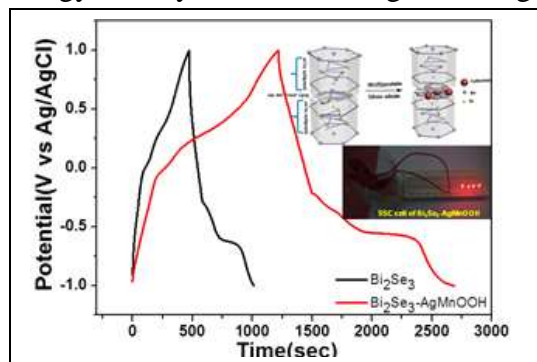
**Intercalation of Ag-Mn(III)Oxyhydroxide in the course of Seed Mediated Growth of Bi<sub>2</sub>Se<sub>3</sub> Disks for High-Rate Capable Symmetric Supercapacitors**

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One of the primary objectives of intercalation chemistry in layered materials is the study of improved electrochemical energy storage performance in supercapacitors. We demonstrate the in-situ intercalation of Ag-MnOOH during seed mediated growth of 2D Bi<sub>2</sub>Se<sub>3</sub> hexagonal nanodisks under controlled reaction environment to give Ag-MnOOH-Bi<sub>2</sub>Se<sub>3</sub> nanocomposite. The as-obtained products have been thoroughly studied by several characterization techniques and a possible growth mechanism based on surface and nucleation controlled chemistry have also been studied. Further, electrochemical measurements were carried out by electrode fabrication in three and symmetric two electrode systems. In addition, we have conducted ex-situ XRD analyses after electrochemical cycling to study structure-electrochemistry relationship. We observed an enhancement in specific capacitance, energy density and power density due to nanocomposite formation, which aids in delivering high-rate retention as a consequence of improved capacitive contribution by intercalation and redox pseudocapacitances. A significant increase in specific capacitance of 734 F g<sup>-1</sup> (three-electrode system) and 146 F g<sup>-1</sup> (two-electrode system) at 1 A g<sup>-1</sup> current density were obtained for Ag-MnOOH-Bi<sub>2</sub>Se<sub>3</sub> nanocomposite compared to bare Bi<sub>2</sub>Se<sub>3</sub> nanodisks, 270 F g<sup>-1</sup> (three-electrode system) at the same current density. In addition, a high energy density of 80.91 Wh kg<sup>-1</sup> at 1 A g<sup>-1</sup> and high power density of 4.99 kW kg<sup>-1</sup> at 10 A g<sup>-1</sup> were



obtained. Thus, by merging the advantages of high-power density and immense charge-storage capacitance behaviour, the designed nanocomposite can be a promising energy-storage material.

Figure: Enhancement of van der Waal's gap of Bi<sub>2</sub>Se<sub>3</sub> host matrix on intercalation of AgMnOOH and its consequent application as a high-performance symmetric supercapacitor.





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POSTER PRESENTATION

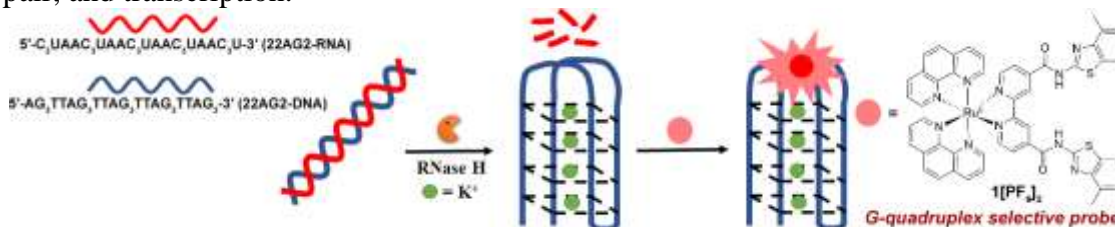
**G-Quadruplex Selective Ru(II) Complex Based Photoluminescent  
'off-on' Probe for RNase H Activity Detection**

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Development of highly selective and sensitive G-quadruplex (GQ) DNA probes have attracted immense attention due to their potential involvement in various biological functions.<sup>1</sup> The GQ DNA architecture is developed as planar motif from four guanine residues combine together *via* Hoogsteen hydrogen bonding and stabilized by metal cations mainly  $K^+$  and  $Na^+$ . GQ sequences forming DNA can be found in telomeres at the ends of chromosomes and in promoter regions of some oncogenes. Identification of GQ DNA by using small molecules become an extremely active area of research for the potential targets in therapeutic intervention. The very rich photophysical properties of luminescent Ru(II) complex such as, long lifetime, large Stokes shift, and tuneable excitation and emission maxima in the visible range has made them perfect candidate for GQ DNA probe.<sup>2</sup> G-quadruplex are applied as a versatile signal transducer for the edifice of label-free detection platforms for environmentally or biologically important analytes. Endolytic nuclease RNase H specifically degrades the RNA strand of a double stranded DNA-RNA hybrid. They involved in numerous important biological processes including DNA replication, DNA repair, and transcription.<sup>3</sup>



Herein we report a bis-heteroleptic Ru(II) complex,  $1[PF_6]_2$  carrying two benzothiazoleamide groups connected to a bipyridine ligand.<sup>4</sup>  $1[PF_6]_2$  demonstrates aggregation caused quenching (ACQ) effect, where the luminescence intensity of  $1[PF_6]_2$  is weakened at higher concentrations or in the aggregated state.  $1[PF_6]_2$  selectively detects GQ DNA over dsDNA and ssDNA. GQ DNA detection ability of  $1[PF_6]_2$  is exploited to established a label-free assay platform for the detection of RNase H activity.

**References:** 1. Bhasikuttan, A. C.; Mohanty, J. *Chem. Commun.* **2015**, *51*, 7581–7597; 2.(a) Khatua, S.; Samanta, D.; Bats, J. W.; Schmittel, M. *Inorg. Chem.* **2012**, *51*, 7075–7086. (b) Sheet, S. K.; Sen, B.; Thounaojam, R.; Aguan, K.; Khatua, S. *Inorg. Chem.* **2017**, *56*, 1249–1263., (c) Sheet, S. K.; Sen, B.; Patra, S. K.; Rabha, M.; Aguan, K.; Khatua, S. *ACS Appl. Mater. Interfaces* **2018**, *10*, 14356–14366; 3. Xia, Y.; Zhang, R.; Wang, Z.; Tian, J.; Chen, X. *Chem. Soc. Rev.* **2017**, *46*, 2824–2843; 4. Khatua, S.; Schmittel, M. *Org. Lett.* **2013**, *15*, 4422–4425.



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POSTER PRESENTATION

**Synthesis of Chemically Stable Au-Fe<sub>2</sub>O<sub>3</sub>-Mn<sub>3</sub>O<sub>4</sub> Composite Nanorod through Redox Guided Shape-transformation of Fe<sub>3</sub>O<sub>4</sub> Nanoflake for Highly Efficient Solid-State Symmetric Supercapacitor Device**

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A facile redox mediated synthetic methodology has been adopted to prepare chemically stable Au-Fe<sub>2</sub>O<sub>3</sub>-Mn<sub>3</sub>O<sub>4</sub> composite nanorod for high-performance supercapacitor application. Pseudocapacitive electrode materials i.e., transition metal oxides, chalcogenides, etc. show poor stability in acidic electrolyte. To overcome the stability concern we have synthesized Au-Fe<sub>2</sub>O<sub>3</sub>-Mn<sub>3</sub>O<sub>4</sub> nanocomposite by a simple redox reaction i.e., the oxidation of Fe<sub>3</sub>O<sub>4</sub> with HAuCl<sub>4</sub> and KMnO<sub>4</sub> solution in a stepwise manner for the first time, which shows excellent stability in acidic electrolyte. Structural and morphological characterisation of the synthesized nanocomposite has been performed in detailed by several experimental techniques (XRD, XPS, IR, Raman, TEM and FESEM etc.). Morphological transformation from Fe<sub>3</sub>O<sub>4</sub> nanoflake to Au-Fe<sub>2</sub>O<sub>3</sub>-Mn<sub>3</sub>O<sub>4</sub> nanorod occurs through dissolution-nucleation-recrystallization growth mechanism has been characterised by FESEM study of the intermediates during the growth process. Electrochemical measurement of the synthesized composite nanorod shows high specific capacitance of 607 F g<sup>-1</sup> at a scan rate of 1 A g<sup>-1</sup> with superior capacity retention at high scan rate (342 F g<sup>-1</sup> at 10 A g<sup>-1</sup>) compared to the mother component Fe<sub>2</sub>O<sub>3</sub> (222 F g<sup>-1</sup> at 1A g<sup>-1</sup> and 67 F g<sup>-1</sup> at 10 A g<sup>-1</sup>) in 0.5 (M) H<sub>2</sub>SO<sub>4</sub> electrolyte within a potential window of 1.2 V. Further, electro kinetic measurements revealed that total charge storage predominantly depends on redox pseudocapacitive (70 % of the total capacitance) along with intercalation pseudocapacitive mechanism (30% of the total capacitance) at scan rate 5 mV s<sup>-1</sup>. The synthesized composite nanorod as an active electrode material for solid-state symmetric supercapacitor device exhibits excellent energy density of 48.71 Whkg<sup>-1</sup> and power density of 4KW

kg<sup>-1</sup> at 1 A g<sup>-1</sup> and 10 A g<sup>-1</sup> current densities respectively. In addition, the composite nanorod as an active electrode material in a solid state symmetric device shows outstanding stability (89%) upto 2000 consecutive charge-discharge cycles at 10 Ag<sup>-1</sup> current densities even in strong acidic electrolyte.

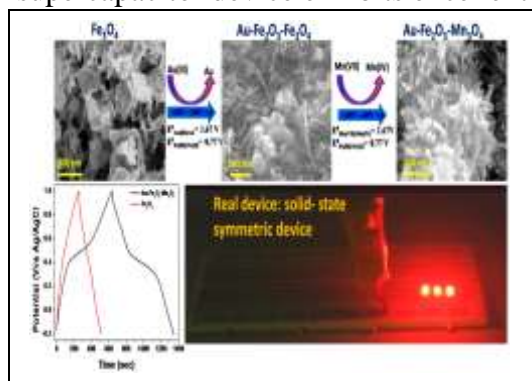


Fig. Synthesis of Au-Fe<sub>2</sub>O<sub>3</sub>-Mn<sub>3</sub>O<sub>4</sub> through shape-transformation for high rate capable symmetric supercapacitor system.



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POSTER PRESENTATION

**Mixed Micellar System of Cationic Gemini Surfactant and Conventional Cationic Surfactants: Effects of Chain Length**

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Mixed micellization and surface properties of cationic Gemini surfactant, bis-N,N-tetradecyldimethyl-m-phenylenediammonium dibromide (14-m- $\phi$ -14), and conventional cationic surfactants, namely, dodecyltrimethylammonium bromide ( $C_{12}$ TAB), tetradecyltrimethylammonium bromide ( $C_{14}$ TAB) and hexadecyltrimethylammonium bromide ( $C_{16}$ TAB) in aqueous medium have been investigated by conductometric, tensiometric, and fluorimetric techniques at 25°C. Clint's and Rubingh's model has been employed to explain the behaviour of the binary mixtures in the light of regular solution theory. The results indicated a non-ideal behaviour which was further confirmed by  $\beta$  values and activity coefficients. The synergism, an attractive interaction, between the surfactant molecules was ascertained and the results showed that the order of the strength of interactions between Gemini and conventional surfactants is  $C_{12}$ TAB >  $C_{14}$ TAB >  $C_{16}$ TAB. The average aggregation number ( $N_{agg}$ ), was evaluated by steady-state fluorescence quenching method. The result suggested that  $N_{agg}$  diminished with increased mole fraction of Gemini surfactant.



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**POSTER PRESENTATION**

**Biophysical and Computational Explorations of Hemoglobin–  
Flavonoid Complexes**

*Sourav Das and Atanu Singha Roy\**

Department of Chemistry, NIT Meghalaya, Shillong 793003, E-mail: souravdas@nitm.ac.in

The binding of small molecules with carrier proteins is an important factor for determining their cellular uptake, transportation, activity, absorption and distribution throughout the circulatory system.<sup>1,2</sup> An accurate understanding of the protein-ligand binding processes in terms of the binding parameters, associated thermodynamic energetics, binding sites and conformational changes is essential for assessing the pharmacokinetics, pharmacodynamics and distribution of the ligands, which are important for designing and developing of new drug molecules in medicinal industries. Flavonoids are the bio-active compounds, known to possess various complementary and alternative medicinal effects that are basically related to their anti-oxidants, anti-cancer and anti-bacterial properties. The distribution of these flavonoids within the body requires the involvement of carrier proteins e.g. hemoglobin, lysozyme, human serum albumin etc. The present work demonstrates the molecular recognition processes of few flavonoids with bovine hemoglobin (BHb) using multi-spectroscopic and computational studies. The flavonoids were found to quench the intrinsic fluorescence of BHb via static quenching mechanism while the binding constant ( $K_b$ ) values were found to be moderate in nature ( $\sim 10^4$ - $10^5$  M<sup>-1</sup>). The alterations in the secondary structure of BHb upon binding with flavonoids were determined with the help of circular dichroism (CD) and fourier-transform infrared spectroscopy (FTIR) measurements. The calculated thermodynamic parameters suggested that different non-covalent binding forces were involved in the interactions of flavonoids with BHb. The flavonoids could inhibit the glucose mediated glycation of BHb. The possibility of energy transfer from the donor (BHb) to the acceptor molecules (flavonoids) was indicated by the FRET studies. Excellent correlations with the experimental studies were observed from the molecular docking and molecular dynamics (MD) simulation studies.<sup>3,4</sup> This study will be helpful in the design of new drug like molecules based on the understanding of protein-drug complexes at molecular level.

**References:** 1) T. Khazaeinia, A. A. Ramsey and Y. K. Tam, *J. Pharm. Pharm. Sci.*, 2000, **3**, 292–302; 2) M. N. Martinez and G. L. Amidon, *J. Clin. Pharmacol.*, 2002, **42**, 620–643; 3) S. Das, A. Karn, R. Sarmah, M. A. Rohman, S. Koley, P. Ghosh and A. Singha Roy, *J. Photochem. Photobiol. B Biol.*, 2018, **178**, 40–52; 4) S. Das, N. Bora, M. A. Rohman, R. Sharma, A. N. Jha and A. Singha Roy, *Phys. Chem. Chem. Phys.*, 2018, **20**, 21668–21684.





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POSTER PRESENTATION

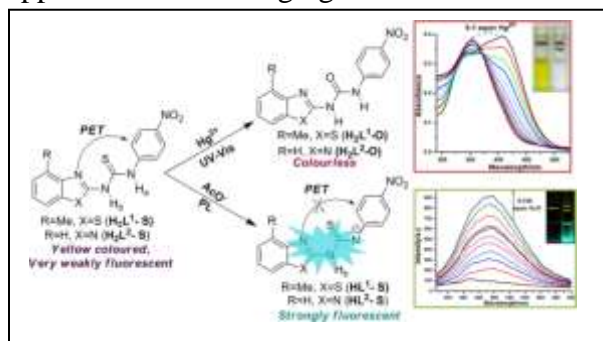
**Thio-Urea based Single Molecular Dual Analyte Probes for Colorimetric  $\text{Hg}^{2+}$  and Fluorometric  $\text{AcO}^-$  Detection and Bioimaging**

*Sumit Kumar Patra and Snehadrinarayan Khatua\**

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Nowadays, the development multi-ion responsive single molecular probe has been attracting a great deal of interest because of its versatility and low cost for practical applications in the environmental and medical fields.<sup>1-3</sup> Among the heavy and transition metal ions,  $\text{Hg}^{2+}$  is one of the most highly potent neurotoxin that leads to many serious human afflictions, such as Minamata, edema and anemia, damage the central nervous system, even a very low concentration.<sup>4</sup> Acetate anion has long been perceived as a crucial cellular molecule for their fundamental role in a wide range of chemical and biological Processes.<sup>5</sup> However till now there is no report of single molecular bifunctional probe for selective detection of two analytes, namely toxic mercury and biologically important acetate anion at two distinct channels through different reaction mechanism.

Herein we present the synthesis of two simple thio-urea based bifunctional probes and their aptness for highly sensitive and selective detection of  $\text{Hg}^{2+}$  and  $\text{AcO}^-$  with two distinct detection methods. These probes selectively detect mercury ion under the UV-vis spectroscopy through the colour change from yellow to colourless associated with a notable blue shift. A distinct fluorescence enhancement is observed only in the presence of  $\text{AcO}^-$  at 493 nm due to the inhibition of photo induced electron transfer (PET). The probes have also low cytotoxicity and are also applied for  $\text{AcO}^-$  imaging in live cells.



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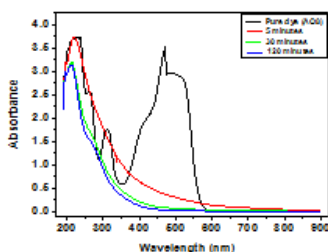
**POSTER PRESENTATION**

**Degradation and COD removal studies of Acid Orange 8 in aqueous medium by Fenton process**

*Tsungom M and Mihir Kumar Sahoo\**

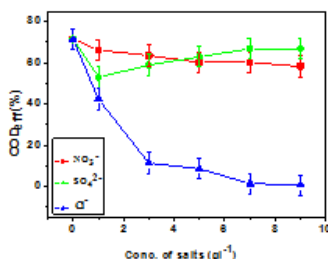
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Degradation and COD removal studies of Acid Orange 8 (AO 8) was carried out by Fenton Process at pH 3 using  $\text{Fe}^{2+}$  as catalyst and  $\text{H}_2\text{O}_2$  (HP) as oxidant. The various optimised operational parameters such as conc. of  $\text{Fe}^{2+}$ , HP, pH etc. for efficient degradation and COD removal efficiency ( $\text{COD}_{\text{eff}}$ ) were found to be:  $[\text{Fe}^{2+}] = 0.3 \text{ mM}$ ;  $[\text{HP}] = 7.0 \text{ mM}$  and pH 3. The  $\text{COD}_{\text{eff}}$  increases from 23.8 to 72.8 % under optimized parameters when we vary the treatment period from 5 to 300 min. It was further observed that the peak at 471 nm decline rapidly with time and no peak was observed at 120 min (Fig 1), thus indicating complete degradation of the dye in 120 min. Thus, it may be inferred that COD removal is a slower process than degradation. The effect of anion such as  $\text{NO}_3^-$ ,  $\text{Cl}^-$  and  $\text{SO}_4^{2-}$  on  $\text{COD}_{\text{eff}}$  were also studied at optimum parameters and it was found that  $\text{COD}_{\text{eff}}$  decreases with an increase in the concentration of  $\text{NO}_3^-$ ,  $\text{Cl}^-$  [1]. However the decreasing effect is more with  $\text{Cl}^-$  than with  $\text{NO}_3^-$ . However, a different trend is observed in the presence of  $\text{SO}_4^{2-}$ . Initially the  $\text{COD}_{\text{eff}}$  decreases to 53% from 71.5% in 120 min of treatment in the presence of  $1.0 \text{ g l}^{-1}$  of  $\text{SO}_4^{2-}$  and on further increase in the concentration of  $\text{SO}_4^{2-}$ , a slow increase in  $\text{COD}_{\text{eff}}$  was observed, i.e the value reached to 66.9% at  $9.0 \text{ g l}^{-1}$  of  $\text{SO}_4^{2-}$  (Fig. 2). Nevertheless, the net effect of  $\text{SO}_4^{2-}$  is retarding. Further, the reactions were carried out in the presence of tert-butyl alcohol, of a known scavenger of  $\text{HO}^\bullet$  radicals. A slow decrease in degradation was observed with increase in the concentration of tert-butyl alcohol and at  $0.7 \text{ mol l}^{-1}$  the degradation was significantly reduced to 10.6 from 99.0% at 90 min of treatment period. This result establishes the role of the  $\text{HO}^\bullet$  radicals in Fenton process [2].



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**Fig.1.** Effect of treatment period on UV-vis spectral changes of AO 8 in  $\text{Fe}^{2+}$  / HP system:  $[\text{AO 8}] = 0.3 \text{ mM}$ ;  $[\text{Fe}^{2+}] = 0.3 \text{ mM}$ ; pH = 3.00.



**Fig.2.** Effect of anions on the  $\text{COD}_{\text{eff}}$  of AO 8:  $[\text{AO 8}] = 0.3 \text{ mM}$ ;  $[\text{Fe}^{2+}] = 0.3 \text{ mM}$ ;  $[\text{HP}] = 7.0 \text{ mM}$ ;  $\text{COD}_0 = 151 \text{ mg/L}$ ;  $\lambda_{\text{max}} = 471 \text{ nm}$ ; Absorbance of pure Dye = 3.542; treatment period = 120 min



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**POSTER PRESENTATION**

**Photocatalytic Oxidation of L- 3, 4 -dihydroxyphenylalanine using Cadmium Sulfide Nanoparticles: A Case of Catechol Oxidase Mimetic Behaviour**

*Wandibahun Warjri, Dipika Saha, Siewdor Diamai and Devendra P.S. Negi*  
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Cadmium sulphide is an attractive visible light photocatalyst since it allows light absorption in the visible region. The photocatalytic activity of cadmium sulfide nanoparticles (CdS NPs) have been evaluated for the oxidation of L-3,4 -dihydroxyphenylalanine (L-Dopa). CdS NPs were synthesized by simple wet chemical approach using sodium hexametaphosphate as a stabilizer. Structural and morphological studies have been done using powder X-ray diffraction (XRD) technique and transmission electron microscopy (TEM). The semiconductor NPs were in the size range of 5-10 nm. The optical property of CdS particles was investigated using the UV-visible absorption spectroscopy and band gap energy of 2.66 eV was evaluated from Tauc plot equation. UV-vis spectroscopy was used to monitor the progress of oxidation of L-Dopa (a diphenol) using CdS NPs as a catalyst under visible light irradiation. The oxidation product of the diphenol was determined by high performance liquid chromatography (HPLC). The results indicated that the substrate L-Dopa had been successfully oxidized leading to the formation of dopachrome. The mechanism of the photocatalytic transformation of L-Dopa to dopachrome suggests the participation of the hydroxyl radicals ( $\cdot\text{OH}$ ) of CdS in the reaction. The formation of hydroxyl radicals ( $\cdot\text{OH}$ ) on the surface of visible-light illuminated CdS NPs was detected by the photoluminescence technique using terephthalic acid as probe molecule. Recently, nanomaterials have been reported to show enzyme mimicking activity, an alternative to natural enzymes. CdS NPs have been suggested to exhibit catechol oxidase like activity and was determined by kinetic analysis employing Michaelis-Menten equation.

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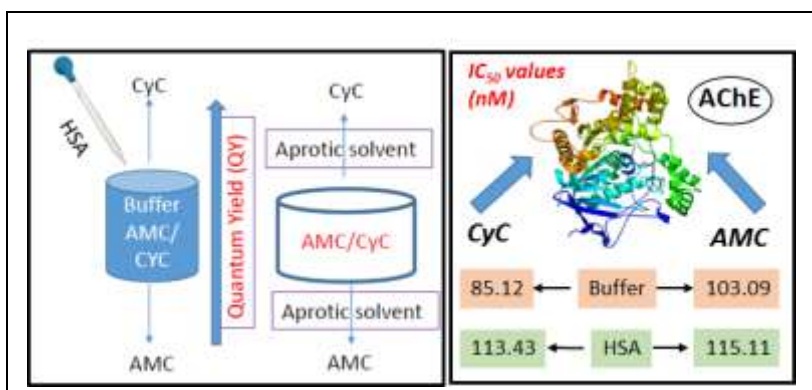
**POSTER PRESENTATION**

**Fluorescence modulation and anti-cholinergic activity of substituted chromones in presence of human serum albumin**

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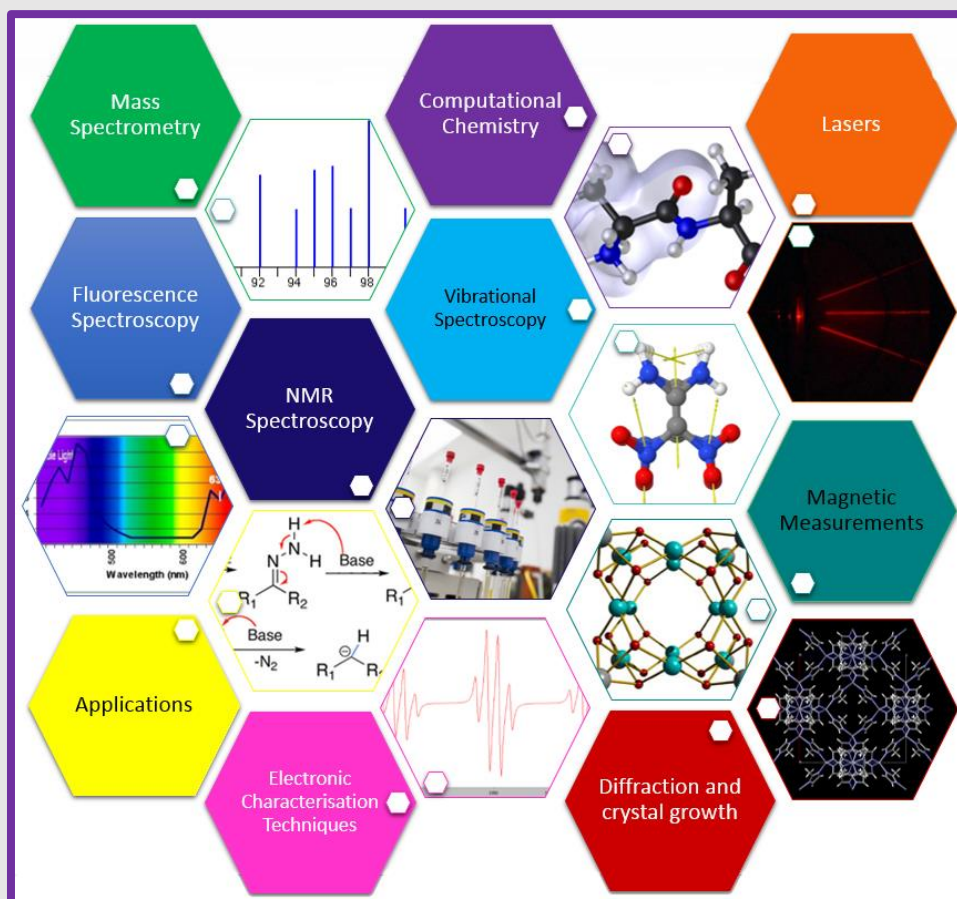
Solvent-dependent photophysical properties of two chromone derivatives, namely 7-amino-2-methyl chromone (AMC) and 3-cyano chromone (CyC), were studied by fluorescence spectroscopy, DFT calculation and MD simulation [1]. Contributions from different solvatochromic parameters were quantitatively estimated using multi-parametric Kamlet-Taft (KT) and Catalán relations. The notable solvatochromic shift in emission peak was estimated for CyC ( $\Delta\lambda=130$  nm) in comparison with AMC ( $\Delta\lambda=53$  nm). The fluorescence emission from both the systems was manipulated by varying the concentration of human serum albumin (HSA) [2]. Both the chromones show significant inhibitory efficiency on acetylcholinesterase (AChE), leading to their use as precursor to potential AD drug. However, substantial difference in  $IC_{50}$  and other kinetic parameters in presence of serum albumin matrix re-emphasize to consider the nature of delivery medium in evaluating drug potency [3].



**Fig. 1.** Diagram showing the modulation in fluorescence behavior and anti-cholinergic activity of AMC and CyC in presence of HSA.

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