1st KIIT CRSI SEMINAR

on

Modern Trends in Chemical Sciences

5th September 2023

PHYSICAL CHEMISTRY

Computational

Dissecting the Molecular Basis of Host Leucine-rich-repeats-containing 15 Mediated Interaction with Receptor Binding Domain of SARS-CoV-2 Spike Protein

Sarbani Mishra, Sanghamitra Pati, Budheswar Dehury*

Department of Biinformatics, ICMR-Regional Medical Research Centre, Chandrasekharpur,
Bhubaneswar-751023, Odisha, India

Email: budheswar.dehury@gmail.com

Abstract: Amid COVID-19 infections, the detection of leucine-rich-repeats-containing 15 (LRRC15),as a connecting link with Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) underscores the possibility of its involvement in differential restriction activity of SARS-CoV-2 pathways[1,2]. However, the structure-function mechanism of LRRC15 involving the receptor binding domain (RBD) of SARS-CoV-2 spike protein and their mode of interaction remains largely unknown. Understanding the dynamics of LRRC15-RBD interaction will aid in achieving critical insights into their molecular binding mechanism and the activity of LRRC15 as an inhibitory attachment factor as well as enhancement factor for modulating SARS-CoV-2 infection[1]. Herein, using state-of-the-art machine-learning approach employed in AlphaFold2 and all-atoms molecular dynamics (MD) simulations, we provide evidences of alternative binding modes of RBD with LRR units of LRRC15 having varied affinities for the first time. Contribution of both the receptor binding regions in RBD, including receptor binding motif in accommodating the LRR domain, towards the C-terminal region, emphasizes over its differential role in modulating host cell receptiveness for SARS-CoV-2, innate immune system as well as antiviral tone. Our findings further highlight the critical role of Arg326 (LRR-12), Glu345 (LRR-13), and Arg376 (LRR-14) residues of LRRC15 in formation of stable complexes with RBD. However, further experimental validations are necessary for unravelling the unknown mechanism and distinctive features of this host cell receptor in COVID-19 pandemic, involving both the transmembrane as well as cytoplasmic domain.

Keywords: horse-shoe; LRRC15; Severe Acute Respiratory Syndrome Coronavirus 2; spike protein

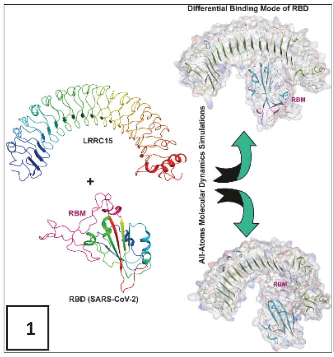


Figure 1: Understanding of the structural basis of host LRRC15 mediated interaction with the receptor binding domain (RBD) of SARS-CoV-2 S-protein is of immense importance in unveiling the multi-functionality of LRRC15 i.e., both as a modulator and inhibitor of SARS-CoV-2.

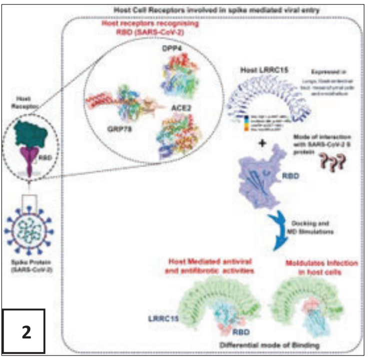


Figure 2: Schematic representation of investigation of the plausible mode of host mediated LRRC15 interaction with RBD through different computational approaches.

References and Notes:

1. J. Shilts, T.W.M. Crozier, A. Teixeira-Silva, I. Gabaev, P.P. Gerber, E.J.D. Greenwood, S.J. Watson, B.M. Ortmann, C.M. Gawden-Bone, T. Pauzaite, M. Hoffmann, J.A. Nathan, S. Pöhlmann, N.J. Matheson, P.J. Lehner, G.J. Wright, LRRC15 mediates an accessory interaction with the SARS-CoV-2 spike protein, PLoS Biol. 21 (2023) 1–28. https://doi.org/10.1371/journal.pbio.3001959.
2. J. Song, R.D. Chow, M.A. Peña-Hernández, L. Zhang, S.A. Loeb, E.Y. So, O.D. Liang, P. Ren, S. Chen, C.B. Wilen, S. Lee, LRRC15 inhibits SARS-CoV-2 cellular entry in trans, PLoS Biol. 20 (2022). https://doi.org/10.1371/journal.pbio.3001805.

Hydrogen Bonding Directed Reversal of ^{13}C NMR Chemical Shielding

Subhrakant Jena, Himansu Sekhar Biswal*

School of Chemical Sciences, National Institute of Science Education and Research (NISER), Bhimpur-Padanpur, Via-Jatni, District, Khurda, 752050, Bhubaneswar, India; Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, India

(E-mail: subhrakant.jena@niser.ac.in, himansu@niser.ac.in)

Abstract: He deshielding or downfield 13C NMR chemical shift of amide carbonyl carbon upon H-bonding is a widely observed phenomenon. This downfield chemical shift is commonly used as a spectroscopic ruler to acquire local environment information such as hydrogen bond strength, micro solvation, electrostatics, and polarity. In this poster, I shall discuss regarding the very first observation of an upfield 13C NMR of thiocarbonyl carbon in thioamides upon H-bonding. The solution phase NMR observations corroborated with various computational calculations explains the physical origin of the reversal of 13C NMR chemical shielding. Further analysis shows that sulfur and selenium-centered H-bonds (S/SeCHBs) induce a shielding effect on the 13CC=S(Se) while changing from amides to thioamides or selenoamides. In addition, natural chemical shielding (NCS) analysis shows that the σ11 and σ22 components of the isotropic shielding tensor (σ) have a crucial role in this unusual shielding. We expect this new finding will encourage other researchers to explore magnetic shielding and deshielding properties of other NCIs commonly observed in chalcogen chemistry.

References and Notes:

1. S. Jena, C. Routray, J. Dutta, H. S. Biswal, *Angew. Chem. Int. Ed.* **2022**, *61*, e202207521

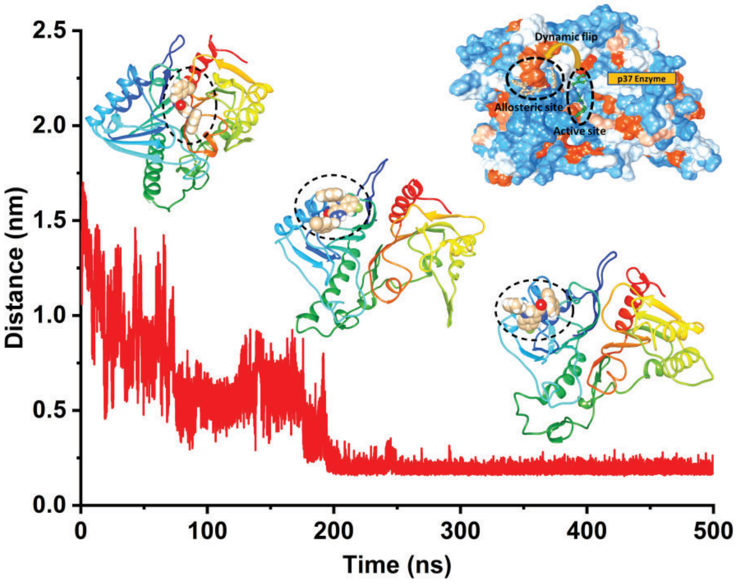
Identification and Investigation of a Cryptic Binding Pocket of the P37 Envelope Protein of Monkeypox Virus by Molecular Dynamics Simulations

Saroj Kumar Panda, Parth Sarthi Sen Gupta, Abhijit Kumar Nayak, and Malay Kumar Rana*

Department of Chemistry, Indian Institute of Science Education and Research (IISER), Berhampur, Odisha, 760010, India

(E-mail: mrana@iiserbpr.ac.in)

Abstract: The spread of the monkeypox virus has surged during the unchecked COVID-19 epidemic. The most crucial target is the viral envelope protein, p37. However, lacking p37's crystal structure is a significant hurdle to rapid therapeutic discovery and mechanism elucidation. Structural modeling and molecular dynamics (MD) of the enzyme with inhibitors reveal a cryptic pocket occluded in the unbound structure. For the first time, the inhibitor's dynamic flip from the active to the cryptic site enlightens p37's allosteric site, which squeezes the active site, impairing its function. A large force is needed for inhibitor dissociation from the allosteric site, ushering in its biological importance. In addition, hotspot residues identified at both locations and discovered drugs more potent than tecovirimat may enable even more robust inhibitor designs against p37 and accelerate the development of monkeypox therapies.



References and Notes:

1. Gupta, P.S.S.^{1}; Panda, S.K.^{1}; Nayak, A.K.; and Rana, M.K., *J. Phys. Chem. Lett.* **2023,** *14*(13), 3230-3235.

Two distinct mode of ligand recognition by extra-cellular domain of TREM2: Insights from all-atoms molecular dynamics simulations

Preety Sthutika Swain, Sarbani Mishra, Budheswar Dehury*

Bioinformatics Division, ICMR-regional Medical Research Centre, Chandrasekharpur,
Bhubaneswar-751023, Odisha, India

Email: budheswar.dehury@gmail.com

Abstract: Triggering receptors expressed on myeloid cells also known as TREMs, are class I receptors expressed on microglial cells in brain are important players in transmission of signals for activation of cells linked to neurodegenerative disorders. Among these TREMs, the extra cellular domain (ECD) of TREM2 plays a decisive role in neurodegenerative diseases such as Alzheimer's disease (AD) and Nasu Hakola disease (NHD) [1]. TREM2 ECD interacts with a range of putative ligands; still the endogenous ligands molecular recognition to this class I receptor are underexplored. Herein, we made an attempt to systematically investigate the mode of ligand recognition in TREM2 ECD by employing docking and computational state-of-the-art all atoms molecular dynamics simulations and free energy calculations. These ligands tend to interact with two distinct interfaces of TREM2 ECD; a group of compounds are seen to be binding to the complementarity-determining regions (CDR), which are key players in maintaining structural integrity of the protein, and interestingly, the others form dense network hydrophobic contacts with the core region residues of β3-β7 region. The reported pathogenic mutation W50C is seen to from hydrophobic contacts can be explored to understand its critical role in ligand recognition. In addition, investigation of observed interaction of the 11 compounds near the CDR loops would be motivating to look at, where variants like R47H and R62H associated with AD tends to disrupt surface interactions[2]. Altogether, our comprehensive study provides deep insights into the endogenous ligand recognition by TRME2 ECD surface and core region, which may pave the way for exploration of other small molecules towards development of novel therapeutics against Alzheimer's disease.

Keywords: neurodegenerative disorders, TREM2 ECD, AD, NHD, complementarity-determining regions, mutation

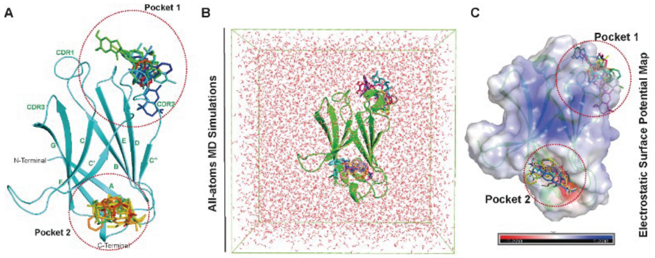


Figure: Potrayal of TREM2-ECD ligand recognition . A. demonstrates the interaction of small molecules bound to TREM2-ECD at two separate places, namely the CDR loop area and the strands A and G**. B**. Illustrates the all-atom simulations of the generated complexes. **C**. Electrostatic surface potential map showcasing charge distribution on the protein surface; pocket 1 flaunts the neutral charge allocation and pocket 2 displays negatively charged site that denotes the hydrophobic region.

Dynamics of nucleophilic substitution reaction at nitrogen center: Reactions of NH_2Cl with different alkoxide ions (HO^-, CH_3O^- and $C_2H_5O^-$)

Siddharth Sankar Dutta and Upakarsamy Lourderaj*
School of Chemical Sciences, National Institute of Science Education and Research (NISER)
Bhubaneswar, An OCC of Homi Bhabha National Institute, P.O. Jatni, Khurda, Odisha, India
(E-mail: siddharthsankar.dutta@niser.ac.in)

Abstract:

The nucleophilic substitution reaction at the nitrogen center is a crucial process for forming C-N bonds, and has applications in both synthetic chemistry and cancer treatment.[1,2] Despite its importance, the mechanism of this reaction is not well understood compared to substitution reactions at the carbon center, which have been extensively studied both experimentally and theoretically.[3-7] In this study, we used various electronic structure calculations to map the potential energy profile for the reaction between chloramine (NH_2Cl) and different alkoxide ions. We found that the potential energy profile exhibits a typical double well potential, similar to the potential energy profile observed in S_N2 reactions at the carbon center. However, the intermediates involved in the pre- and post-transition state are hydrogen-bonded intermediates that differ from those observed in S_N2 potential energy profiles at carbon centers.

We also observed a competitive proton-abstraction pathway and a front-side S_N2 attack pathway. Our benchmarking using MP2-full/aug-cc-pVTZ geometries showed that both S_N2 and proton-abstraction products were exothermic in all cases. The back-side S_N2 and proton-abstracted pathway had a submerged transition state for all three reactions, while the front-side S_N2 transition state had a high barrier transition state. Additionally, we used ab-initio on-the-fly classical trajectories simulations at MP2/aug-cc-pVDZ level of theory to study the reaction of NH_2Cl with CH_3O^- and observed both proton-abstracted and S_N2 products, supporting the experimental observations.[8]

References

1. Ulbrich, R.,Famulok, M.,Bosold, F.,Boche, G., Tetrahedron Lett. 1990, 31, 1689-1692.
2. Helmick, J.S., Martin, K. A., Heinrich, J. L., Novak, M., J. Am. Chem. Soc. 1991, 113, 3459-3466.
3. Glukhovtsev, M. N., Pross, A., Radom, L., J. Am. Chem. Soc. 1995, 117, 9012–9018.
4. Viggiano, A. A., Arnold, S. T., Morris, R. A., Ahrens, A. F., Hierl, P. M., J. Phys. Chem. 1996, 100, 14397–14402.
5. Mann, D. J., Hase, W. L., J. Phys. Chem. 1998, 102, 6208 – 6214.
6. Anbar, M., Yagil, G., J. Am. Chem. Soc. 1962, 84, 1790 –1796.
7. Beak, P., Li, J., J. Am. Chem. Soc. 1991, 113, 2796 –2797.
8. Gareyev, R., Kato, S., Bierbaum, V. M., J. Am. Soc. Mass Spectrom. 2001, 12, 139-143.

Natural polyphenols as effective antivirals for monkeypox virus: Insights from machine learning and all-atoms MD simulations

Madhusmita Rout, Sarbani Mishra, Sanghamitra Pati, Budheswar Dehury*

ICMR-Regional Medical Research Centre, Chandrasekharpur, Bhubaneswar-751023, Odisha, India

Email: budheswar.dehury@gmail.com

Abstract: The resurgence of monkeypox (MPX) poses a new worldwide threat in the context of the COVID-19 pandemic. Despite its potential for mildness, MPX has the potential to cause serious health problems [1,2]. F13, a critical protein of MPXV, is involved in the production of viral particles [3]. Drugs that target F13 are crucial. Natural polyphenols, which have antiviral characteristics, are being investigated as alternatives to standard therapies [4]. Advanced machine learning approaches were used to predict a very precise 3-dimensional structure of F13, as well as unveil pivotal binding regions on the protein surface [5–7]. A comprehensive virtual screening of 57 potent natural polyphenols with antiviral activities followed by state-of-the-art all-atoms molecular dynamics simulations [8] are performed to determine the ligand recognition mechanism of F13 [9,10]. Six polyphenols with higher binding affinity to F13 are chosen based upon Glide SP, XP and MM/GBSA scores for structural dynamics of ligand bound states of F13 [11,12]. Close inspection of docked and simulated snapshots of F13-complexes reveals the importance of critical amino acid residues i.e. Glu^{143}, Asp^{134}, Asn^{345}, Ser^{321}, and Tyr^{320} in polyphenol recognition. These findings are well supported by per residue binding free energy decomposition analysis. Our study suggests that the small-molecule binding site of F13 is predominantly hydrophobic in nature. Two polyphenols viz., myricetin and demethoxycurcumin forms dense network of non-bonded contacts with the receptors binding site signifying their importance as potent inhibitors of F13. Nonetheless, further research under controlled settings i.e., *in vitro* and *in vivo* are required to validate these findings.

Keywords: Monkeypox, polyphenols, demethoxycurcumin, drugs

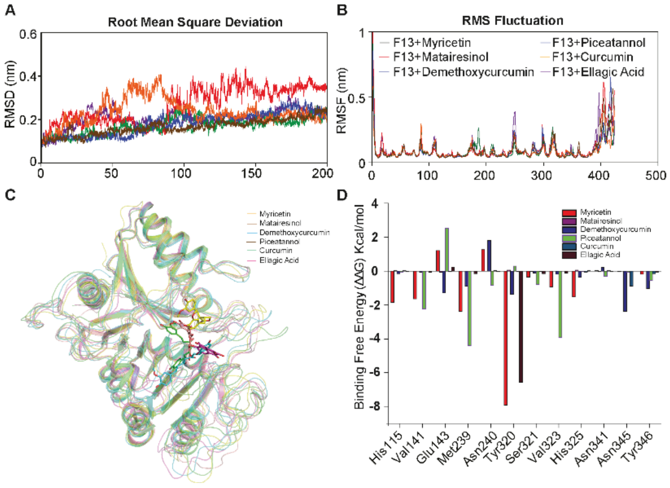
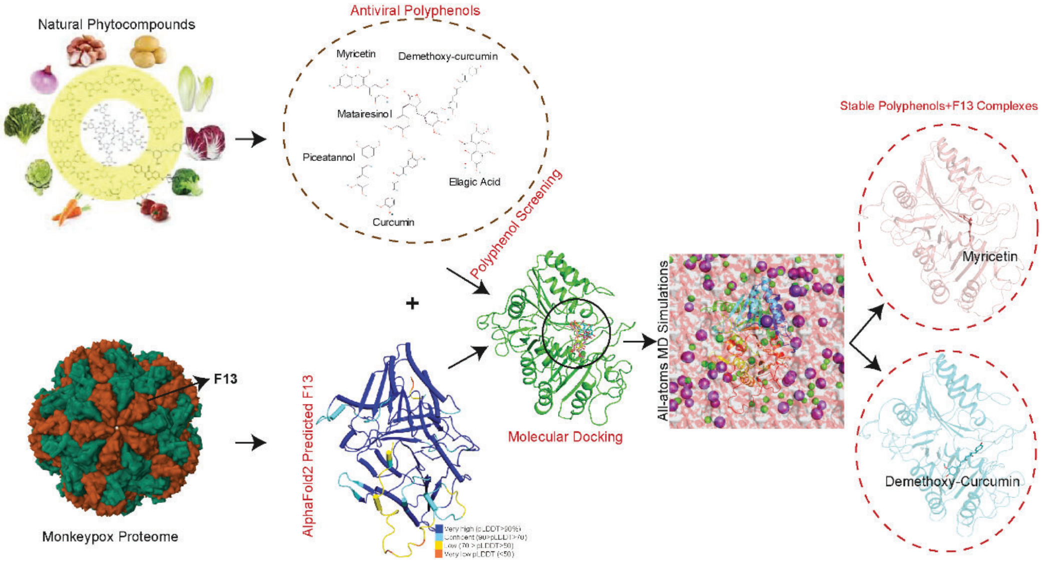


Figure 1. Dynamics of F13-polyphenol complexes reveals the stability and conformational flexibility during all-atoms molecular dynamics simulation over a time scale of 200 ns. (**A**) Backbone RMSD of polyphenol+F13 complexes observed throughout 200 ns MD simulation. (**B**) Fluctuation in each region of F13 observed throughout the MD run upon

ligand binding. (**C**) Top cluster representative of polyohenol-F13 complexes. (**D**) Plot representing decomposed binding free energy of each key residue involved in polyphenol binding.



Scheme: Schematic representation portraying the detailed workflow of screening antiviral polyphenols against MPX viral F13 surface protein using machine learning mediated structure prediction followed by molecular docking and all-atoms MD simulations.

References and Notes:

1. B.W. Petersen, I.K. Damon, Orthopoxviruses: Vaccinia (Smallpox Vaccine), Variola (Smallpox), Monkeypox, and Cowpox, Mand. Douglas, Bennett's Princ. Pract. Infect. Dis. 2 (2014) 1694-1702.e3. https://doi.org/10.1016/B978-1-4557-4801-3.00135-1.
2. D. Mileto, A. Riva, M. Cutrera, D. Moschese, A. Mancon, L. Meroni, A. Giacomelli, G. Bestetti, G. Rizzardini, M.R. Gismondo, S. Antinori, New challenges in human monkeypox outside Africa: A review and case report from Italy, Travel Med. Infect. Dis. 49 (2022). https://doi.org/10.1016/j.tmaid.2022.102386.
3. G.L. Smith, A. Vanderplasschen, M. Law, The formation and function of extracellular enveloped vaccinia virus, J. Gen. Virol. 83 (2002) 2915–2931. https://doi.org/10.1099/0022-1317-83-12-2915.
4. M.F. Montenegro-Landívar, P. Tapia-Quirós, X. Vecino, M. Reig, C. Valderrama, M. Granados, J.L. Cortina, J. Saurina, Polyphenols and their potential role to fight viral diseases: An overview, Sci. Total Environ. 801 (2021) 149719. https://doi.org/10.1016/j.scitotenv.2021.149719.
5. J. Jumper, R. Evans, A. Pritzel, T. Green, M. Figurnov, O. Ronneberger, K. Tunyasuvunakool, R. Bates, A. Žídek, A. Potapenko, A. Bridgland, C. Meyer, S.A.A. Kohl, A.J. Ballard, A. Cowie, B. Romera-Paredes, S. Nikolov, R. Jain, J. Adler, T. Back, S. Petersen, D. Reiman, E. Clancy, M. Zielinski, M. Steinegger, M. Pacholska, T. Berghammer, D. Silver, O. Vinyals, A.W. Senior, K. Kavukcuoglu, P. Kohli, D. Hassabis, Applying and improving AlphaFold at CASP14, Proteins Struct. Funct. Bioinforma. 89 (2021) 1711–1721. https://doi.org/10.1002/prot.26257.

6. R.A. Laskowski, J.M. Thornton, PDBsum extras: SARS-CoV-2 and AlphaFold models, Protein Sci. 31 (2022) 283–289. https://doi.org/10.1002/pro.4238.
7. D.T. Jones, J.M. Thornton, The impact of AlphaFold2 one year on, Nat. Methods. 19 (2022) 15–20. https://doi.org/10.1038/s41592-021-01365-3.
8. H. Bekker, H. Berendsen, E. Dijkstra, S. Achterop, R. Van Drunen, D. Van der Spoel, A. Sijbers, H. Keegstra, B. Reitsma, M. Renardus, Gromacs: A parallel computer for molecular dynamics simulations, Phys. Comput. 92 (1993) 252–256.
9. V.A. Shiryaev, M.Y. Skomorohov, M. V. Leonova, N.I. Bormotov, O.A. Serova, L.N. Shishkina, A.P. Agafonov, R.A. Maksyutov, Y.N. Klimochkin, Adamantane derivatives as potential inhibitors of p37 major envelope protein and poxvirus reproduction. Design, synthesis and antiviral activity, Eur. J. Med. Chem. 221 (2021) 113485. https://doi.org/10.1016/j.ejmech.2021.113485.
10. M. Rout, S. Dey, S. Mishra, S. Panda, M.K. Singh, R. Sinha, B. Dehury, S. Pati, Machine learning and classical MD simulation to identify inhibitors against the P37 envelope protein of monkeypox virus, J. Biomol. Struct. Dyn. (2023). https://doi.org/10.1080/07391102.2023.2216290.
11. R.A. Friesner, R.B. Murphy, M.P. Repasky, L.L. Frye, J.R. Greenwood, T.A. Halgren, P.C. Sanschagrin, D.T. Mainz, Extra precision glide: Docking and scoring incorporating a model of hydrophobic enclosure for protein-ligand complexes, J. Med. Chem. 49 (2006) 6177–6196. https://doi.org/10.1021/jm051256o.
12. M.P. Jacobson, D.L. Pincus, C.S. Rapp, T.J.F. Day, B. Honig, D.E. Shaw, R.A. Friesner, A Hierarchical Approach to All-Atom Protein Loop Prediction, Proteins Struct. Funct. Genet. 55 (2004) 351–367. https://doi.org/10.1002/prot.10613.

Halogen bonding interactions of 3,5-bis(3-pyridyl)-1,2,4-oxadiazole with molecular iodine and iodonium ion

Niharika Nath, Sweety Moharana, Himansu Sekhar Sahoo*
Department of Chemistry
College of Basic Science and Humanities, OUAT, Bhubaneswar-751003
(E-mail:himansusekhars@gmail.com, niharikanathchem@gmail.com)

Abstract:

Supramolecular chemistry deals with the study of complex chemical systems which involve non-covalent interactions for their formation. Parallel to hydrogen bonding in the field of non-covalent interactions there exists another interaction between atoms of different molecules, known as halogen bonding. According to IUPAC, halogen bonding occurs when there is net attractive interaction between an electrophilic region associated with a halogen atom in a molecular entity and nucleophilic region in another or the same molecular entity. Due to the uneven distribution of electron density around halogen, there exists a sigma hole (where electrostatic potential is positive) and it creates a cap of depleted electron density which is used as electron acceptor centre from N, O, and S atoms of other molecules. The highly directional nature of halogen bonds can be used for the formation of halogen-organic frameworks (XOF) and are free from metal ions which leads to a more environment-friendly alternative to MOF.

In this work, we have highlighted the halogen bonding interaction of bidentated 3,5-bis(3-pyridyl)-1,2,4-oxadiazole, L with molecular iodine as well as with iodonium ions. A comparison of bonding of 3,5-bis(4-pyridyl)-1,2,4-oxadiazole, L_1 with $AgNO_3$ and metal-free interaction of L_1 with iodonium ion is also discussed. Interaction of molecular iodine with ligand L results in two-dimensional linear polymeric structures that stack on each other resembling English single quotation marks. The presence of halogen bonding favours hydrogen organic framework (HOF) in $L\cdots I_2$ crystal packing in solid state. We have studied the interaction of iodonium ions with L_1 in the solution state and found halogen bonding interaction as observed from ^{1}H NMR and DLS studies.

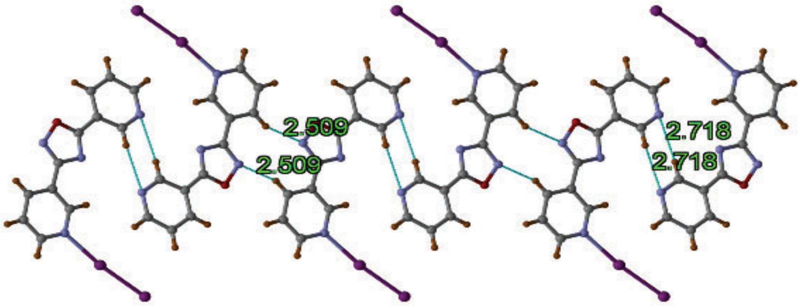


Figure: Halogen bonding interaction of L with iodine.

Model structure of C5aR2 in complex with β-arrestin1

Pulkit Kr. Gupta[1], Aurosikha Das[1], Aditi Singh[1], Soumendra Rana[1]

[1]*Chemical Biology Laboratory, School of Basic Sciences, IIT Bhubaneswar*

E-mail: pkg12@iitbbs.ac.in

Abstract: Complement component fragment 5a (C5a) is a potent pro-inflammatory glycoprotein of the complement system that binds to two genomically related G protein-coupled receptors (GPCRs), such as C5aR1 and C5aR2. Initiation of further downstream signaling in tissues requires the recruitment of heterotrimeric G-proteins and β-arrestins by the binary complexes of C5a-C5aR1/C5aR2. Compared to C5aR1, C5aR2 is established as a non-canonical GPCR, as it signals through β-arrestins rather than G-proteins. Moreover, C5aR2 demonstrates both anti-inflammatory and pro-inflammatory signaling. Notably, structural data establishing the interaction of C5a with C5aR2 and C5a-C5aR2 with β-arrestins is currently unknown. In the absence of structural data, we had recently developed highly refined model structures of C5aR2 bound to the CT-peptide of C5a (meta-active state) and C5a (active form) embedded in a model POPC bilayer. The current study has attempted to generate a highly refined, fully-active ternary model complex of the C5a-C5aR2-β-arrestin1 utilizing the C5a-C5aR2 complex published earlier from our laboratory. The data obtained from the computational modeling, 500 ns molecular dynamics (MD), and principal component analysis (PCA), including the Molecular Mechanics Poisson-Boltzmann Surface Area (MMPBSA) studies, indicate that the C5a-C5aR2-β-arrestin1 complex, based on an experimentally testable hypothesis, is of high quality, which will further enrich the current structural understanding related to the interaction of β-arrestins with the C5a-C5aR2 system. In addition, the ternary complex illustrates two targetable active sites located at the extracellular and intracellular sides of the C5aR2. Targeting the extracellular active site through β-arrestin biased ligands can be helpful to exploit the anti-inflammatory signaling of C5aR2. Conversely, selective targeting of the intracellular active site of C5aR2 may prevent its interaction with β-arrestins, which may attenuate pro-inflammatory signaling under pathological conditions.

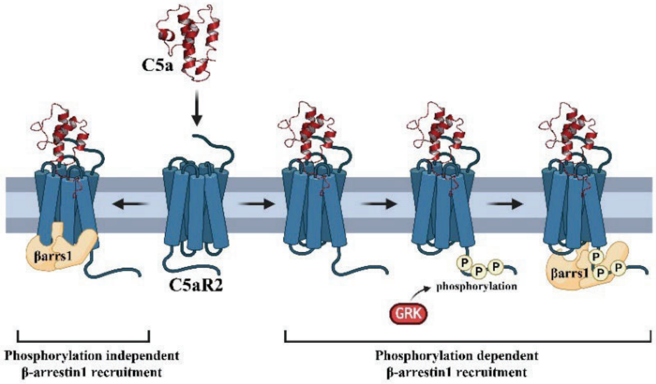


Figure: Schematic illustration of recruitment and activation of β-arrestin1 by the C5a-C5aR2 binary complex based on the established arrestin activation mechanism reported for other GPCRs.

References:

1. Gupta, P. K.; Das, A.; Singh A.; and Rana S., Ternary model structural complex of C5a, C5aR2, and β-arrestin1. *J. Biomol. Struct.* **2023**, 1–17
2. Das, A.; Gupta, P. K.; and Rana, S., C5aR2 receptor: The genomic twin of the flamboyant C5aR1. *J. Cell. Biochem.* **2022** 123(11), 1841–1856.

Computational insights into Manganese Catalyzed Vinyl Cyclopropane Ring Expansion Cascade

Prativa Behera, Dr. Lisa Roy*
Department of Chemistry
Institute of Chemical Technology Mumbai-IOC Odisha Campus Bhubaneswar, 751013, India
(E-mail: L.Roy@iocb.ictmumbai.edu.in)

Abstract:

Cyclopentene is one of the fundamental building blocks of natural products and pharmaceutical ingredients. Computational investigation based on density functional theory (DFT) at the B3LYP/D3(BJ)/def2-TZVPP/SMD(toluene) level of theory unravelled the mechanism of acyl cyclopentene formation from phenyl cyclopropyl alcohol (**1a**) and pentamethyl acetophenone (**2a**). Manganese-catalyzed hydrogen borrowing oxidation of cyclopropyl alcohol (**1a**) is enabled through a strong O-…H-N hydrogen bonding interaction. The phenyl cyclopropyl ketone (**17a**) subsequently undergoes aldol condensation with pentamethyl acetophenone (**2a**) to form vinyl cyclopropene species (**6a**). Single electron transfer (SET) initiation through in situ generated radical anion species triggers a ring expansion rearrangement to form the ultimate cyclopentene product.[1] The cascade process is independent of the manganese catalyst. Additionally, the alcohol **2a** assisted dehydrogenation of **MnH_2** occurs at relatively low barrier kinetics that arrest further hydrogenation of the cyclopropene (**6a**) or the targeted cyclopentene product (**3a**) (Figure 1). [2-4]

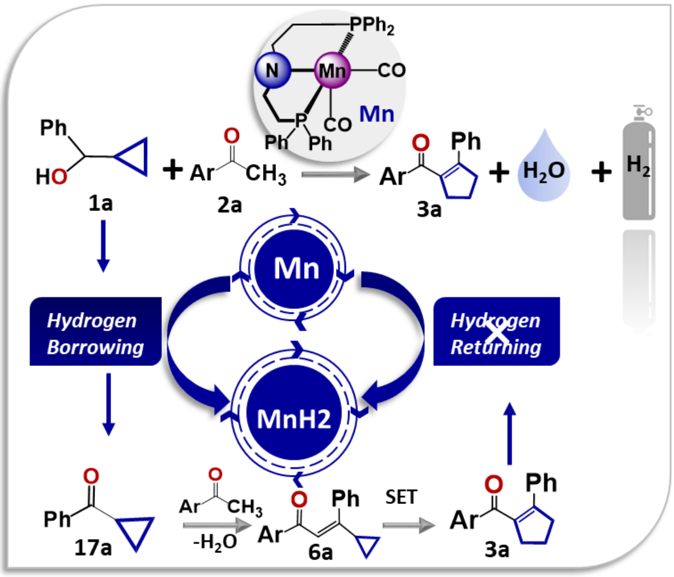


Figure 1: Catalytic pathway for cyclopentane formation from cyclopropane.

References:

[1] Wübbolt, S.; Cheong, C. B.; Frost, J. R.; Christensen, K. E.; and Donohoe, T. J. A., *Angew. Chem. Int. Ed. Engl.* **2020**, *59*, 11339-11344.
[2] Luque-Urrutia, J. A.; Solà, M.; Milstein, D.; and Poater, *J. Am. Chem. Soc.* **2019**, *141*, 2398-2403.
[3] Roy, L.; Paul, A., *Chem. Commun* **2015**, *51*, 10532-10535.
[4] Sarkar, K.; Behera, P.; Roy, L; and Maji, B., Manuscript in preparation.

Surface water acidification due to anthropogenic activity : Bhubaneswar smart city – a case study.

Ranjita Biswal

Abstract: This paper presents the seasonal analysis reports of the chemistry of surface water, rain water and fog of Bhubaneswar city for three years.july 2019 to June 2022.In this study 880 rain water samples, 340 fog samples and 650 surface water samples have been collected from twelve different areas such as, Acharya Vihar , Bapuji Nagar , Patra pada, Nalco chhak, Dumduma,Sailashree vihar,Chandaka Forest range, Baramunda, Khandagiri,Pandara, Kausalyaganga. The occurance of acid rain is known from the present study of acid rain, smog and formation of fog and their rate of contamination to the suface water changing its pH and nutrient content . The watert sample collected from Acharya vihar , Bapuji Nagar and Sailashree vihar area were found to be highly acidic in nature (pH < 5.2). It has been observed that pH of the rain water varies within the range of 5.0 to 4.3 and fog water sample in the range of 4.7 to 4.1 respectively. It has been found that the water sample obtained from other areas are slightly acidic in nature where the pH of the surface water remains in the range of 5.8 to 5.4 . It has been observed that the water sample in high acidic area is found to be more loaded with heavy metal in comparison to the water obtained from low acidic area. An correlation has been established by the critical analysis of both the water samples(atmospheric and surface).

A Mechanistic Investigation of Arylation of Heterocycles through Photoactivation of a Charge-Transfer Assembly

Sanat Kumar Mahapatra[1], Lisa Roy[1]
[1]*Institute of Chemical Technology Mumbai-IOC Odisha Campus Bhubaneswar, 751013, India*
(E-mail: che22sk.mahapatra@stuiocb.ictmumbai.edu.in)

Abstract: In the area of natural products, bioactive compounds, pharmaceuticals and functional materials synthesis, methods facilitating arylation of heterocycles plays a crucial role. Photoredox-catalyzed arylation of heterocycles are primarily done with precious metals like Ir and Ru[1]. Herein, we propose a novel photoredox system comprising of sodium iodide, triphenyl phosphine, tetramethylethylenediamine and diaryliodonium reagent (DAIR) that can form a tetrameric electron donor-acceptor charge transfer assembly (CTA) for efficient arylation of heterocycles. Interestingly, the CTA furnish aryl radicals upon irradiation with blue light-emitting diodes (Figure 1) which could be further utilized for arylation of azauracil. In depth investigation with density functional theory (DFT) at B3LYP-D3(BJ)/SMD {HFIP:H_2O = 4:1}/6-311+G(d,p) and time-dependent DFT (TD-DFT) calculations at M06L/SMD {HFIP:H_2O=4:1}/6-311+G(d,p) level of theory provide understanding about the mechanistic intricacies and highlight the role of weak non-covalent interactions (NCIs) that facilitate formation of the CTA[2,3,4]. Moreover, NCIs such as H-bond networks provided through explicitly added HFIP and water molecules favour a lower energetic pathway for the target product formation.

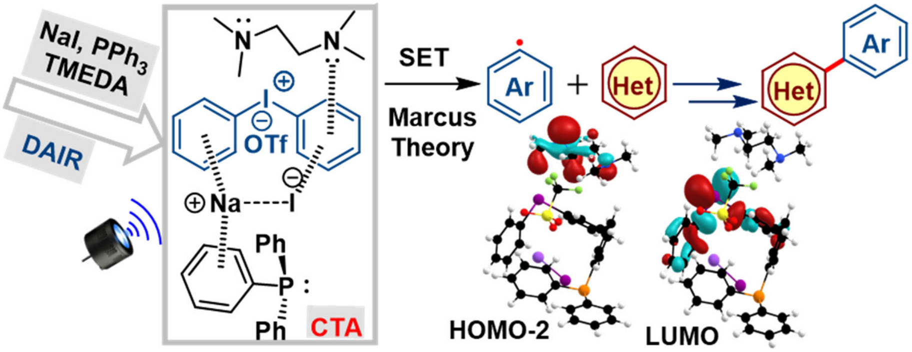


Figure:1 Photoinduced arylation of azauracil derivative via a CTA complex.

References:

1. Neufeldt, S.R.; Sanford, M. S.; *Adv. Synth. Catal* **2012**, *354*, 3517-3522
2. Fu, M. C.; Shang, R.; Zhao, B.; Wang, B.; Fu, Y.; *Science* **2019**, 363, 1429–1434
3. Mallojjala, S. C.; Nyagilo, V. O.; Corio, S.A.; Adili, A.; Dagar, A.; K. A. Loyer, K.A.; Seidel, D.; Hirschi, J. S.; *J. Am. Chem. Soc.* **2022**, 144, 17692−17699
4. Das, S.; Parida, S.K.; Mandal, T.; Hota, S.K.; Roy, L.; Sarkar, S.D.; Muraka, S. *Org. Chem. Front.*, **2021**, 8, 2256

Spectroscopy

ZIFs: A Raman Study of Temperature Induced Structural Transformation

Anulipsa Priyadarshini, Jaykishon Swain, Raghabendra Samantaray*, Rojalin Sahu*

School of Applied Sciences, Kalinga University of Industrial Technology (KIIT), Deemed to be University, Bhubaneswar, Odisha, India-751024

Email: rsahufch@kiit.ac.in

Abstract: Zeolitic Imidazolate Frameworks (ZIFs) are porous, crystalline frameworks in which the tetrahedral metal ions are linked by imidazolate (Im) units. ZIFs possess a structure similar to conventional aluminosilicate zeolites, where the Zn^{2+} ion replaces silicon, while imidazolate anions imitate oxygen, producing metal–imidazole–metal bridges an angle of ~145°. The crystaline structure of ZIFs play a strong role in guiding physical properties such as surface areas, unimodal micropores, abundant functionalities and exceptional thermal and chemical stabilities. The molecular vibration have been shown to greatly influence the many of the aforementioned behaviors. However, the sturtural characterisation used in the literature has been limited to techniques like XRD, FTIR, FESEM, UV-DRS. In particular, variable temperature Raman has been overlooked. We feel that this is urgently needed to understand properties such as gas adsorption, which strongly correlates with the puckering motions of the imidazole group. In this study, we have undertaken variable temperature Raman and UV-DRS with the goal of establishing the structure-function relation on the basis of the possible puckering motions and structural transformations therin. These studies have indeed revealed a distinct stuctural transformation owing to metal-nitrogen bond of the imidazole groups.

Keywords: ZIFs, Phase transition, Structural transition, Raman study, Ring puckering motion

A comparative study on pyrolysis kinetics and thermodynamic parameters of little millet and sunflower stem biomass using thermogravimetric analysis

Abinash Mishra, Manasi Dash*

Department of PBG, CA, OUAT, Bhubaneswar-3, Odisha

Email: mdpbgouat@gmail.com

Abstract: Several biochemical and thermochemical routes including pyrolysis, liquefaction, combustion and gasification are used to convert biomasses to several bioproducts and green fuels. The current investigation included two biomasses namely, little millet and sunflower stem, whose potentiality as useful feedstocks are largely unexplored. The presence of considerable level of cellulose accumulation (approx. 30.00%), volatiles (approx. 67%) and HHV (approx. 14MJ/kg) in both the biomass, inferred their potentiality to be used as useful feedstocks in the pyrolysis process. The estimate of E_α for LMS was reported as 191.14 kilo joule per mole (FWO), 191.46 kilo joule per mole (KAS) whereas, For SS, the E_α was estimated as 166.52 kilo joule per mole (FWO), 162.68 kilo joule per mole (KAS). The difference between ΔH and E_α was small (5-6 kilo joule per mole) for both the biomasses, indicating the feasibility of combustion process. From $Z(\alpha)$ analyses, the experimental curve was seen passing through different theoretical curves, indicating complex nature of pyrolysis process for both the biomass.

INORGANIC CHEMISTRY

Inorganic Synthesis

Structural Optimization of Luminescent Sulfur Dots for Solar Light Induced Efficient and Selective Oxidative Coupling Reactions of Aromatic Amines: A Complete Metal Free Approach

Srayee Mandal, Bramhaiah Kommula, Santanu Bhattacharyya*

Department of Chemical Sciences, Indian Institute of Science Education and Research, Berhampur,
Odisha-760010, India

(E-mail: srayeem@iiserbpr.ac.in)

Abstract: It is highly desirable to perform aerobic oxidation of aromatic amine to imines through green photocatalytic approach. Therefore, development of metal free complete green photocatalyst is extremely important in this regard. Herein, we have synthesised two different types of luminescent sulfur dots (S dots) from totally earth abundant bulk sulfur with different structural and elemental features through a simple chemical etching method, followed by solvent extraction based post growth mechanism. The structural and elemental features of both the S dots are further correlated with the underpinning photophysics through in-depth steady state and time resolved spectroscopy. It is further supported by detailed electrochemical and photoelectrochemical studies. Notably, light absorption cross-section, charge separation and free carrier accumulation are maximum for the specific type of S dots with almost defined crystalline nature and maximum extent of molecular sulfur as the constituent elements, while normal S dots shows polycrystallinity and predominantly S-based functional groups. Finally the as synthesised S dots have been utilized for the photocatalytic coupling reactions of benzylamine at complete ambient conditions. The optimized S dots show almost ~90 % conversion with ~99.5 % selectively for the production of specific aromatic imines. The photocatalytic mechanism was crucially investigated by tracking the photoinduced free radicals and intermediates.

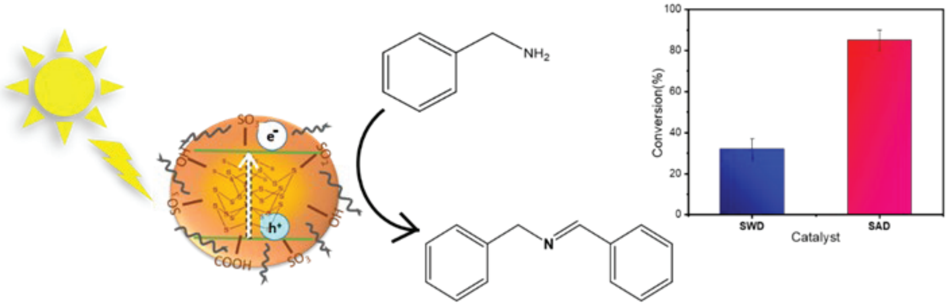


Figure 1: photocatalytic aerobic oxidative coupling reaction of benzylamine to imine

References and Notes:

1. Mondal, S.; Sahoo, L.; Vinod, C. P.; Gautam, U. K., *Appl. Catal. B Environ.* **2021**, *286.*
2. Wang, H.; Wang, Z.; Xiong, Y.; Kershaw, S. V.; Li, T.; Wang, Y.; Zhai, Y.; Rogach, A. L., *Angew. Chemie - Int. Ed.* **2019**, *58* (21), 7040–7044.

Selective aerobic oxidation of biomass model compound veratryl alcohol catalyzed by air-stable copper(II) complexes in water

Suraj kumar Maharana

National Institute of Science Education and Research (NISER), Bhubaneswar 752050 Odisha, India.

Abstract: Air-stable square pyramidal copper(II) bromide complexes 1, 2 and 3 with NNS, N(NH)S and NNO ligand frameworks, respectively, were synthesized and successfully utilized as effective catalysts for the aerobic oxidation of biomass model compound veratryl alcohol in water as a green and sustainable reaction medium. Complex 2 displayed the best catalytic activity. The oxidation reactions were successfully conducted under ambient conditions (40 °C) in the presence of a catalytic amount of copper catalyst and TEMPO ((2,2,6,6-tetramethylpiperidin-1-yl)oxyl) utilizing air as a sustainable oxidant. Addition of an external base is required to obtain a quantitative yield and complete selectivity towards the desired aldehyde product. The oxidation reaction can also be conducted in the absence of base; however, selectivity declined, with the formation of an over-oxidation product, veratric acid. Acetonitrile is the most commonly used solvent in oxidation reactions, and various green solvents such as methanol, ethanol, acetone and ethyl acetate were also used for the same purpose. Although acetonitrile and water gave similar catalytic efficiency, we selected water after considering the green and sustainable aspects. Optimized reaction conditions in water were utilized for the oxidation of other lignin biomass-derived alcohols as well as various other substituted benzylic alcohols to the corresponding aldehydes. Aldehyde products were easily isolated by simple workup processes (filtration and evaporation). Complex 2 is highly recyclable and quantitative isolated yields of product were obtained even after ten consecutive runs. The present catalytic protocol produced less waste as reflected in the low E-factor (4.16). Finally, the sustainable credentials of various optimized reaction protocols were evaluated with the help of the CHEM21 green metrics toolkit.

Post-synthetic Modification of Zr-based Metal-organic Frameworks with Imidazole: Variable Optical Behavior and Sensing

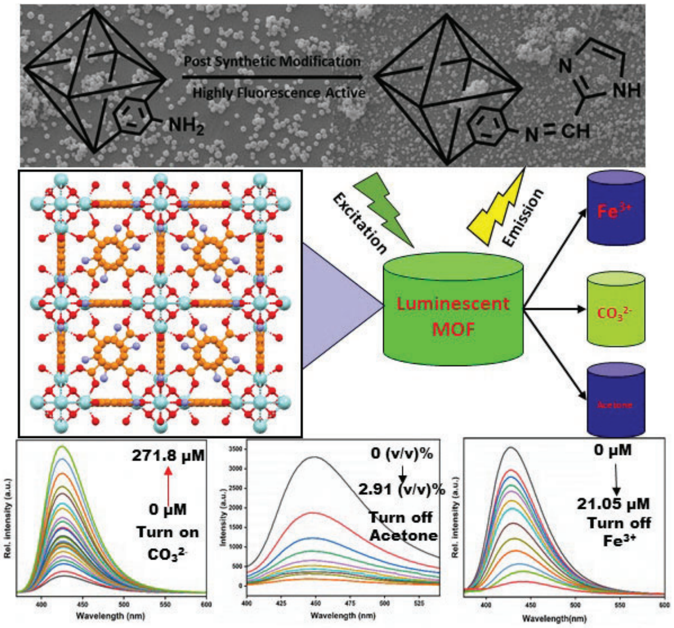
Dipankar Singha , Dibya Prakash Biswal , , Dr. Jagannath Panda, Dr. Malay Kumar Rana

Department of Chemical Sciences, Indian Institute of Science Education and Research

(IISER), Berhampur, Berhampur 760010, Odisha, India

Abstract: UiO-66-NH_2-IM, a fluorescent metal-organic framework (MOF), was synthesized by post-synthetic modification of UiO-66-NH_2 with 2-imidazole carboxaldehyde via a Schiff base reaction. It was examined using various characterization techniques (PXRD, FTIR, NMR, SEM, TGA, UV-Vis DRS, and photoluminescence spectroscopy). The emissive feature of UiO-66-NH_2-IM was utilized to detect volatile organic compounds (VOCs), metal ions, and anions, such as acetone, Fe^{3+}, and carbonate (CO_3^{2-}). Acetone turns off the high luminescence of UiO-66-NH_2-IM in DMSO, with the limit of detection (LOD) being 3.6 ppm. Similarly, Fe^{3+} in an aqueous medium is detected at LOD = 0.67 µM (0.04 ppm) via quenching. On the contrary, CO_3^{2-} in an aqueous medium significantly enhances the luminescence of UiO-66-NH_2-IM, which is detected with extremely high sensitivity (LOD = 1.16 µM, i.e., 0.07 ppm). Large Stern-Volmer constant, Ksv, and low LOD values indicate excellent sensitivity of the post-synthetic MOF. Experiments supported by density functional theory (DFT) calculations discern photo-induced electron transfer (PET), resonance energy transfer (RET), inner filter effect (IFE), or proton abstraction as putative sensing mechanisms. NMR and computational studies propose a proton abstraction mechanism for luminescence enhancement with CO_3^{2-}. Moreover, the optical behavior of the post-synthetic material toward analytes is recyclable.

Scheme:



References and Notes:

1. Biswal, Dibya Prakash, Singha, Dipankar, Panda, Jagannath, Rana, Malay Kumar, *ChemPhysChem* 2023, e202300311.

Single step site-selective reaction and optoelectronic properties of Ag_4, Ag_2Au_2-*N*-heterocyclic carbene(NHC) supramolecular organometallic

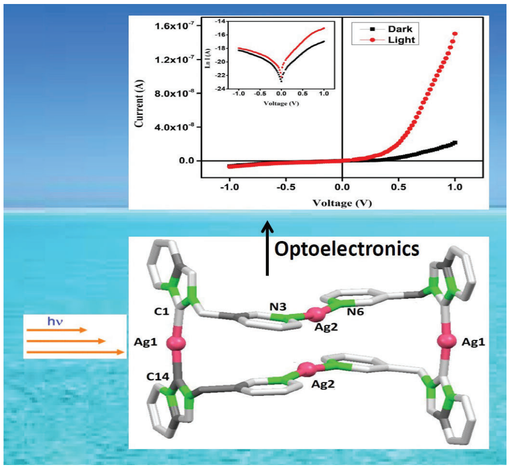
Pooja Das and Joydev Dinda*

Department of Chemistry, Utkal University, Vani Vihar, Bhubaneswar-751004

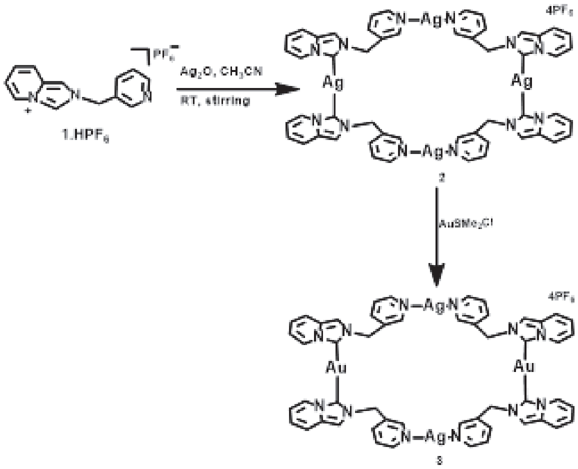
(E-mail: joydevdinda@gmail.com)

Abstract: A Novel Ag(I) cluster complex $[Ag_4(1)_2][PF_6]_4$, 2 and Ag(I)-Au(I) cluster complex $[Ag_2Au_2(1)_2][PF_6]_4$, 3 has been synthesized from *N*-heterocyclic carbene (NHC) precursor 3-(pyridylmethyl)imidazo[1,5-a]pyridin-4-yliumhexafluorophosphate, ($1.HPF_6$) which were further characterized by spectroscopic techniques. Transmetallation by Au(I) to Ag_4 macrocycle leads to Ag_2Au_2 macrocyclic cluster where Au(I) selectively binds with $C_{carbene}$. Geometrics of 2 and 3 were established by single crystal X-ray diffraction studies. Optoelectronic studies revealed the scope of 2 and 3 as photovoltaic cells. Further, MS-junction potential directs the use of 2 and 3 as semiconductor devices where 2 is more effective than 3.

Figure:



Scheme:



Zirconium Quantum Dots (Zr QDs): A New Class for Hydrogen Peroxide Sensor

Amit Sahoo and Achyuta N. Acharya*

Department of Chemistry, Odisha University of Technology and Research, Bhubaneswar-751029, Odisha, India.

(E-mail: aacharya@outr.ac.in ; amitsahoochemistry@gmail.com)

Abstract: Zirconium QDs have been synthesised by the chemical reduction method. The EDS and EDX studies were attempted to confirm the purity of the Zr QDs. The XRD data reveal that Zr QDs are both in cubic and hexagonal lattice configurations. The HRTEM and FESEM studies supported that Zr QDs are homogeneous, tiny, spherical QDs with a diameter of 5 nm to 6 nm. It exhibited chemiluminescence; the quantum yield of the QDs is ~ 68.72% (abs.). It showed H2O2 sensitivity. The Stern-Volmer equation is satisfied by the variations in the intensity of the emission spectra of Zr QDs at different wavelengths (406 nm, 430 nm, and 413 nm), making them fascinating candidates for application to biological science and as energy materials.

Keywords: Zirconium, Zirconium QDs, Fluorescence, PCCS, H2O2.

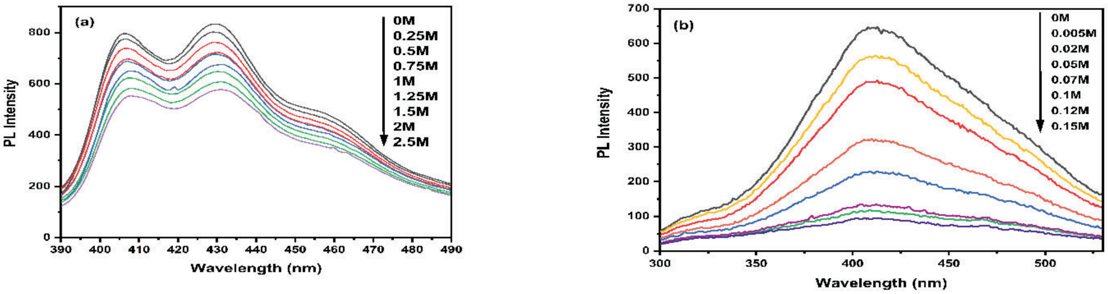


Figure 1. (a) Emission patterns of H_2O_2 sensors under various [H_2O_2] at wavelengths of 406 and 430 nm, and (b) Emission profiles of H_2O_2 sensors under various [H_2O_2] at wavelength of 413 nm.

References and Notes:

1. Acharya, A.N.; Sahoo, A., *J. Mater. Sci.* **2023**, 58, 12976–12992. https://doi.org/10.1007/s10853-023-08812-w
2. Ahmed S.R.; Kang S.W.; Oh S.; Lee J.; Neethirajan S., *Heliyon* **2018**, 4, 1–17. https://doi.org/10.1016/j.heliyon.2018.e00766

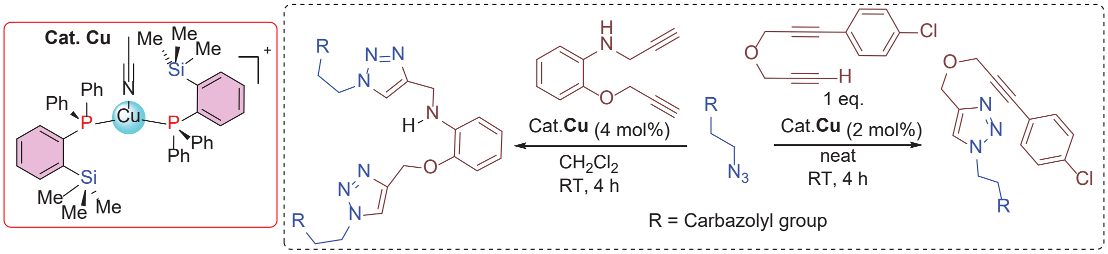
Coinage Metal Complexes of Silylated-Phosphines; New Molecular Catalysts for Alkyne-Azide Cycloaddition Reactions

Amiya Kumar Sahoo, Bhagyashree Das, and Adinarayana Doddi*

Department of Chemical Sciences/ Indian Institute of Science Education and Research Berhampur/ Transit Campus, Industrial Training Institute, Engineering School Road, 760010, Berhampur, Odisha

Email: adoddi@iiserbpr.ac.in

Abstract: Lewis acidic main-group element functionalized phosphines have attracted widespread attention as potential and superior ligands over the normal phosphines as such species facilitate in tuning electronic and steric properties of the attached metal centers. Additionally, several reports showed their use in the preparation of more soluble metal complexes.[1,2] Due to the presenc of group 14 element groups in the close proximity of metal atoms, this class of ligands facility oxidative addition, and reductive elemination reactions which are in the domain of organometallic chemistry and catalysis.[3] In this work, a series of coinage metal (Cu & Ag) complexes featuring ortho-silylated phosphine(s) have been isolated, and structurally characterized. Neutral, and mono-cationic copper complexes were obtained by the reactions of silylated phosphine with suitable copper(I) sources. Different varieties of cationic silver complexes were also prepared by treating the silylated phosphine with various silver salts AgX (X = BF4, NO3) in 2:1 ratio. The homoleptic tris(silylphosphinochalcogenide)copper(I) complexes were also synthesized, and these complexes were employed as molecular catalysts in the azide-alkyne cycloaddition reactions in a sustainable solvent free approaches (Scheme). [4] All the neutral, caitonic copper complexes exibhited excellent catalytic performances, and this work has demonstrated applications of silylated-phosphines as pontential ancillary ligands in homogeneous catalysis. Synthesis, and catalytic and mechanistic investigations of this work will be presented.



Scheme. Copper(I) catalyzed cycloaddition reactions.

References and Notes:

1. (1) G. Bouhadir and D. Bourissou, *Chem. Soc. Rev.*, 2016, **45**, 1065–1079.
2. (2) T. Komuro, Y. Nakajima, J. Takaya and H. Hashimoto, *Coord. Chem. Rev.*, 2022, **473**, 214837.
3. (3) P. Gualco, S. Ladeira, K. Miqueu, A. Amgoune and D. Bourissou, *Angew. Chem. Int. Ed.*, 2011, **50**, 8320–8324
4. (4) **A. K. Shoo**, A. K. Sahoo, B. Das, S. Panda, C. S. Purohit, and A. Doddi. *Manuscript under revision*

Synthesis and Application of Cobalt Oxide (Co_3O_4)/rGO-Impregnated banana Biochar for the Removal of dyes and heavy metal chromium (VI)

Amrita priyadarsini1, Chirasmayee Mohanty2, NigamanandaDas2*, Nandita Swain1, Pradip kumar Jena

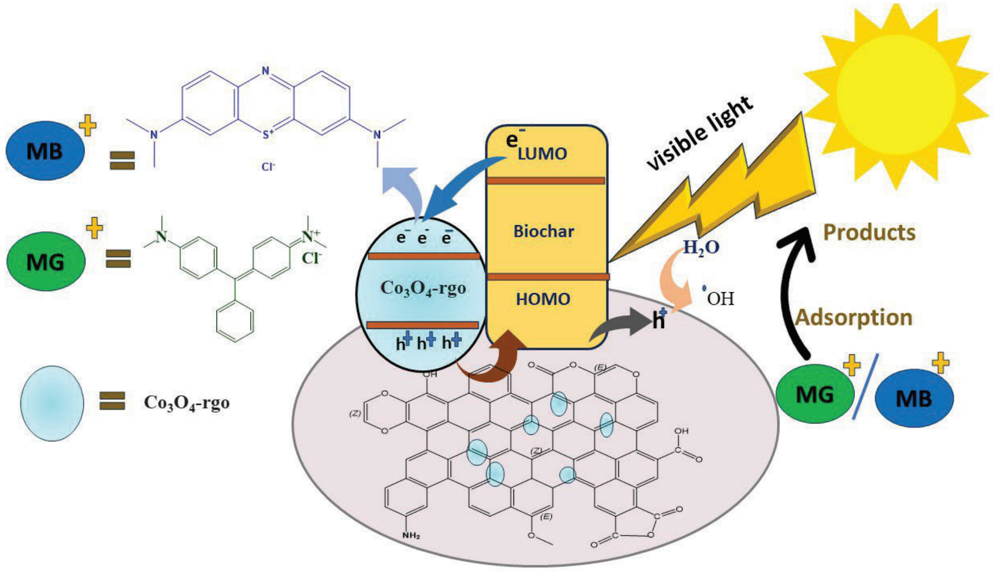
[1][1]Department of Chemistry, College of Basic Science and Humanities, Odisha University of Agriculture and Technology*

[2] Department of Chemistry, Utkal University, Bhubaneswar 751004, Odisha

Abstract: An rising global concern is the massive buildup of heavy metals and dyes in agricultural land as a result of increased soil toxicity levels. Chromium pollution, among other metals, has a significant impact on plant and human health via the food chain. In this study, cobalt oxide -rgo -doped biochar (CBG) hybrid composite was synthesised using the coprecipitation method for the photodegradation of the dyes (Methylene blue (MB), Malachite green (MG)) and heavy metal Chromium (VI). They were then characterised using a number of analytical techniques (PXRD, FTIR, SEM, EDX, TEM PL, BET and XPS). The results showed that MG and MB dyes degraded by around 92% and 94% in 60 minutes under visible light exposure when cobalt oxide and rgo were added to biochar. The CBG Catalyst was utilised to degrade Cr (VI) ions from simulated wastewater solutions at various pH, adsorbate, temperature, and dose concentrations. Nearly 98.7% of the Cr (VI) ions were eliminated at a dosage of 20 mg/L, a pH of 6 and at room temperature. It was found that the photocatalytic performance of the catalysts as made was greatly improved by 10% doping of Biochar and rgo and 70% loading of cobalt oxide (Co_3O_4). After five cycles, the synthetic hybrid catalysts maintained their high stability. CBG structure was unaffected by the modification, resulting in a small band gap, a light source with a long wavelength, efficient e^-/h^+ pair separation, and significant photocatalytic activity. The radical-trapping studies supported the theory that the significant improvement was caused by the production of OH, h^+, e^- and $O_2^{\cdot -}$. It was also suggested that a viable mechanism for the photocatalysis of cobalt oxide-rgo over biochar hybrid catalysts under UV-vis irradiation.

Keywords: Photocatalysis, heavy metal (Cr (VI)), MB, MG and CBG

Schematic figure :



Facile Synthesis of N-CDs for selective detection of Pd^{2+} in water

Chinmaya Chirasundar Behera, Tanmayee Mohanta and Ashis Kumar Jena*

Department of Chemistry, Maharaja Sriram Chandra Bhanja Deo University, Baripada, Odisha

(E-mail: jenaashis016@gmail.com, chinmayabehera64@gmail.com)

Abstract: Now-a-days, Carbon Dots (CDs) have attracted many researchers due to their excellent photoluminescence properties, easy synthetic route, lox toxicity, high chemical and photo-stability, solubility in water and bio-compatibility nature.[1] Due to these unique properties, CDs have large number of applications in the fields of catalysis, sensing, biomedicine, bioimaging and opto-electronic devices etc.[2,3] Herein, we have synthesized Nitrogen Doped Carbon dots (N-CDs) from 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) and Ethylene diamine by hydrothermal method (Fig. 1). Further, the as synthesized N-CDs was characterized by different analytical techniques and the stability of the N-CDs was investigated. Recently, researchers have developed many methods for detection of transition and post-transition metal ions due to their hazardous nature and biological importance on human health. Pd^{2+} is a transition metal ion used in treatment of cancer, jewelry, dental crowns and as a catalyst for many reactions. Thus, detection of Pd^{2+} in water, food or drugs is highly demandable since the residue of Pd^{2+} left in these substances can lead to many adverse effects on human health. A number of analytical techniques such as high-performance liquid chromatography (HPLC), atomic absorption spectroscopy (AAS) and X-ray fluorescence (XRF) have been applied for the detection of Pd^{2+}. However, these techniques have many disadvantages and high instrument cost. Thus, there is an urgent need for an easy, economic, simple and fast method for selective detection of Pd^{2+}. The detection of Pd^{2+} in aqueous medium is based on fluorescence quenching mechanism by N-CDs. As the concentration of Pd^{2+} increased from 0-100 μM, the fluorescence intensity of N-CDs decreased and the intensity of N-CDs quenched to 80% at 100 μM concentration of Pd^{2+}.

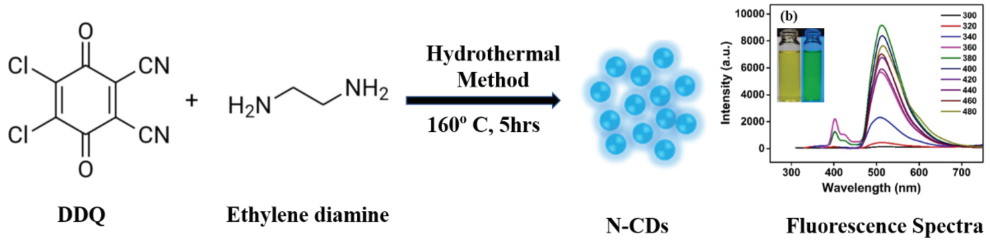


Fig. 1 Synthesis of N-CDs for selective detection of Pd^{2+}

References and Notes:

1. Li, L.; Zhang, R.; Lu, C.; Sun, J.; Wang, L.; Qu, B.; Li, T.; Liu, Y.; Li, S. In Situ Synthesis of NIR-Light Emitting Carbon Dots Derived from Spinach for Bio-Imaging Applications. *J. Mater. Chem. B* **2017**, *5* (35), 7328–7334.
2. Swain, S.; Jena, A. K.; Mohanta,T.Ratiometric Fluorescence/Colorimetry/Smartphone Triple-Mode Real-Time Detection of Doxorubicin by Nitrogen-Doped Carbon Dots. *ACS Appl. Opt. Mater*. **2023**, 1, 1236-1244.
3. Lu, H.; Li, C.; Wang, H.; Wang, X.; & Xu, S. Biomass-derived sulfur, nitrogen co-doped carbon dots for colorimetric and fluorescent dual mode detection of silver (I) and cell imaging. *ACS omega*, **2019**, *4*(25), 21500-21508.

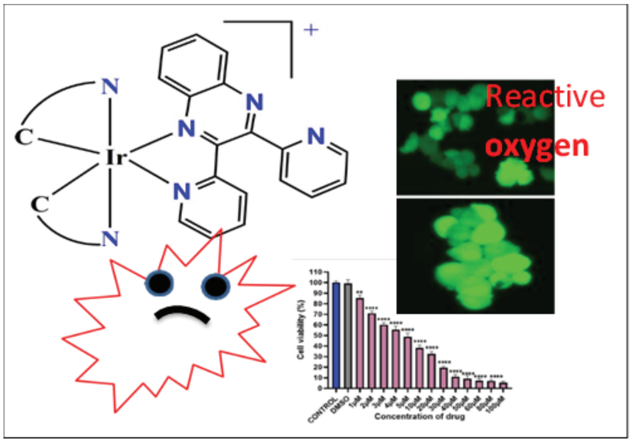
Cationic iridium(III)organometallic complexes containing2,3-di(pyridine-2-yl)quinoxaline ancillary ligand and their bioactive behaviour

Kahnu Charan Pradhan*[a], Satyanarayan Pal[a]

[a]*P. G. Dept. of Chemistry, Utkal University, Bhubaneswar, Odisha-751004, India*

Abstract: Novelcationic iridium(III) complexes **Ir5** to **Ir8** of formula [Ir(C^N)$_2$(pyrquinox)]PF$_6$ {where C^N=2-phenylpyridine (ppy), 2-(2,4-difluorophenyl)-5-(trifluoromethyl)pyridine (F$_2$CF$_3$ppy), 2,5-diphenylbenzoxazole (phox), 2,3-diphenylquinoxaline (phquinox) and pyrquinox = 2,3-bis(2-pyridyl)quinoxaline} were synthesised and characterised through FT-IR, ^{1}H NMR, mass spectroscopy, UV-Vis, emission spectroscopy and cyclic voltammetry studies. Further,**Ir5** structure was confirmed from single crystal X-ray structure analysis and it appeared to be bis-heterolepticIr(III) mononuclear octahedral complex of formula [Ir(ppy)$_2$(pyrquinox)]PF$_6$. The spectroscopic and analytical data suggest a similar formulation for the other three complexes (**Ir6-Ir8**) too.On irradiation, all four complexes produced emissions at higher wavelength close to orange and red light region.The cytotoxicity effect of these complexes was evaluated on the MCF-7 cell line and found to have high cytotoxicity properties for complex **Ir5** and **Ir6**.

Figure:



Tetrapyridoresorcin[4]arene cavitand: Synthesis, Characterization and pH sensing application

Manas Ranjan Swain[a], Manini Nayak[a], Anita Pati[a]*

[a]*Department of Chemistry, School of Applied Sciences, Kalinga Institute of Industrial Technology, Bhubaneswar-751024, Odisha*

(Email: anitapatifch@kiit.ac.in)

Abstract: Resorcin[4]arenes are a distinct class of supramolecular building blocks that are typically formed by the acid-catalyzed condensation reaction of resorcinol and aldehydes. Resorcin[4]arenes are distinguished by their well-defined cyclic tetrameric cavity with rich in π electron environment. Simple substitutions at the upper and lower rims, as well as their multiple hydroxyl (-OH) groups, expand the synthetic possibilities for the generation of a new class of resorcin[4]arene cavitands, and their applications in host-guest chemistry, nanoscience, catalysis, medicinal chemistry, and so on. A review of the literature reveals that pyridine-substituted resorcin[4]arene cavitands have a wide range of applications. It was also observed that the water soluble tetrakis(4-pyridinyl)resorcin[4]arene cavitand shows pH sensing ability due to presence of both donor (hydroxyl) and acceptor (pyridine) groups. The real time pH sensing application has been carried out through naked eye colorimetric experiment using both solution phase and C-4-pyridyl resorcin[4]arene based pH paper. A colour change from orange to pink is observed in basic medium. This naked eye colorimetric experiment eliminates the need for sophisticated instrument for data collection and verification. There are many acid-base pH indicators reported till date among which the most commonly used basic indicator in laboratories is phenolphthalein having pH sensing range within 8.2-10 and it is alcohol soluble. Though there are many pH indicators reported, most of them are water insoluble and not having a wide pH sensing range. The synthesized tetrakis(4-pyridinyl)resorcin[4]arene cavitand is highly water soluble and it changes its colour from orange to pink in all basic pH range of solutions.

Keywords: resorcinarene, cavitand, pH indicator

Effect of composition variation of microwave-assisted $CuBi_xIn_{1-x}Se_2$ microrod flowers on various properties for the optoelectronic applications

P. Priyadarshini[1*], R. Naik[1]
[1]*Institute of Chemical Technology, Indian Oil Odisha Campus, Bhubaneswar, 751013, India*
(E-mail: priyanka.priyadarshini2019iocb@gmail.com)

Abstract:

$CuInSe_2$ (CIS), as an I-III-VI_2 material, has been used as a commercial product for solar cell applications and is well known for being an effective light absorber. High potential solar energy conversion of this semiconductor is due to its band gap (1.04 eV), being at the red edge of the solar spectrum, large Bohr exciton radius (10.6 nm), high absorption coefficient, high radiation stability (compared to CdTe), and defect tolerance. [1,2] Variation in the composition is also a suitable method to approach controllable properties, greater efficiencies, and stability. The $CuIn_xGa_{1-x}Se_2$ (CIGS), $CuIn_{1-x}Fe_xSe_2$ (CIFS), and $CuIn_{1-x}Al_xSe_2$ (CIAS) are well-known alternative semiconductors in substituting Ga, Fe, and Al for In to enhance PV efficiency. [3,4] However, Bi as a trivalent cation dopant improves the absorbance performance and physical and chemical properties. Doping of such type of heavy ion element with a bigger radius of Bi^{3+} results in lattice mismatch and increases structural disorders.[5] Here, the $CuBi_xIn_{1-x}Se_2$ microrod flowers (x = 0, 0.4, 0.8) are synthesized by microwave synthesis procedure by taking different Bi/In concentrations. The variation in Bi/In concentration allows alterations in structural, morphological, and optical behaviors. The microwave-assisted $CuInSe_2$ showed polycrystalline nature with the appearance of $CuInSe_2$, CuSe, and InSe phases (in Figure 1(a)), while Bi incorporation led to the appearance of the Bi_2Se_3 phase along with the same. Slight shift in the Raman vibrational bands with varying Bi/In content suggests the composition variation induced structural rearrangements inside the matrix. Morphological study deliberates the transit from micro rods to clustered microrod flowers (in Scheme. 1) due to compositional change among bismuth and indium. The optical absorption response in Figure 1(b) is slightly enhanced with the increase in Bi content in the expense of In, which might be due to densification with larger radii Bi addition. This tends to reduce the optical band gap (E_g) by creating more disorder and defects over the gap region. Broad absorbance over visible regions and reduced E_g make them more appealing for photovoltaic applications. In order to study its potentiality for photodetector applications, the current-voltage measurement of all samples was done by illuminating 9W white LED bulb by varying the DC voltage at room temperature. The I-V characteristics of samples-based devices have been obtained under both dark and illumination conditions. The photocurrent of the device based on all synthesized materials has been significantly improved under illumination conditions from dark conditions. The observed photocurrent in the case of $CuInSe_2$ is in the μA range. The photosensitivity slightly increased with a change in Bi content, which showed the potential to be an applicant for photodetector applications. However, the photocurrent gradually reduced from mA to nA with an increase in Bi content replacing In concentration.

Figure:

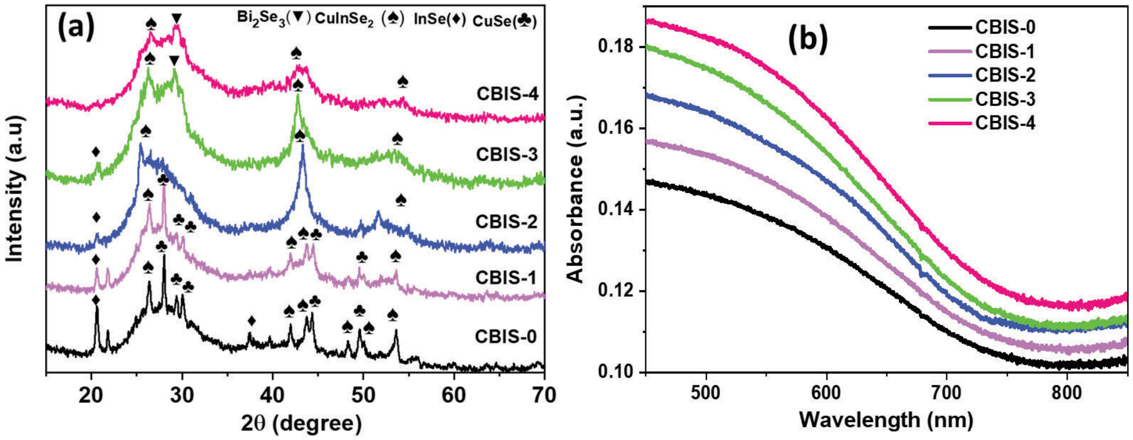
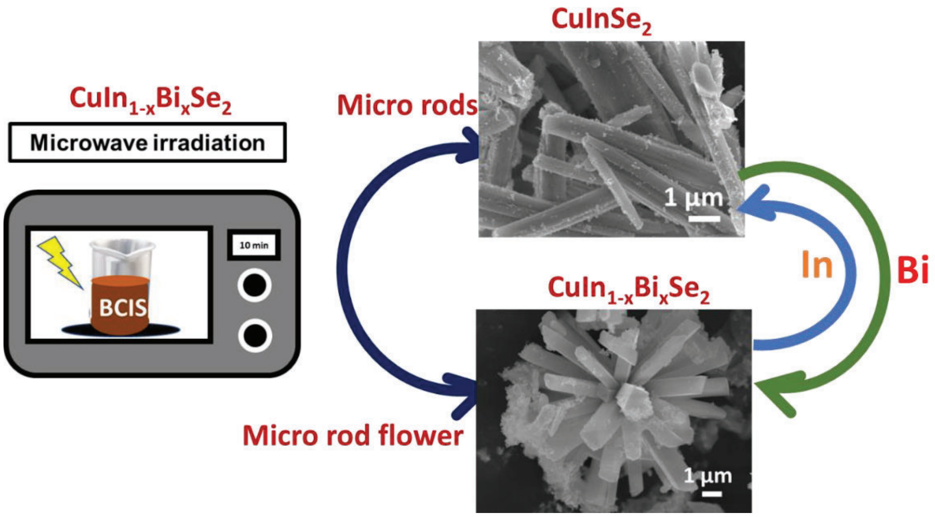


Figure 1. (a) XRD pattern and (b) Absorbance tuning of CBIS MFs.

Scheme:



Scheme. 1. Schematic presentation of morphological change from micro rod to micro rod flower with Bi/In composition variation.

References and Notes:

[1] Lian, W.; Tu, D.; Hu, P.; Song, X.; Gong, Z.; Chen, T.; Song, J.; Chen, Z.; Chen, X., Nanotoday **2020,** 35, 100943.

[2] Priyadarshini, P.; Senapati, S.; Bisoyi, S.; Samal, S.; Naik, R., J. Alloys Compd. **2023,** 945, 169222.

[3] Goncalves, B. F.; Lagrow, A. P.; Pyrlin, S.; Baird, B. O.; Botelho, G.; Marques, L. S. A.; Ramos, M. M. D.; Kovnir, K.; Mendez, S. L.; Kolenko, Y. V., Nanomaterials **2021,** 11(5), 1148.

[4] Odin, I. N.; Gapanovich, M. V.; Chukichev, M. V.; Novikov, G. F., Mendeleev Commun. **2020,** 30, 666-668.

[5] Kazmi, J.; Ooi, P. C.; Goh, B. T.; Lee, M. K.; Mohd, M. F.; Wee, R.; Karim, S. S. A.; Raza, S. R. A.; Mohamed, M. A., RSC Adv. **2020,** 10, 23297-23311.

Modulating Porosity and Hetero-atom Functionalities in Carbon Dot Grafted g-C_3N_4 for Dual Mode of Photocatalysis: Boosting Both Photocatalytic Solar to Green Hydrogen and Chemical Energy Conversion

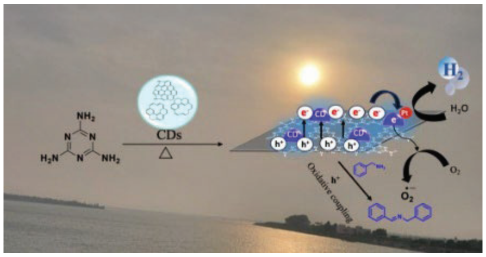
Ramesh Mandal [a] and Santanu Bhattacharyya [a]*

Department of Chemistry, [a] Department of Chemical Sciences, IISER Berhampur, Berhampur, Odisha-760010

(E-mail: rameshm@iiserbpr.ac.in)

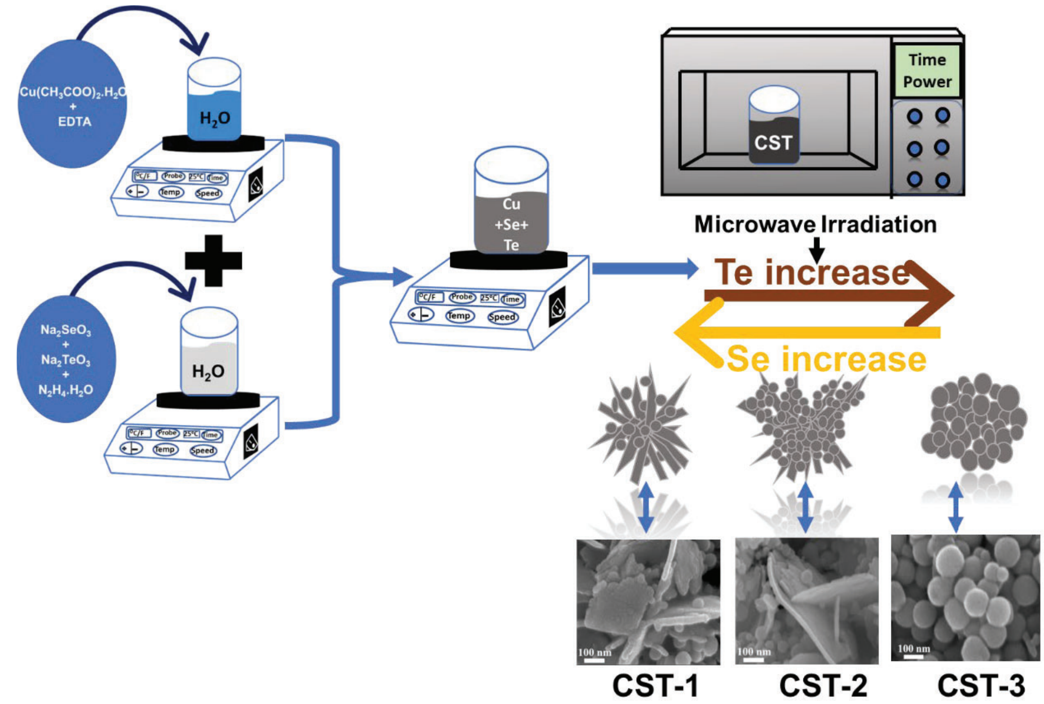
Abstract: Herein, we have intrinsically modified the structural and elemental features of g-C_3N_4 by incorporating two different types of citric acid based carbon dots with defined N-atom functionality.[1,2] It is observed that incorporation of carbon dots having more amorphous content and specific nitrogen atom functionalities at the edge sites improves the porosity, hetero atom functionality, visible light absorption and effective active sites of the g-C_3N_4 matrix for photocatalysis. Details structural and elemental features along with surface area as well as surface porosity studies have been investigated by transmission electron microscopy, X-ray photoelectron spectroscopy and N_2 adsorption-desorption isotherms. The intriguing structural modifications of g-C_3N_4 by grafting carbon dots was further correlated with the ongoing photophysical properties through steady state and time resolved spectroscopy. All the composites are further utilized for photocatalytic solar hydrogen production. Photocatalytic H_2 production was calculated to be 12 mmol/g after 12 hrs of continuous irradiation with external quantum efficiency of almost 30% for the final optimized composites. In addition, the optimized photocatalyst was also used to generate solar H_2 even from raw sea water. Photocatalytic H_2 production data was finally supported by in depth electrochemical study and band gap analysis from valence band X-ray photoelectron spectroscopy. Finally based on the fundamental structure-property correlation and band gap alignments, those all carbon based composites are chosen for selective organic transformation of benzylamine to imine derivatives where both the photoinduced electrons and holes are simultaneously used. The product formation was almost 85%. In depth mechanism was revealed by detailed NMR and Mass spectroscopy. Overall, we have developed all carbon based composites made of g-C_3N_4 and specific N-functionalized amorphous carbon dots with dual mode of photocatalytic activities, *i.e.*-a) highly efficient green hydrogen production and b) selective organic transformation.

Scheme:



References and Notes:

1. Bhuyan, R.; Bramhaiah, K.; Bhattacharyya, S., J. Colloid Interface Sci. 2022, 605, 364–372.
2. Bramhaiah, K.; Bhuyan, R.; Mandal, S.; Kar, S.; Prabhu, R.; John, N. S.; Gramlich, M.; Urban, A. S.; Bhattacharyya, S., J. Phys. Chem. C 2021, 125 (7), 4299–4309.



Scheme 1. Schematic representation of the microwave-assisted synthesis of CST nanomaterial.

References:

1. Das, S; Senapati, S; Pradhan, G. K.; Varadharajanperumal, S; and Naik, R., ACS Appl. Nano Mater. 2023, 6, 7, 5298–5312
2. Krishnan, N. N.; Vijayakumar, S.; Gnanadurai, P.; Shabu, R.; and Preetha, K. C., J. Nanosci. Tech. 2018, 04, 345−347.
3. Singh, S.; Katyal, S. C.; and Goswami, N., Appl. Phys. A: Mater. Sci. Process. 2019, 125, 638.
4. Cao, M.; Wang, X.; Cao, W.; Fang, X.; Wen, B.; and Yuan, J. Small 2018, 14, 1800987.
5. Saadi, H.; Benzarti, Z.; Rhouma, F. I. H.; Guermazi, S.; Khirouni, K.; and Vieira, M. T., J. Mater. Sci.: Mater. Electron. 2021, 32, 1536−1556.

Adsorption of methylene blue dye on chemically and physically modified rice straw derived biomass

Soumyaranjan Senapati[1], Jyotirmayee Giri[1], Prasanta Rath[1], Tapan Kumar Bastia[1] and Alok Kumar Panda[1] *

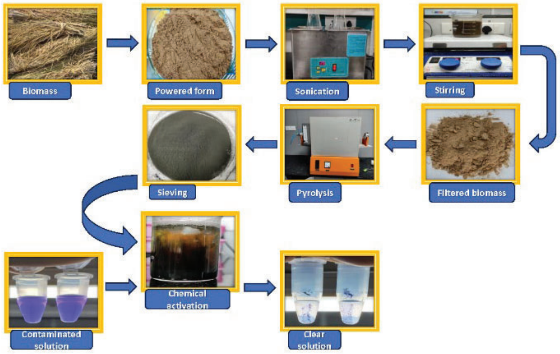
[1] *Environmental Science Laboratory, School of Applied Sciences, KIIT Deemed to be University, Bhubaneswar, 751024, Odisha, India*

* Correspondence: alok.pandafch@kiit.ac.in

Abstract: The planet needs water to survive, but fresh water is becoming scarce because of the increasing human population and the modernization of various sectors such as agriculture, industry, and health. One of the major sources of water pollution is the dyes that are used in different industries such as textiles, pharmaceuticals, leather, cement, etc. Dyes are very harmful to the environment and living beings because they can cause cancer, toxicity, and other problems. Even a small amount of dyes can affect the natural balance of plants and animals in the water. Therefore, it is very important to treat the wastewater that contains dyes before releasing it into the environment. One of the methods that is widely used for wastewater treatment is adsorption, which is a process where a substance sticks to the surface of another substance. Adsorption is preferred because it is simple, cheap, effective, and eco-friendly. Biochar (BC) is a type of adsorbent that is made from organic waste such as plant or animal matter. It is a porous material that has rich in carbon and aromatic compounds and can remove dyes from water. In this study, we used biochar prepare from rice straw to remove methylene blue, which is a common dye causes water pollution. We have used a tubular furnace to prepare the biochar and analyse its properties using different characterization techniques such as XRD, FESEM-EDAX, FTIR, and Raman. We have also studied mechanism of adsorption process and the factors like pH, PZC, dose and dye concentration that affects in the adsorption process. Different mathematical isotherm models like Langmuir Isotherm, Freundlich isotherm have studied as well as different kinetic model like Pseudo second kinetics and Pseudo first order kinetics have studied and fitted in their corresponding equations. Also, checked the diffusion process of dye through the biochar by using different diffusion models like film diffusion and intraparticle diffusion.

Keywords: Wastewater, Adsorption, Dye, Methylene blue, Biochar, Isotherm, Kinetic, XRD, SEM, EDAX, FTIR, Raman, Intraparticle diffusion, Film diffusion.

Graphical Abstract:



References:

1. Lonappan, L., Rouissi, T., Das, R. K., Brar, S. K., Ramirez, A. A., Verma, M., and Valero, J. R. *Waste Management* **2016**, 49, 537-544.
2. Sahu, S., Pahi, S., Tripathy, S., Singh, S. K., Behera, A., Sahu, U. K., and Patel, R. K. *Journal of Molecular Liquids*, **2020**, 315, 113743.

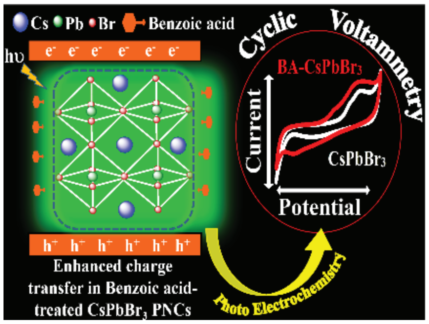
Exploring the Role of Short Chain Acids as Surface Ligands on Photoinduced Charge Transfer Dynamics from the $CsPbBr_3$ Perovskite Nanocrystals

Subarna Biswas[a] , Dr. Nimai Mishra[b]

[a,b]Department of chemistry, ICT Bombay,Indian Oil Odisha Campus Bhubaneshwar,odisha-751013

E-mail: subarna.nanochem@gmail.com

Abstract: Recently the scientific world have seen an enormous rise of research activities on Cesium lead halide perovskites nanocrystals[PNCs] in various areas like of solar cells , light-emitting diodes,photodetector, scintillators and photocatalysis. Although most of these PNCs are adopted successfully in photovoltaic and optoelectronic devices, the use of it as a photocatalyst remains particularly challenging. This arises mainly due to the effective surface passivation of both amines and carboxylic acids during the colloidal synthesis which limits the access of electron and hole acceptor to the active sites of PNCs. Most literature on both optoelectronic and photocatalytic properties perovskite focus on tuning it`s properties by engineering the the inorganic core by cation or anion Exchange and impurity doping,but the surface chemistry dependent interfacial charge transfer and the dynamics of exciton between CsPbX3 PNCs and molecular acceptor has not been studied much. . Here in this study, we have done post-treatment on CsPbBr3 PNCs with short-chain ligands Benzoic acid [BA] and Ascorbic acid [AA] and observed that both acids treated PNCs show enhanced stability, as well as optical properties but BA-treated PNCs, shows highest charge transport rate due to its conjugating nature. The photoelectrochemical measurements also show the most efficient electron flow across the surface of the PNC with BA-treated PNCs. Higher carrier lifetime along with fast charge transfer makes BA-treated PNCs an ideal candidate for real-life device application.



References:

1. Biswas et al. *J. Phys. Chem. Lett.* 2023, 14, 7, 1910–1917

Symmetrical organic cation based one dimensional halide perovskite ferroelectric semiconductor

Prabhanjan Pradhan[1], Biplab K. Patra[1]

[1] *CSIR-Institute of Minerals and Materials Technology*

*prabhanjan.p@immt.res.in

Abstract: Halide perovskites with organic cations at A site are generally referred to an organic inorganic halide perovskite (OHIP). Through deliberate manipulation of the A-site constituents using various organic cations, a diverse spectrum of OIHPs can be synthesized, each exhibiting distinct and tunable characteristics. One of the recent phenomena discovered in these halide perovskites is the presence of the presence of ferroelectricity. Ferroelectricity arises in these OIHPs, either due to the presence of polar/asymmetrically aligned A cation or due to displacement of B site cation from its original position. But in most of OIHPs reported till now, ferroelectricity originates due to the alignment of polar/ asymmetric organic A site cation. Here we report first time a phosphonium based ferroelectric halide perovskite with symmetrical A site cation, micro tubes. These rods are synthesized at room temperature under ambient air. These materials show notably high phase transition temperature of 685K with notable remanent polarization and maximum polarization. Ferroelectricity in our material is generated due to distortion in PbBr6 octahedra rather than aligning of A site cation as shown by conventional OIHPs. It absorbs solar light in the UV-visible region with a direct bandgap of 3.3 eV and highly ordered crystalline oriented structures. We have done theoretical calculations of band structures and crystal orientation in space to compare and confirm our experimental findings. Synthesized rods retain their properties and morphology for months under natural environment. They do not lose their properties under normal condition storing for longer times.

Keywords: Halide perovskite, Asymmetric, Ferroelectricity, Polarisation

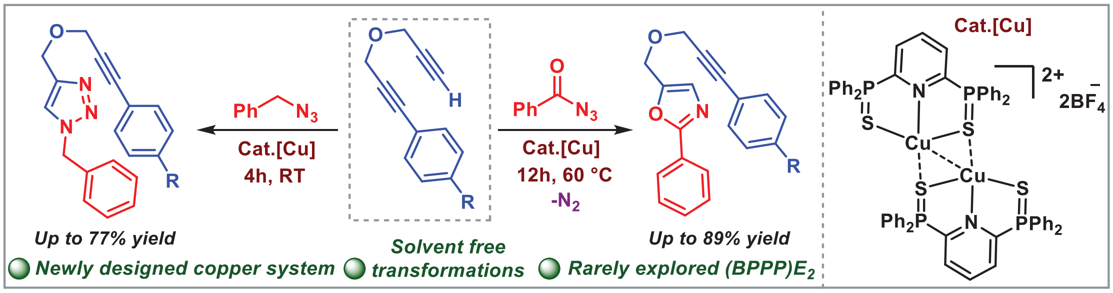
Copper(I) Complexes Bearing Electronically Tuned ENE (E = S, Se) Pincer Ligands; Synthesis and Applications in Cyclization of 1,6-diynes

Bhagyashree Das, Amiya Kumar Sahoo, and Adinarayana Doddi*
Department of Chemical Sciences, Indian Institute of Science Education and Research Berhampur, Industrial Training Institute, Engineering School Road, 760010, Berhampur, Odisha
(E-mail: adoddi@iiserbpr.ac.in)

Abstract:

***P*NP** pincer ligand namely BPPP (bis(diphenylphosphino)pyridine) has played a tremendous role in the coordination and organometallic chemistry because of its effective ligating character, which has been employed in the isolation of numerous transition metal complexes of mono, di and multimetallic systems. The reaction chemistry and application of the corresponding chalcogenophosphoryl species of the type $[Ph_2P(E)(C_5H_3N)P(E)Ph_2]$ (E = S (**1**), & Se (**2**)) synthesized from BPPP species have not been studied in a great deal.[1] Dark orange solids of dicationic copper(I) complexes of the type $[\{(BPPP)E_2\}Cu]_2[BF_4]_2$ (E = S (**3**), Se (**4**)) were prepared by the reactions of $(BPPP)E_2$ (E = S, Se) with $[Cu(CH_3CN)_4]BF_4$. These complexes were fully characterized by various spectroscopic techniques.

The single crystal X-ray structures showed the presence of cuprophilic (Cu···Cu) interactions between the two mono-cationic Cu(I) units. Subsequently, the catalytic activity of these two complexes were studied in the synthesis of biologically active heterocyclic oxazole and triazole derivativies in good to excellent yields.[2] Varities of substrates were screend, for instance carbonyl azides and internal terminal alkynes for the synthesis of 2,3-disubstituted oxazoles bearing alkyne-phenyl propargylic ether substituents.[3] Furthermore, the detailed mechanistic investigations were performoed by using mass spectral analysis. The complete details of the structures, and catalytic studies will be discussed in this poster presentation. [4]



Scheme. Catalytic applications of cheap and Earth-abundant copper(I) complexes in oxazoles and triazoles synthesis.

References

1. R. Sevcik, M. Necas, J. Novosad, *Polyhedron* **2003**, *22*, 1585.
2. I. Cano, E. Álvarez, M. C. Nicasio, P. J. Pérez, *J. Am. Chem. Soc.* **2011**, *133*, 191.
3. V. K. Tiwari, B. B. Mishra, K. B. Mishra, N. Mishra, A. S. Singh, X. Chen, *Chem. Rev.* **2016**, *116*, 3086.
4. **B. Das**, A. K. Sahoo, S. K. Banjare, S. K. Panda, C. S. Purohit and A. Doddi, *Dalton. Trans.* **2023, *accepted manuscript; doi.org/10.1039/D3DT01989F***

Design and synthesis of Binary Cobalt ferrite/poly(m-aminophenol) hybrid nanocomposites for high-performance photocatalytic degradation of dyes /Chromium(VI)

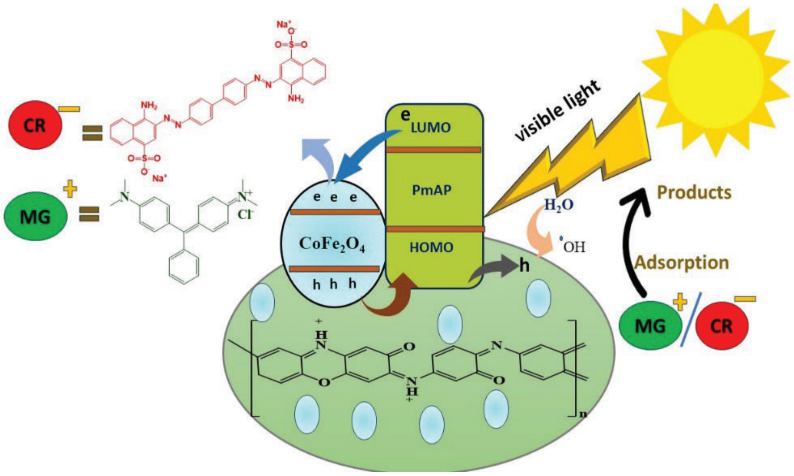
Chirasmayee Mohanty[1], Ajaya K. Behera[1] and Nigamananda Das[1*]

[1]Department of Chemistry, Utkal University, Bhubaneswar, Odisha, India-751004

Abstract: Recent years have been a persistent interest in an effective, affordable, environmentally friendly and easily separable catalyst to treat environmental toxins due to their enormous potential for environmental protection and cleanup. The remarkable ability of the Poly(m-amino phenol)(PmAP)activated heterojunction Cobalt ferrite (CoFe2O4) catalyst to degrade Congo red(CR) /Malachite green(MG) dyes and hexavalent Chromium Cr(VI)in an aqueous solution under ambient conditions is reported here. The nano photocatalyst was synthesized via facile Chemical oxidative polymerization process. PXRD, FTIR, SEM, HRTEM, XPS, EDX, and DRS techniques were used to confirm the synthesized catalyst's physicochemical characteristics and structural details. The synthesized catalyst demonstrated accelerated degradation of dyes approximately 98% for the dye concentration of 20 ppm within an hour at ambient conditions with catalyst loading of 1 g/L. The heterostructure catalyst's practical uses for water remediation at ambient conditions may be facilitated by its facile synthesis, simple separation by an external magnet, robust reusability, and high degrading capability. In the present study MG /CR and Cr(VI)degradation in aqueous solution under visible-light irradiation (420nm to 800nm) is used to assess the photocatalytic activity of photocatalysts as-synthesised. The photogenerated holes in the valence band (VB) of CoFe2O4 that can transfer directly to the HOMO of PmAP and the excited state electrons in PmAP that can migrate to the conduction band (CB) of CoFe2O4 are responsible for the dramatic increase in photoactivity. This effectively prevents the direct recombination of electrons and holes. The findings demonstrate that CoFe2O4-PmAP nanocomposites are more Photo catalytically active and stable than both pure PmAP and naked Cobalt ferrite. According to the results of the current study, CoFe2O4-PmAP hybrid nanocomposite is a pertinent and sustainable adsorbent for treating wastewater and eradicating aqueous dyes.

Keywords: Cobalt ferrite, poly-m-aminophenol, hybrid nanocomposites, dye degradation, Cr(VI) reduction

Schematic figure



Fabrication and characterizations of luffa sponge fiber reinforced soy-based composites

Diptiranjan Behera*, Shruti S. Pattnaik, and Ajaya K. Behera

Department of Chemistry, Utkal University, Vani Vihar, Bhubaneswar, Odisha-751004

(E-mail: ranjandipti538@gmail.com)

Abstract: Luffa sponge fiber is a waste lignocellulosic material required attention from researcher for the development of eco-friendly biodegradable composite as an alternant of nondegradable thermoplastic. In this study, luffa sponge fiber reinforced composites were produced using soy and different weight percentages of poly (vinyl alcohol) (PVA) resins. Due to chemical interaction, the luffa-soy-PVA composite attained maximum tensile strength of 45.8 MPa, flexural strength of 42.7 MPa, and storage modulus of 2322 MPa. After water absorption, the mechanically optimized composite absorbed just 32.9 % of the water. Weight loss of composites following various degradation durations, as well as subsequent fourier transform infrared characterization and field emission scanning electron micrographs, demonstrated that created composites are entirely biodegradable. As luffa, and soy are the prime components of fabricated composite and biodegradable in nature, hence their concerned composite was also found completely biodegradable and after service periods can be easily mixed with soil improving its fertilization capacity unlike non degradable plastic.

Keywords: Luffa sponge fiber; Soy resin; Poly (vinyl alcohol); Ecofriendly; Biodegradation

Scheme/Figure:

References:

1. Gupta, V. K., Agarwal, S., Singh, P., & Pathania, D. (2013). Acrylic acid grafted cellulosic Luffa cylindrical fiber for the removal of dye and metal ions. *Carbohydrate polymers*, *98*(1), 1214-1221.
2. Behera, A. K., Sen, R., & Adhikari, B. (2022). Environment-friendly fully biodegradable jute-poly (vinyl alcohol) modified soy composite development as plastic substitute. *Journal of Natural Fibers*, *19*(3), 905-914.

Triazine skeletal covalent organic frameworks: A versatile highly positive surface potential triboelectric layer for energy harvesting and self-powered applications

[1]**Jagannath Panda**, [2]Sugato Hajra, [3]Jaykishon Swain, [2]Hang-Gyeom Kim, [2]Manisha Sahu, [1]Malay Kumar Rana, [3]Raghabendra Samantaaray, [2,4]*Hoe Joon Kim, [5]*Rojalin Sahu

[1]*Department of Chemical Sciences, Indian Institute of Science Education and Research, Berhampur-760010, India*

[2]*Department of Robotics and Mechatronics Engineering, Daegu Gyeongbuk Institute of Science and Technology, Daegu-42988, South Korea*

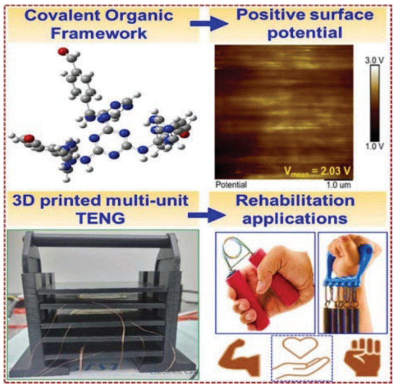
[3]*School of Chemical Technology, Kalinga Institute of Industrial Technology (KIIT), Deemed to be University, Bhubaneswar- 751024 India*

[4]*Robotics and Mechatronics Research Center, Daegu Gyeongbuk Institute of Science and Technology, Daegu-42988, South Korea*

[5]*School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT), Deemed to be University, Bhubaneswar- 751024 India*

(E-mail: jagannathp@iiserbpr.ac.in)

Abstract: Covalent organic frameworks (COFs) with triazine skeleton have been developed via reticular chemistry. In this present work, a triazine-based nitrogen-rich organic moiety has been used for the synthesis of the COF and then tested for the output performance of a triboelectric nanogenerator (TENG). The synthesized COF has been characterized by several physical characterization techniques. For the first time, the surface potential of the prepared COF material was tested experimentally using Kelvin probe force microscopy which indicates a very high positive triboelectric potential of 2.03 V. The single unit of COF-based TENG delivered 70 V, 0.6 μA, and 38 nC as an electrical output. In the case of multi-unit TENG, the current and voltage values are boosted as the parallel connection of four units of TENG gave the peak-to-peak current output rises by 6.3 μA while the series connection of four units of TENG gave a high peak-to-peak voltage of 175 V. This work describes the synthesis of N-rich COF material, the facial construction, fabrication of the TENG, and the excellent energy harvesting performance with the realization of low-cost self-powered hand strengthening with a self-powered device. This result paves the way to achieve fruitful exercise monitoring units towards improving lifestyle.



References:

1. Hajra, S., Panda, J., Swain, J., Kim, H.G., Sahu, M., Rana, M.K., Samantaray, R., Kim, H.J. and Sahu, R., *Nano Energy*, **2022**.*101,107620.*

Synthesis, characterization and adsorption of novel magnetic activated carbon for effective removal of Cr(VI) from aqueous solution

Jyotirmayee Giri[1], Soumyaranjan Senapati[1], Prasanta Rath[1], Tapan Kumar Bastia[1*] and Alok Kumar Panda[1*]

[1]Environmental Science Laboratory, School of Applied Sciences, KIIT Deemed to be University, Bhubaneswar, 751024, Odisha, India
[*]Correspondence: tapan.bastiafch@kiit.ac.in and alok.pandafch@kiit.ac.in

Abstract

This study aims to synthesize activated magnetic biochar using a single-step approach and explore solute-solvent mechanisms for removing hexavalent chromium [Cr(VI)] from the aqueous solution. The removal of a toxic contaminant like Cr(VI) from the water via green adsorbents like biochar and activated carbon is an eco-friendly technique. In this paper, using agricultural waste rice straw was synthesized and activated carbon as a raw material, pre-treated using magnetic ferric oxide/activated carbon at different ratios (SW_10, SW_30, SW_50, SW_100) was prepared by the chemical co-precipitation method, and Cr(VI) adsorption in water was applied and pyrolyzed at 500° C. The synthesized materials were characterized by advanced characterization techniques including XRD, and SEM. In aqueous solutions, Cr(VI) break down to HCrO4− , CrO42− , and Cr2O72− ions. However, at low pH (~1 − 4), HCrO4− ion attributes electrostatic force of attraction, which encourages higher adsorption of Cr(VI) ions. Overall, batch experiments demonstrated that the initial Cr(VI) concentration, pH, different dosages, and adsorption time on the adsorption effect of Cr(VI) were evaluated. Therefore, electrostatic interaction and ion exchange dominates Cr(VI) adsorption onto activated magnetic biochar at low pH. Results illustrated that the maximum Cr(VI) adsorption was achieved by different ratios of iron (SW_10, SW_30, SW_50, SW_100) with a removal rate of 90.8% at the optimum pH of 2.0 at 25^0C and an adsorption time of 4hr. The results of XRD, and SEM characterization analysis of Cr(VI) before and after adsorption suggested that the adsorption mechanism is mainly based on chemisorption, supplemented by physical adsorption, accompanied by electrostatic attraction and complexation. Overall, the activated magnetic biochar synthesized from rice husk was more efficient than raw biochar in removing Cr(VI) ions from the aqueous solution.

Keywords: Magnetic synthesized biochar, Adsorption, Metal removal, XRD analysis, SEM analysis

GO-TiO_2 nanocomposite-An efficient catalyst for the synthesis of trisubstituted Imidazole derivatives

Kanyanjali Samal, Manas Ranjan Swain, Anita Pati*

Department of Chemistry, School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT) University, Bhubaneswar-751024, Odisha, India

Email: anitapatifch@kiit.ac.in

Abstract: A flexible, reliable, and effective method for the synthesis of a wide variety of highly functionalized 2, 4, 5-trisubstituted Imidazole derivatives are reported. It involves a one-pot, multicomponent process using a variety of aldehydes, ammonium acetate, and benzil /benzoin in the presence of non-toxic, readily accessible, affordable, reusable and unexplored catalysts, GO-TiO_2. This ultrasonication one-pot synthesis method has numerous benefits, including benign reaction conditions, a quick reaction time, low catalyst loading, efficient productivity with better atom economy and functional group tolerance, which makes this methodology realistic. TiO_2 is known for its excellent catalytic activity for many organic reactions, however GO-TiO_2 nanocomposite is yet to be explored in the field of heterocyclic synthesis. In the present work GO-TiO_2 nanocomposite has been introduced as a catalyst for the synthesis of Imidazole derivatives in both conventional as well as ultrasonication methods and among the TiO_2 and GO-TiO_2 catalysts, GO-TiO_2 exhibited better catalytic efficiency and provided great substrate scope with α-hydroxy ketone (benzoin) as well as 1, 2-diketone (benzil).

Ortho C-H Bond Activation by Pyridine-2-Aldoxime in a Iridium(III) Metal Complex

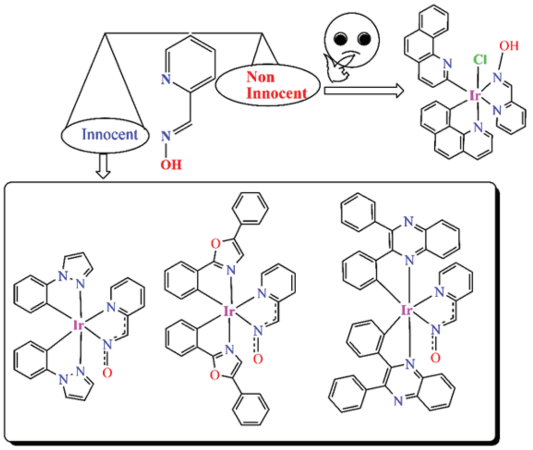
Madhusmita Jadab, Kahnu Charan Pradhan, Satyanarayan Pal*

Department of Chemistry

Utkal University, Bhubaneswar: 751004

(E-mail: snpal@utkaluniversity.ac.in)

Abstract: A series of Ir(III) complexes of formula $[Ir(C^\wedge N)_2(pyrald)]$ were designed and synthesised from the reaction of $[(C^\wedge N)_2Ir(\mu\text{-}Cl)_2Ir(C^\wedge N)_2]$ and pyridine-2-aldoxime (pyrald) {C^N=1-phenylpyrazole (phpyr), 2,5-diphenylbenzoxazole (phox), 2,3,-diphenylquinoxaline (phquinox), 7,8-benzoquinoline (benzq)}. All the complexes were characterised through ^{1}H NMR, UV-Vis, emission spectroscopy, mass analysis and cyclic voltammetric studies. The molecular structure of iridium complex derived from 7,8-benzoquinoline ligand, [Ir(benzq-κN, κC^{10})(benzq-κC^2)(Hpyrald)(Cl)], confirmed first ortho C-H bond activation in a iridium coordinated 7,8-benzoquinoline moiety. It was suspected that pyridine-2-aldoxime played a decisive role in causing such C-H activation. To explore such possibility, more number of iridium complexes were prepared from three more different cyclometallating ligands and characterised. However, the complexes with other cyclometallating ligand did not display such unusual C-H activation. Thus, the role of pyridine-2-aldoxime in C-H bond activation remains inconclusive and requires more investigation.



References and Notes:

1. K.C. Pradhan, M. Jadab, S. Barik, N. Behera, B. Bag, S. Pal, J. Mol. Struct., **1271**, 133998, (2023).
2. K.C. Pradhan, H.K. Kisan, S.Pal, *RSC Adv.*, **11**, 12578-12582 , (2021).

Spent Catalyst Derived Mo-MOF: Triboelectric Nanogenerator and Energy Harvesting

[1#]Jaykishon Swain, [#2]Sugato Hajra, [#1]**Niharika Das**, [3*]Pankaj Parhi, [2]Swati Panda, [1]Anulipsa Priyadarshini, [1]Jagannath Panda, [4]Alok Kumar Sahu, [4]Perumal Alagarsamy, [5]Vivekananthan Venkateswaran, [2*]Hoe Joon Kim, [1*]**Rojalin Sahu**

a Department of Robotics Engineering, Daegu Gyeongbuk Institute of Science and Technology, Daegu-42988, South Korea. E-mail: joonkim@dgist.ac.kr

b Department of Physics, Indian Institute of Technology, Guwahati, Assam-781039, India

c School of Applied Sciences, Kalinga Institute of Industrial Technology (Deemed to be University), Bhubaneswar-751024, India. E-mail: rsahufch@kiit.ac.in

d Department of Electrical Engineering, Siksha 'O' Anusandhan (Deemed to be University), Bhubaneswar-751030, India

Email: rsahufch@kiit.ac.in/rojalinsahu.chem@gmail.com

Abstract: The spent catalysts discarded during chemical manufacturing can be a source of pollution and classified as hazardous waste. Looking at the bright sides of the mission of waste management such as recycling, reducing, reuse such types of the spent catalyst can be chemically treated to extract valuable salts and metals. Such a process not only reduces waste disposal issues but also promotes a circular economy ecosystem. This present study aims at the extraction of MoO_3 from the spent petroleum catalyst, Mo–Ni/Al_2O_3, and further processing of Mo-MOF particles using extracted MoO_3 and imidazole acting as an organic binder. The structural, morphology, and thermal properties of the Mo-MOF were evaluated. The surface roughness and positive surface potential of the Mo-MOF were achieved. The Mo-MOF/Kapton-based TENG generated a 148 V voltage, 470 nA current, and 17 nC charge. Further, TENG was utilized to charge the capacitors, and powering of the electronic devices was demonstrated. The repetition of the boxing punches and the impact of punches can be monitored using TENG paves the way towards intelligent sports.

Keywords: Recycle, spent catalysts, triboelectric, exercise monitoring

References and Notes:

1. Spent Catalyst Derived Mo-MOF: Triboelectric Nanogenerator And Energy Harvesting" (Research Article, No. ente.202300498R1) to Accepted in Energy Technology, 2023, Wiley

Disinfection of antibiotic resistant bacteria from municipal tap water using Fenton-like process

Abstract: Water borne illness are of important concern in the emerging world. Many dreadful pathogens are carried and spread through water. At the same instant, these pathogens are developing resistance to most of the antibiotics. This alarming situation calls for development of some techniques which not only eliminates the microbes but also destroys its antibiotic resistant genes. Advanced oxidation process is considered as a good option to this tackle this. The production of reactive oxygen species is the key feature of this type of process. They disinfect the bacteria from water along with eliminating their drug resistant gene. Here, the disinfection of *Shigella dysenteriae* in tap water using Fenton like process is reported. Different process parameters were optimised to obtain the best result. Hydrogen peroxide and Iron based nanoparticles were used along with ultrasound to catalyse the disinfection of *S. dysenteriae* from municipal tap water. The impact of treatment on the real water setup (tap water) was evaluated to explore its real life applications.

Presented by: Pranjal

Supervisor: Dr. Suraj Kumar Tripathy

KIIT School of Biotechnology.

KIIT DU

Unexpected structural preference with metallophilic Ag--- Au contacts in silver(I)-N heterocyclic carbene cluster; experimental and theoretical approach

Priyanka Sahu and Joydev Dinda*

Department of Chemistry

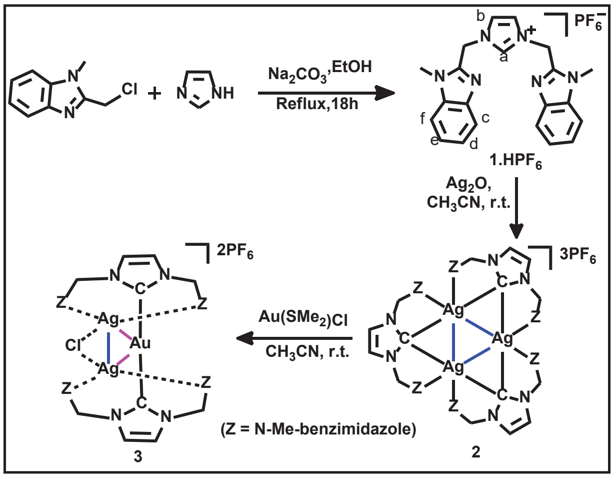
Utkal University, Vani Vihar, Bhubaneswar-751004

(E-mail: joydevdinda@gmail.com)

Abstract: A novel synthetic site-selective approach has been adopted for the synthesis of a heterobimetallic cluster of a new *NCN*-pincer 1,3-bis-(1-methyl-1H-benzo[d]imidazol-2-yl)methyl)-1H-imidazol-3-ium hexafluorophosphate (**1**.HPF_6). The complex $[Ag_3(\mathbf{1})_3][PF_6]_3$, **2** has been prepared *via* the Ag_2O route; which undergoes transmetallation to yield a cluster that seems to be the first example of the heterobimetallic trinuclear system $[Au\text{-}Ag_2(\mathbf{1})_2Cl][PF_6]_2$, **3**. Finally, trinuclear cluster geometries of **2** and **3** were confirmed by SCXRD studies. Interestingly, Au(I) binds with $C_{carbene}$ selectively that transmetallated from the cluster of **2**. In both the trinuclear clusters, M---M interactions were further inspected by Gauge Independent Atomic Orbital (GIAO) computations. Both, **2** and **3** are luminescent and possess σ-aromaticity, the NICS values support that **3** is more aromatic than **2**.

Figure:

Scheme:



Deoxygenative Hydrogenation of Amides to Amines Using Lewis Acidic Boron Appended Ruthenium Carbene Complexes

Raju Sharma, Prosenjit Daw*

Department of Chemistry

Indian Institute of Science Education and Research, Berhampur

(E-mail: rajus19@iiserbpr.ac.in)

Abstract: Amine compounds are present as a key structural motif in many biologically active natural products and widely used in dyes, agrochemicals, and pharmaceuticals.[1] The common method to synthesize amines involves the use of naturally occurring amides or artificially via the amination of carboxylic acid derivatives.[2] Compared with the other carboxylic derivatives, amides are less electrophilic and thus need the over-stoichiometric amount of external Lewis acid additives for their activation. Traditional organic approach for the reduction of amides involves the use of external borane (B_2H_6), $LiAlH_4$, or $NaBH_4$, however, such reagents are highly toxic, hazardous, and restrict functional group tolerance.[3] Thus, the development of ambient and efficient catalytic hydrogenation systems is highly preferable for sustainable amine synthesis. Herein, a new Ru-bidentate carbene complex appended with pinacolato borane as Lewis acidic arm and piperidine as Lewis basic arm in the secondary coordination sphere was synthesized and its reactivity study towards amide deoxygenative hydrogenation was explored. Using 1 mol% of Ruthenium-catalyst with silane as a hydride source up to 97% NMR yield of amine was obtained under optimized reaction conditions. The optimized reaction conditions were used further to synthesize various tertiary amides with different electronic substituents.

References and Notes:

1. B, Li.; Sortais, J.B.; Darcel C., *RSC Adv.* **2016,** 6, 57603-57625.
2. Werkmeister, S.; Junge, K.; Beller, M., *Org.Process Res. Dev.* **2014,** 18, 289-302.
3. Chardon, A.; Morisset, E.; Rouden, J.; Blanchet, J., *Synth.* **2018**, 50, 984–997.

E-stilbene embedded Diphyrin(6.0.1.0) and its B^{III} Complex

Rampal Vishwakarma and A. Srinivasan*

Department of Chemistry

NISER, OCC of HBNI, Bhubaneswar, Odisha, India 752050

(E-mail: rampal.vishwakarma@niser.ac.in)

Abstract: The macrocycle with four pyrrole units directly connected with four *meso*-carbon atoms is known as Porphyrin. It has 18π electrons in the conjugation pathway and follows the Hückel aromatic character. Based on the structural modification, the porphyrin analogues can be categorized as larger congeners called expanded porphyrins and smaller ones known as contracted porphyrins.[1] By replacing one or more pyrrole / *meso*-carbon atoms in the porphyrin core affords contracted porphyrinoids. The macrocycle with four pyrrole units and three *meso*-carbon atoms are known as Corrole which constitutes a bridge between porphyrin and corrin units. The trianinoic inner core of corrole is effectively utilized to stabilize higher oxidation state metal ions and are widely applied in sensors, catalysis and dye-sensitized solar cells.[2] The macrocyclic core with three pyrrole unit and three *meso* carbons are coined as Triphyrins. The triphyrin core is stabilized in the form of B^{III} complex and adopt a nonplanar cone-shaped conformation.[3] To the best of my knowledge, the simplest contracted porphyrin, Diphyrin(6.01.0) (**1**) with two pyrrole units, is hitherto unknown in the literature. In this poster presentation, we wish to report the synthesis, spectral and structural analysis of *E*-stilbene embedded Diphyrin(6.0.1.0) and its B^{III} Complex (**2**) (Figure1).

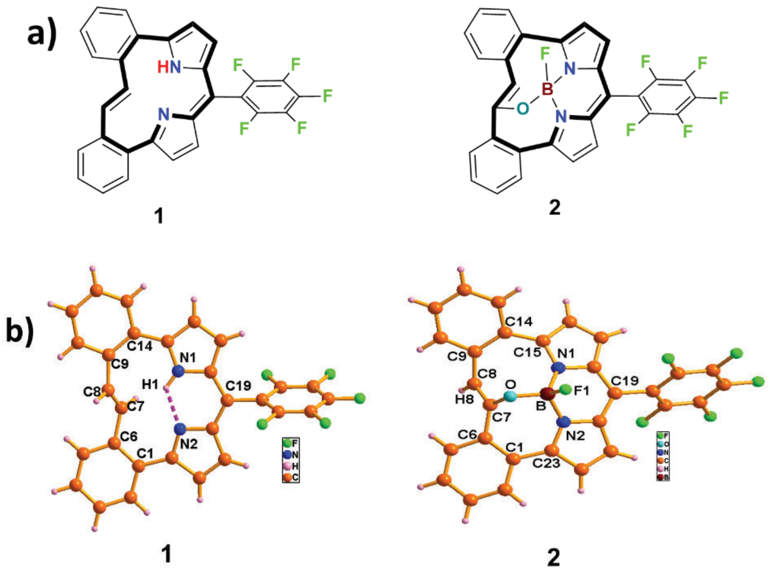


Figure 1. a) Structures of Diphyrin(6.0.1.0) (**1**) and respective B^{III} Complex (**2**). b) Single Crystal X-ray structures of **1** and **2**.

References and Notes:

1. Sessler, J. L.; Gross, Z.; and Furuta, H., *Chem. Rev*. **2017**, *117*, 2201−2202.
2. Orłowski, R.; Gryko, D.; and Gryko, D. T., *Chem. Rev*. **2017**, *117*, 3102−3137.
3. Shimizu, S., *Chem. Rev*. **2017**, *117*, 2730−2784.

Catalytically induced nanographites in boron-doped diamond films by nickel-ion implantation/annealing for enhanced microplasma illumination

S. S. Sethy[1], K. J. Sankaran[1], K. Devarani[2], K. Asokan[2], J. P. Thomas[3], K. Haenen[4]

[1]*CSIR-Institute of Minerals and Materials Technology, Bhubaneswar-751013, Odisha.*

[2]*Inter-University Accelerator Centre, New Delhi-110 067.*

[3]*WATLab and Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L3G1, Canada.*

[4]*Institute for Materials Research (IMO), Hasselt University, 3590 Diepenbeek, Belgium.*

(E-mail: salila.s@immt.res.in)

Abstract: Diamond films are investigated systematically for their application as microplasma illumination owing to their negative electron affinity and low effective work function[1]. While the physical properties of these films depend on the intrinsic structure of the materials, their electrical properties are more closely related to the microstructure of the films. The decrease in diamond grain size increases the proportion of grain boundaries, which contain non-diamond carbon phases such as amorphous carbon (*a-C*) or *trans*-polyacetylene phases[2]. These non-diamond carbon phases act as conducting channels, facilitating easy tunneling of electrons through a 'grain boundary conduction emission' mechanism and thus improving the microplasma illumination characteristics of diamond films. Ion implantation is a possible way to alter the electrical properties of materials via controlled doping with a wide variety of dopant species[3]. By proper selection of the implantation energy and dose, the sp^2/sp^3 ratio of diamond and related carbon materials can be tailored. The sp^2-bonded carbon induced during ion implantation and post-annealing treatments of diamond films is the conductivity promoter, which enables the electrons to move freely inside the films. In the present study, the effect of nickel ion implantation and post-annealing processes on the electrical conductivity and microplasma illumination properties of boron-doped diamond (BDD) films was investigated. A high dose Ni ion implantation (10^{15} ions/cm^2) with the implantation energy of 50 keV induced the formation of electron trap centers inside the diamond grains as well as *a-C* in grain boundaries for both BDD films. Post-annealing at 600°C healed the defects, eliminated the electron trap centers, and converted the *a-C* into nanographitic phases. Micro-Raman spectroscopic and X-ray photoelectron spectroscopic examinations indicated that, there presence of abundant nanographitic phases in the grain boundaries of Ni-implanted BDD films as compared with those in undoped BDD films. The nanographitic phases formed an interconnected path for efficient electron transport and thus improved the electrical conductivity and microplasma illumination properties of nickel-implanted BDD films more profoundly, which makes these films a potential cathode material for applications in high-brightness plasma devices.

References and Notes:

1. S. C. Lou, C. Chen, K. Y. Teng, C. Y. Tang, and I. N. Lin, *J. Vac. Sci. Technol*. **2013,** 31, 02B109.
2. S. Kunuku, K. J. Sankaran, K. C. Leou, and I. N. Lin, *Mater. Res. Express* **2017**, 4, 025001.
3. S.K. Sethy, K. J. Sankaran, P. Gupta, J. P. Thomas, A. Dash, J. V. Kennedy, K. T. Leung,and K. Haenen, *Phys. Status Solidi A* **2023**, 2300157.

Effective Renewable Hydrogen Production from Biomass-derived Feedstocks Using Bifunctional Ruthenium Catalyst

Satabdee Tanaya Sahoo and Prosenjit Daw*

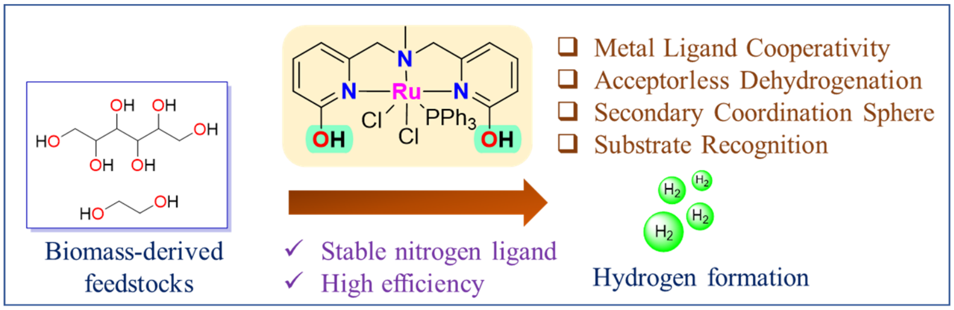
Department of Chemistry

Indian Institute of Science Education and Research Berhampur, Odisha, India -760010

(E-mail: satabdeets@iiserbpr.ac.in)

Abstract: Environmental issues and high alerts in energy security due to the acute stain in current energy infrastructure led to the transition from conventional non-renewable fossil fuels to reliable, clean, greener, affordable, and efficient energy sources.1 Currently, seminal research interest has been developed in biomass as a source of net-zero carbon energy feedstocks which will open a new avenue to generate energy in a more sustainable way.2 Homogeneous cooperative catalysts have gained widespread interest in developing highly efficient new-generation catalysts and strategies on the basis of metal-ligand cooperativity.3 Herein a bifunctional cooperative NNN-Ru pincer catalyst bearing a proton-responsive arm (-OH) in ligand scaffold has been synthesized liable for switchable metal-ligand cooperativity though lactam-lactim tautomerization as well as secondary coordination sphere hydrogen bonding interaction for proper substrate orientation. The catalytic efficiency of this air-stable Ru complex for hydrogen production from biomass-derived feedstocks such as sorbitol and ethylene glycol was found to be highly efficient with a maximum TON of 35359 and 25225 respectively. During ethylene glycol reforming this developed bifunctional catalyst features high selectivity in the production of hydrogen and glycolic acid as value-added products in two tuneable operating conditions. A series of control experiments and NMR studies have revealed the significant participation of functionalized protic arms during catalysis. The catalyst remained efficiently active for up to 8 runs over a period of 192 h during the aqueous phase reforming of sorbitol and a total of 1.4 L of H2 gas was collected from solvent-free reforming of ethylene glycol.4,5

Figure:



References and Notes:

1. Rana, J.; Sahoo, S. T.; Daw, P. *Tetrahedron* **2021**, 99, 132473.
2. Kumar, A.; Daw, P.; Milstein, D. *Chem. Rev.* **2022**, 122 (1), 385–441.
3. Shimbayashi, T.; Fujita, K. I. Catalysts 2020, 10 (6), 635.
4. Sahoo, S. T.; Mohanty, A.; Sharma, R.; Rout, S. R.; Dandela, R.; Daw, P. *Organometallics* **2023**, 42 (9), 745–751.
5. Sahoo, S. T.; Mohanty, A.; Sharma, Raju Daw, P. *Dalt. Trans.* **2023**. https://doi.org/10.1039/D3DT01671D.

Fabrication and characterization of banana peduncle fibre reinforced biodegradable soy composite

Shruti Swaroop Pattnaik* and Ajaya Kumar Behera

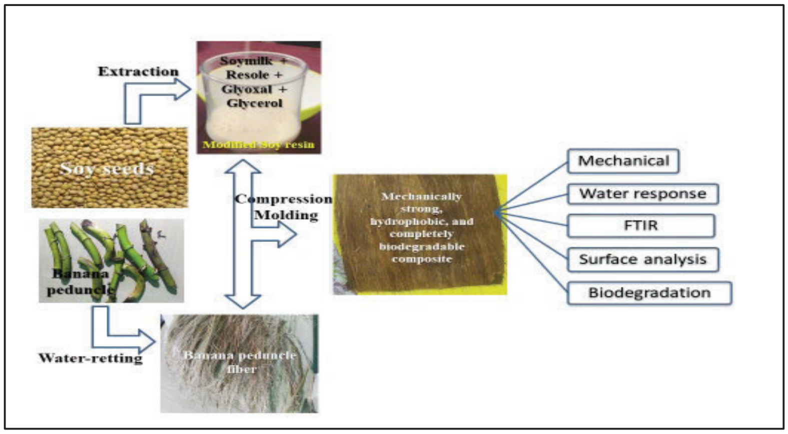
Department of Chemistry, Utkal University, Vani Vihar, Bhubaneswar, Odisha-751004

(E-mail: shrutipattnaik96@yahoo.com)

Abstract: Since banana peduncles have a high cellulose content and a modest tensile strength, they have lately been recognised as a viable raw material. The peduncle fibres from discarded banana peduncles were separated, and then reinforced using biodegradable soy resin, phenol-formaldehyde (resole), and soy-resole resins via thermal moulding (compressing) process, in order to create multiple lots of biodegradable composite. Because of the significant interaction/bonding between the functional groups of the two natural materials utilised here, the peduncle fibre reinforced soy-resole composite displayed maximum tensile strength of 43.5 MPa and flexural strength of 36.2 MPa. The water sorption test that was performed on all composites revealed that they are generally hydrophobic by nature since after 24 hours, they only absorbed 10.2 to 28.2% of water. Given that they mostly decomposed in the soil after 2 months and that they all dropped roughly 70% of their initial weight, these composites demonstrated that they were both environmentally benign and compostable. It is projected that interior furniture, packaging, and computer cabinets will use these composites in place of plastic, thus reducing environmental hazards.

Highlights: Banana peduncle fiber was extracted from agro-wastes and used as reinforcement.The highest tensile strength of the composite was achieved as 43.5 MPa.The water absorption of composite was found to be as low as 10.2% in 24 hours. Composite lost 70.8% of its original weight under 2 months of soil burial degradation.Developed composites can be a good eco-friendly substitute to plastic packaging and wood, hence saving environment.

Scheme/Figure:



References and Notes:

1. Pattnaik, S. S.; Mohapatra, S. K.; Mohanty, C.; Behera, A. K.; and Tripathy, B. C., *Fibers and Polymers* **(2023),** *24*(1), 265-274.
2. Bishoyi, K. C.; Pattnaik, S. S.; Behera, D.; and Behera, A. K., *Polymer Composites* **(2023)**, https://doi.org/10.1002/pc.27583
3. **Acknowledgements:** We gratefully acknowledge the support provided by OURIIP seed fund, CHSE, Govt. of Odisha, and DST-FIST, Govt. of India for some part of this work.

Investigation on the Influence of Pyrolysis Parameters on Biochar Yield from Water Hyacinth Biomass

S.P. Palai[1], B.P. Sahoo[2], P. Parhi[1*], T.K. Bastia[1*] and P. Rath[3]

[1]*School of Applied Sciences*

[2]*KIIT-TBI, KIIT Deemed to be University, Bhubaneswar, Odisha, India-751024*

[3]*Department. of Chemistry, F.M. University Balasore-756089*

(Email- drtkbastia@gmail.com , prathfch@kiit.ac.in, parhipankaj@gmail.com)

Abstract: Synthesis of biochar from water hyacinth (WH) biomass (one of the invasive aquatic species) can adeptly resolves the issues due to the invasive aquatic species disposal vis-a-vis its conversion into biochar which may offer a sustainable and cost-effective adsorbent solution. Nevertheless, to attain the maximum yield of biochar from water hyacinth biomass via pyrolysis, process optimization is imperative. Initially three primary input process parameters were identified that includes pyrolysis temperature, residence time, and heating rate. These parameters were systematically explored to evaluate their impact on the biochar yield. The assessment of biochar yield encompasses both quantitative and qualitative analyses, involving measurements of bulk density, residual solid weight, as well as observations using morphological analysis using SEM. During pyrolysis, 20g finely ground biomass was used with APS of 0.15µm. The temperature range from 400 to 700°C (heating rate ranging from 5 to 10°C/min) and residence times from 60 to 180 minutes was maintained in pyrolysis. The results revealed that as the pyrolysis temperature increased, the amount of solid residue diminished irrespective of variations in residence time and heating rate. Interestingly, the highest amount of solid residue was observed at the lowest combinations of pyrolysis temperature of 400°C, heating rate of 5°C/min, and residence time 60min. Nonetheless, the particular sample which exhibited the highest bulk density (0.19g/cm^3) that was subjected to pyrolysis at the temperature of 700°C with a heating rate of 5°C/min, and a residence time of 90 minutes. To investigate this anomaly, SEM analysis was conducted and it was observed that the biochar generated at parametric combination of 700°C-5°C/min-90min. showed the presence of cube shaped crystals with micropores distributed throughout the heterogenous structure of biochar. While no such crystal formation was noticed in the biochar generated under 400°C-5°C/min-60min parametric combination. In addition, the atomic wt.% of carbon was highest (84%) in the former case. The increasing in the pyrolysis temperature lead to elevate the volatilization processes and so as the loss of organic compounds, thus producing micropores/voids. Higher temperature facilitates the crystallization as well. Although, maximum biochar mass yield was obtained at a parametric combination of 400°C-5°C/min-60min, the higher density along with microporosity was noticed in case of sample pyrolyzed under 700°C-5°C/min-90min condition.

Effect of varying chain length and functional group on photophysical photocatalytic properties of self-assembled thiophene oligomeric nanoparticles for green hydrogen production

Soham Ghosh, Subhajit Kar, Santanu Bhattacharyya*

Department of Chemical Sciences, Indian Institute of Science Education and Research, Berhampur, Odisha-760010, India

(E-mail: sohamg20@iiserbpr.ac.in)

Abstract: Small organic oligomers in the form of self-assembled nanoparticles can be useful for spectroscopic and photocatalytic applications. In this work, three thiophene-based oligomers were chosen, namely 2,2'-Bithiophene-5,5'-dicarboxaldehyde (BTDA), 2,2':5',2"-Terthiophene-5,5"-dicarboxaldehyde (TTDA) and 2,2':5',2"-Terthiophene (TTT) wherein the first two molecules differ structurally by one extra thiophene unit and TTT is devoid of aldehyde functionality. The self-assembled nanoparticles of these molecules in aqueous medium formed by reprecipitation show distinctly different opto-electronic and photocatalytic properties. The photophysical characterization is done for the nanoparticles. The observations indicate fundamental phenomenon, namely J-aggregation for BTDA nanoparticles and H-aggregation for TTDA and TTT nanoparticles. The time-resolved emission decay and time-resolved anisotropy study has been done. TTDA nanoparticles have prominent anisotropy with a shorter fast component and longer slow component with some residual anisotropy. These results suggest that the packing conformation of TTDA nanoparticles is such that it has long-lived charge carriers that shows persistent polarized emission. These properties has definite impact on photocatalysis and TTDA nanoparticles has stable photocatalytic H_2 production with excellent rate. Finally it can be concluded that varying the chain length of the oligomer and presence of aldehyde functionality has immense impact on the photophysical and photocatalytic properties of the self-assembled nanoparticles.

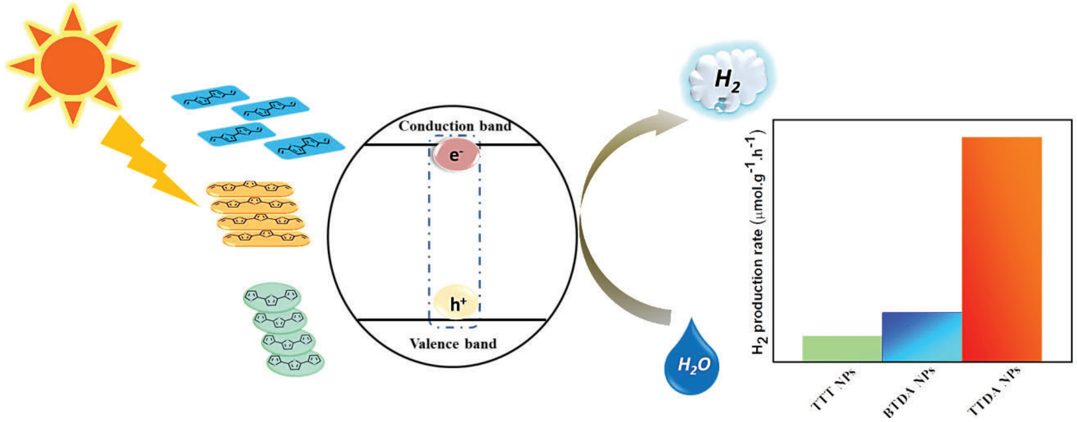


Figure 1: Photocatalytic hydrogen production from self-assembled organic nanoparticles.

References and Notes:

1. Guo, Y.; Zhou, Q.; Zhu, B.; Tang, C.T.; and Zhu, Y., *EES Catal.*, **2023**, *1*, 333-352.
2. Bayda, M.; Dumoulin, F.; Hug, G.L.; Koput, J.; Gorniak, R.; and Wojcik, A., *Dalton Trans.*, **2017**, *46*, 1914-1926.

Study on bioenergy potential of *Oriza sativa* biomass

Spandan Nanda, Manasi Dash, Pradip Kumar Jena*

Department of Chemistry CBSH, Department of PBG, OUAT, Bhubaneswar-3, Odisha

Email: Pradip_callme@yahoo.co.in

Abstract: Pyrolysis is a major method for producing biogas, bio-oils, and charcoal. The current study used three common rice varieties with varying maturity durations to perform thermo-gravimetry and determine the influence of maturity length on kinetic parameters. Rice straw contains cellulose (32.55%), volatiles (64.7%), and 15.71 MJ/kg HHV. The average activation energy (E_a) values for medium (194.57 kJ/mol) and mid-early (180.31 kJ/mol) varieties were greater than for late duration (173.53 kJ/mol) types. For the late duration variation, A values of 10^{12}-10^{15}, 10^{12}-10^{15}, 10^{13}-10^{15} and 10^{13}-10^{15} were reported under FWO, KAS, Starink, and Tang, respectively. Under alternative models, the A values for the other two kinds were determined to be as high as 10^{22}. D4 and D3 diffusion models were determined to be the best fit models using Coats-Redfern and master plot (Z-α) analyses. The values of ΔH increase with the amount of conversion for Mahalaxmi and CR-D-304, suggesting the endothermic nature of rice straw combustion.

Robust Optical Detection of Ga^{3+} by a Rhodamine and Coumarin-based Proficient Probe: Theoretical Investigations and Biological Applications

Suvam Kumar Panda and Akhilesh Kumar Singh*
Department of Chemistry
School of Basic Sciences, IIT Bhubaneswar, Khurdha, 752050
(E-mail: skp19@iitbbs.ac.in)

Abstract:

Gallium(III) is one of the rarest widely dispersed metals, which is well-known for its distinct physical and chemical properties.[1, 2] Gallium compounds are frequently used in the treatment of various malignant disorders and could be used as an imaging agent for identifying inflammation.[2] Therefore, detection of Ga^{3+} is essential and fluorescence is a cost-effective, easy-to-use and sensitive technique that can be used for the easy detection of Ga^{3+}.

The current investigation focuses on a rhodamine-coumarin-based probe (RC) for the selective detection of Ga^{3+} over other metal ions in the DMSO/ H_2O (9:1, *v/v*) environment. SC-XRD analysis for the probe and its Ga^{3+} complex provided the solid-state structures and the binding mode of RC with Ga^{3+}. The ligand-to-metal binding ratio in the RC-Ga^{3+} complex was found to be 2:1 in both solid-state and solution-state. The excitation wavelength (λ_{ex}) of the probe for Ga^{3+} detection was set to 522 nm, and a massive emission (λ_{em}) at 584 nm with a 105-fold increase was observed. The detection limit (LOD) was found to be as low as in nanomolar level (10 nM). Fluorescence lifetime experiments and quantum yield measurements on both the probe and its Ga^{3+} complex were also carried out. DFT and TD-DFT calculations were performed in the gas phase and in the solution phase in DMSO to elucidate the optical and electronic characteristics of the probe and its Ga^{3+} complex. Finally, the live cell imaging for both compounds was done in the HaCaT cell line, and outstanding findings were observed. Interestingly, Ga^{3+} could be measured in intracellular organelles such as lysosomes using the probe, RC.

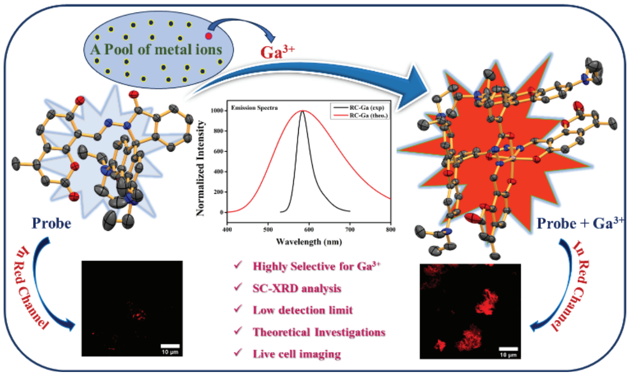


Figure 1. Pictorial representation of sensing ability of the probe towards Ga^{3+} detection.

References and Notes:

1. L. Zhang and Z. Xu, *Environmental Science & Technology*, 2016, **50**, 9242-9250.
2. N. Gómez-Cerezo, E. Verron, V. Montouillout, F. Fayon, P. Lagadec, J. M. Bouler, B. Bujoli, D. Arcos and M. Vallet-Regí, *Acta Biomaterialia*, 2018, **76**, 333-343.

Doped Laser-Induced Graphene for Electrochemical Detection of Heavy Metal ions

Yogesh Chaudhary[1,2#], Shradha Suman[1,2], Benadict Rakesh[1,2], K.J. Sankaran[1,2*]

[1] *CSIR-Institute of Minerals and Materials Technology, Bhubaneswar 751013, India.*

[2] *Academy of Scientific and Innovative Research (AcSIR), CSIR-HRDC Campus, Ghaziabad 201002, India.*

Email: kjsankaran@immt.res.in

Abstract:

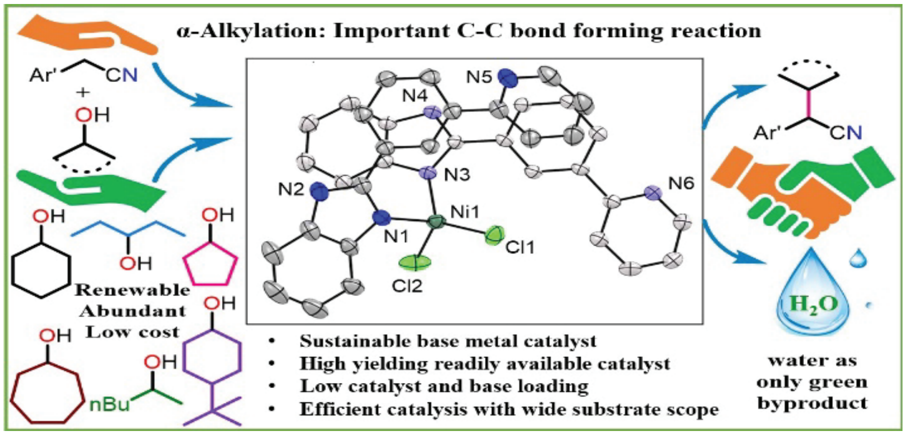
Monitoring water quality to prevent several diseases caused by heavy metal poisoning. Mankind, there is an urge to seek portable, easy-to-operate, and rapid quantitative methods for heavy metal ions (HMIs) detection via electrochemical sensors. Graphene is one of the potential candidates as an electrochemical sensor because of its high electrical conductivity, large specific surface area, and excellent chemical stability. However, the various graphene synthesis and its fabrication routes use hazardous chemicals, toxic to the environment and also time-consuming. In comparison to conventional fabrication methods of graphene, laser-induced graphene (LIG) is fabricated by a direct laser writing method on a polyimide film by exposure to an infrared CO_2 laser.

In this work, boron and nitrogen co-doped LIG (BN-LIG) electrodes are fabricated and utilized for the individual and simultaneous electrochemical detection of lead (Pb^{2+}) and cadmium (Cd^{2+}) ions using a square wave voltammetry technique is elaborated. H_3BO_3 and NH_2CONH_2 are used as precursors for the incorporation of N and B heteroatoms into LIG. The BN-LIG exhibits remarkably improved sensing performance due to the synergistic effect of N and B co-doping. The sensor has a sensitivity of 0.725µA/µM and 0.661 µA/µM for Pb^{2+} and Cd^{2+} ions respectively, low limit of detection (0.21 µM and 0.25 µM for Pb^{2+} and Cd^{2+}), wide linear ranges (8.0 to 80 µM for Pb^{2+} and Cd^{2+} ions) and high linearity of $R^2 = 0.99$. Finally, the measurement of concentrations of heavy metal ions in tap water was performed for Pb^{2+} and Cd^{2+} ions. This work opens a new avenue for fabricating doped LIG with several heteroatoms that can be used in various electrochemical sensing studies.

Nickel-Catalyzed *α*-Alkylation of Arylacetonitriles with Challenging Secondary Alcohols

Ratnakar Saha and Bidraha Bagh

Abstract: The fast depletion of fossil fuel-based resources and growing environmental concern has instigate the need to explore renewable and sustainable alternatives for synthesizing valuable compounds.[1] The basic principles of sustainability are more obeyed when starting substrates are easily accessible at a lower cost and the reaction's by-products are environmentally friendly.[2] With these considerations in focus, the primary goal is the development of eco-friendly synthetic methods that felicitate the formation of C-C bonds by using renewable feedstocks.[3] Hence, we have developed a readily available, air-stable and sustainable nickel(II) complex (**1**) was utilized as an expedient catalyst for the α-alkylation of arylacetonitriles with challenging secondary alcohols in presence of base. Arylacetonitriles with a wide range of functional groups were tolerated and various cyclic and acyclic (including symmetric and asymmetric) secondary alcohols were utilized to yield a large number of α-alkylated products. Plausible mechanism involves the base promoted activation of precatalyst **1** to an active catalyst **2** (dehydrochlorinated product) which activates the O-H and C-H bond of the secondary alcohol in a dehydrogenative pathway.[4]



References:

1. M. Maji, D. Panja, I. Borthakur and S. Kundu, *Org. Chem. Front.*, 2021, **8**, 2673–2709.
2. P. T. Anastas and J. C. Warner, *Green Chemistry: Theory and Practice*, Oxford University press, New York, 1998.
3. C. Gunanathan and D. Milstein, Science, 2013, **341**, 1229712.
4. (a) S. Panda, R. Saha, S. Sethi, R. Ghosh and B. Bagh, *J. Org. Chem.*, 2020, **85**, 15610–15621; (b) R. Saha, S. Panda, A. Nanda and B. Bagh, *J. Org. Chem.* 2023. DOI: 10.1021/acs.joc.2c02026.

In pursuit of Water Oxidation over Catalyst Deactivation by Mononuclear Nickel and Copper complexes: A Computational Study

Ajeet Kumar Singh[a] and Dr. Lisa Roy[a]
[a]*Institute of Chemical Technology Mumbai- IOC Odisha Campus Bhubaneswar*
Email: che20a.singh@stuiocb.ictmumbai.edu.in

Abstract:

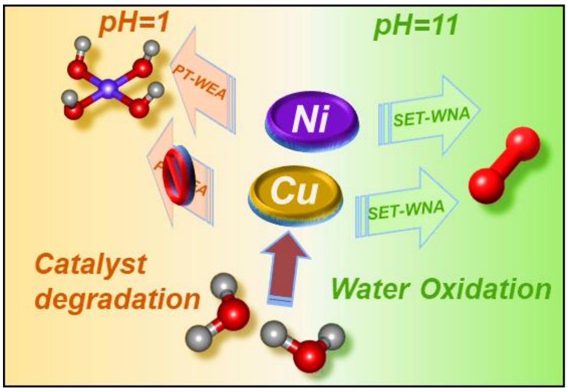


Figure1. Graphical representation of water oxidation versus catalyst degradation by Ni and Cu bis(oxamidate) complexes.

Water splitting is a promising strategy to generate solar fuels such as H_2 and mitigate the current global energy demand. However, out of the two redox processes: water oxidation and proton reduction, the former requires high thermodynamic potential ($E° = 1.23$ V vs NHE) as is considered as the bottleneck in its practical implementation. Herein, we used Density Functional Theory (DFT) to probe the reactivity of nickel and copper complexes with a tetra-anionic tetradentate amide ligand of the type $[(L1)M^{II}]^{2-}$, where L1 = *o*-phenylenebis(oxamidate) for water oxidation and catalyst deactivation. Interestingly, nickel complexes feature the possibility of water oxidation as well as molecular complex degradation due to reversibility of the O-O bond formation. This is primarily facilitated by OH^-/H^+ attack on the $2e^-$ oxidized anionic intermediate $[(L1^{\bullet})Ni^{III}(OH)]^{1-}$. On the contrary, the analogous copper intermediate, $[(L1^{\bullet})Cu^{II}(OH^{\bullet})]^{1-}$, feature radical character on the -OH ligand that enhances its electrophilicity and promote exclusive water oxidation.

References:

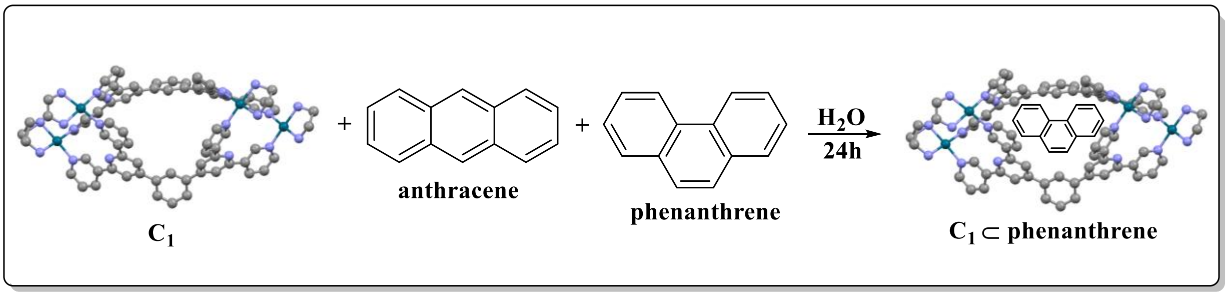
1. Garrido-Barros, P.; Grau, S.; Drouet, S.; Benet-Buchholz, J.; Gimbert-Suriñach, C.; Llobet, A., *ACS Catal.* **2019**, *9*(5), 3936–3945.
2. Garrido-Barros, P.; Funes-Ardoiz, I.; Drouet, S.; Benet-Buchholz, J.; Maseras, F.; Llobet, A., *J. Am. Chem. Soc.* **2015**, *137*(21), 6758–6761.
3. Singh, A.K.; Roy, L., *Eur. J. Inorg. Chem.* **2023**, e202300412.

Selective separation of isomorphic hydrophobic organic pairs in water

Raghunath Singha,[ab] Ayush Bhadani,[ab] and Dipak Samanta*[ab]
[a] *School of Chemical Sciences, National Institute of Science Education and Research (NISER), Bhubaneswar, Odisha 752050, India.*
[b] *Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai 400094, India*
(E-mail: ayush.bhadani@niser.ac.in, dsamanta@niser.ac.in)

Abstract:

Developing confined chemical microenvironments with properties different from the bulk phases yields the synthesis of hollow, nanometre-scale molecular "container compounds." These compounds can solve several reluctant chemical issues, such as separating isomorphic pairs, stabilizing and selectively encapsulating unstable molecular species, and photodimerization of photoswitches like azobenzene, DASA, etc. One such group of confined molecules is coordination cages, and a subset of it is Water-soluble coordination cages (WSCCs). Likewise, the well-defined hydrophobic inner cavities of WSCCs, similar to the nano environments in natural systems, offer a suitable enclosed region extracted from the hydrophilic environment that acknowledges the selective trapping, sequestering, and release of guests with control over their chemical reactivity. Herein, we report a water-soluble $[Pd_4L_2]^{8+}$ (C_1) molecular boat with unprecedented structural topology formed by coordination self-assembly of a flexible donor 1,3-bis([4,2':6',4''-terpyridin]-4'-yl)benzene(L) with a cis-blocked Pd(II)acceptor. This water-solubility results in the hydrophobic cavity, which can potentially encapsulate different PAHs in water. More importantly, this molecular boat (C_1) structure mimics the way biological system works for molecular recognition. Binding studies of this guest-induced cage ($C_1 \subset$ phenanthrene) were found to be 1:1 with the host inclusion complex. Moreover, this metal-organic vessel also demonstrated the ability to purify phenanthrene to >98% from an equimolar mixture of isomeric anthracene and phenanthrene in an aqueous medium. A water-soluble coordination design with the potential for simple and effective separation of phenanthrene from anthracene is exemplified by C_1. This is a particular case of a coordination receptor capable of selective, multi-cycle aqueous phenanthrene extraction from anthracene.



References

1. Edmundo G. Percástegui, Tanya K. Ronson, and Jonathan R. Nitschke., *Chem. Rev.* 2020, 120, 13480−13544.
2. Arppitha Baby Sainaba, Mangili Venkateswarulu, Pallab Bhandari, Kasun Sankalpa Athukorala Arachchige, Jack K. Clegg, and Partha Sarathi Mukherjee., *J. Am. Chem. Soc.* 2022, 144, 7504−7513.

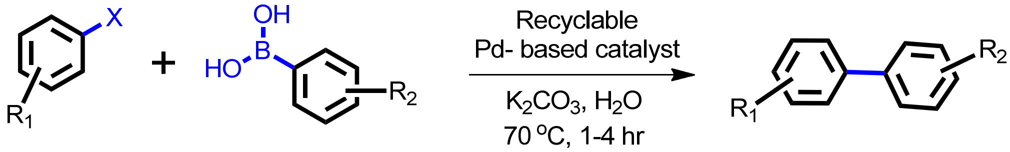
Recyclable Palladium-Catalyst in Suzuki Coupling: Application in Biaryl Synthesis

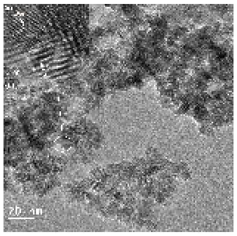
Smitabala Panda, Sagarika Patra, and Bibhuti Bhusan Parida*

P. G. Department of Chemistry, Berhampur University, Berhampur, Odisha, 760007

(Email: bbp.chem@buodisha.edu.in)

Abstract: C-C bond formation plays an important strategy in constructing various scaffolds in natural products synthesis. Coupling two aryls partners for C-C bond formation through transition metal catalysed cross coupling reactions are well explored. Palladium based cross coupling reaction in biaryl synthesis is much efficient among other transition metals. The Palladium based cross coupling through Suzuki reaction offers versatile and robust process for stitching two aryl moieties found in many natural products. Recovering such palladium based catalysts in traditional Suzuki reactions further enhances the scope of catalyst due to its recyclability and repeated use without significant loss of activity. Various substrate scopes was examined to showcase the synthetic utility of catalyst and reaction methodology in constructing biaryl based products.





Defect Engineered White Light Emitting Single-Phase Phosphors

Asish K. Dehurya,b, Rajeswari Kaindaa,b Santosh K. Beheraa, Satya K. Chirauria and Yatendra. S. Chaudharya, b*

[a]*Materials Chemistry Department, CSIR-Institute of Minerals and Materials Technology, Bhubaneswar-751013, Odisha, India*

[b]*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad - 201 002, India.*

Email ID: yschaudhary@immt.res.in,7205755894

Abstract: Intrinsically balanced white light-emitting materials can overcome disadvantages arising in conventional phosphors due to their color-balance emission in the visible region of the electromagnetic spectrum. By tailoring the defects in phosphors, the red emission can be instigated eventually giving white light emission in combination with the blue-green emissions of the host materials. Therefore, to evaluate the unexplored optical and spectroscopic properties of Cu doped-ZnS and orthovanadate phosphor hence to instigate the red emission to get intrinsic white light emission has been investigated. The aforementioned phosphors emit intense white light emission by tailoring the excitation wavelength, the stoichiometry of dopant ion, and defect states by varying the vacuum pressure, the optimized ZSC-3 (3% Cu2+-doped-ZnS) displays the origin of clear blue, green, and red emission bands, consequently giving rise to white light emission (CIE values: 0.345:0398) and PLQE 5.98% whereas the homogeneous thermal zone generated at the molecular level by microwave radiation gives rise to tunable distortion in the tetrahedral VO_4^{-3} and oxygen vacancies in orthovanadate, eventually enabling intrinsic white light emission with CIE(0.31,0.38) and high photoluminescence quantum efficiency (PLQE) (35%). This prompted the fabrication of LED prototypes that exhibit high CRI (97), and warm CCT (4538 K) for Cu doped-ZnS and (CRI) (85), correlated color temperature (CCT) (5217 K) for orthovanadate phosphor - meeting highly desired values for a white light emitting phosphor for different lighting applications and electroluminescence applications. This phosphor enables a large gap in the energy efficiency of white-emitting phosphor-converted light-emitting diodes.

Effect of solvent and auxiliary ligand on catecholase activities of Mn(III) complexes: A comparative study

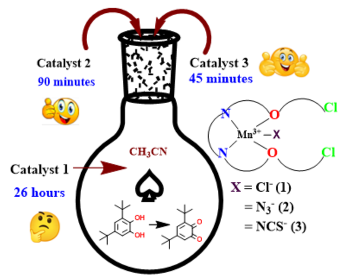
Rashmi Rekha Tripathy, Samaresh Jana*, Sohini Sarkar*

Department of Chemistry, School of Applied Science

(E-mail: sohini.sarkarfch@kiit.ac.in)

Abstract: Three mononuclear Mn(III) complexes named as $[Mn^{III}L(Cl)]$ (1), $[Mn^{III}L(N_3)(CH_3OH)]$ (2) and $[Mn^{III}L(\mu_{1,3}\text{-}NCS)]_n$ (3) were prepared using a Schiff base ligand (H_2L). With variation of auxiliary ligand, a notable change has been observed in structure as well as catalytic efficiencies of them. All of the three complexes behaved as bio-functional models of catechol oxidase toward oxidation of 3,5-di-tert butyl catechol (3,5-DTBC) to 3,5-di-tert butyl quinone (3,5-DTBQ) in open air. Formation of the quinone has been confirmed by UV-Vis, ^{1}H-NMR and ESI-MS spectroscopic techniques. The turn-over numbers of the catalytic processes have been determined using Michaelis-Menten model of enzyme catalysis and the kinetic experiment was performed in UV-Vis spectrophotometer. The progress of catechol oxidation for each complex was monitored by ^{1}H-NMR spectroscopy with the reaction mixtures containing complex (1 or 2 or 3) and substrate (3,5-DTBC). Both the studies have been carried out in different solvents, like, methanol, methanol-water mixture (for 1), acetonitrile and N, N′ -Dimethyl formamide (for 2 and 3). Role of solvent is quite interesting during the oxidation process. The studies indicated toward acetonitrile as the most effective medium in presence of which the turn-over numbers followed the order 3>2>1. From this observation, it may be concluded that complex 3 is the most efficient catalyst in comparison to 1 and 2 toward the catecholic oxidation in acetonitrile. 3 is capable of completing the reaction just in 45 minutes while for 1 and 2, the same were found as 26 hours and 90 minutes, respectively. To propose a tentative mechanism, the ESI-MS spectroscopic studies have been performed with the catalyst-substrate mixtures in acetonitrile for 2 and methanol for 3. In both cases a catechol bound intermediate has been detected in the scale of mass spectra. However, in absence of aerial oxygen, very less amount of formation of the quinone may confirm the compulsory role of oxygen for regeneration of the catalyst to complete the catalytic cycle. Notably, in absence of any of these complexes, oxidation of 3,5-DTBC to 3,5-DTBQ is negligible even after twenty-four hours of mixing in any solvent. This observation is a clear indicative of high catalytic efficiencies of the prepared complexes.

Scheme:



References and Notes:

1. Tripathy, R. R.; Jana, S.; Maji, S. K.; and Sarkar, S., *Chemistry Select* **2022**, 7, 1-10.
2. Tripathy, R. R.; Jana, S.; and Sarkar, S., *J. Mol. Struct.* **2023**, 1290, 135903.

Facile Synthesis of N-CDs for Selective Detection of Pd^{2+} in Water

Chinmaya Chirosundar Behera, Tanmayee Mohanta and Ashis Kumar Jena*
Department of Chemistry
Maharaja Sriram Chandra Bhanja Deo University, Baripada, Odisha-757 003
(E-mail:jenaashis016@gmail.com, chinmayabehera64@gmail.com)

Abstract:

Now-a-days**,** CarbonDots (CDs) have attracted many researchers due to their excellent photoluminescence properties, easy synthetic route, lox toxicity, high chemical and photo-stability, solubility in water and bio-compatibility nature.[1] Due to these unique properties, CDs have large number of applications in the fields of catalysis, sensing, biomedicine, bioimaging and opto-electronic devices etc.[2,3]Herein,we have synthesized Nitrogen Doped Carbon dots (N-CDs) from 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) and Ethylene diamineby hydrothermal method (Fig. 1). Further,the as synthesized N-CDs was characterized by different analytical techniques and the stability of the N-CDs was investigated. Recently, researchers have developed many methods for detection of transition and post-transition metal ions due to their hazardous nature and biological importance on human health. Pd^{2+} is a transition metal ion used in treatment of cancer, jewelry, dental crowns and as a catalyst for many reactions. Thus, detection of Pd^{2+}in water, food or drugs is highly demandable since the residue of Pd^{2+} left in these substances can lead to many adverse effects on human health.A number of analytical techniques such ashigh-performance liquid chromatography (HPLC), atomic absorption spectroscopy (AAS) and X-ray fluorescence (XRF)have been applied for the detection of Pd^{2+}. However, these techniques have many disadvantages and high instrument cost. Thus,there is an urgent need for an easy, economic, simple and fast method for selective detection of Pd^{2+}. The detection of Pd^{2+}in aqueous medium is based on fluorescence quenching mechanismby N-CDs.As the concentration of Pd^{2+}increased from 0-100 µM, the fluorescence intensity of N-CDs decreased and the intensity of N-CDsquenched to 80% at 100 µM concentration of Pd^{2+}.

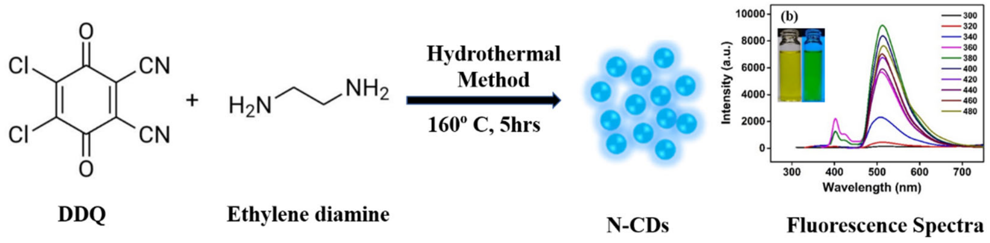


Fig. 1 Synthesis of N-CDs for selective detection of Pd^{2+}

References:

1. Li, L.; Zhang, R.; Lu, C.; Sun, J.; Wang, L.; Qu, B.; Li, T.; Liu, Y.; Li, S. In Situ Synthesis of NIR-Light Emitting Carbon Dots Derived from Spinach for Bio-Imaging Applications. *J. Mater. Chem. B***2017**, *5* (35), 7328–7334.
2. Swain,S.; Jena, A. K.; Mohanta,T.RatiometricFluorescence/Colorimetry/Smartphone Triple-Mode Real-Time Detection of Doxorubicin by Nitrogen-Doped Carbon Dots. *ACS Appl. Opt. Mater*. **2023**, 1, 1236-1244.
3. Lu, H.; Li, C.; Wang, H.; Wang, X.;& Xu, S.Biomass-derived sulfur, nitrogen co-doped carbon dots for colorimetric and fluorescent dual mode detection of silver (I) and cell imaging. *ACS omega*, **2019**, *4*(25), 21500-21508.

Material Chemistry

Photocatalytic dye degradation by $BaTiO_3$/zeolitic imidazolate framework composite

Jaykishon Swain[1], Anulipsa Priyadarshini[1], Sugato Hajra[2], Rojalin Sahu[1]*

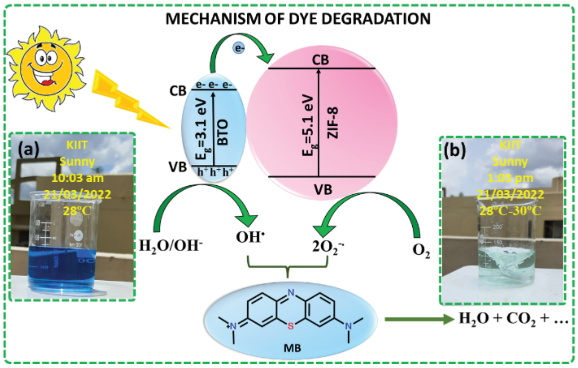
[1]*School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT), Bhubaneswar 751024, India*

[2]*Department of Robotics and Mechatronics Engineering, Daegu Gyeongbuk Institute of Science and Technology, Daegu 42988, South Korea*

(E-mail: rsahufch@kiit.ac.in)

Abstract: Chemical dyes present in wastewater generated from textile and paint industries can cause serious environmental and health hazards if not adequately treated. Photocatalytic degradation, an eco-friendly water treatment method, utilizes charge carriers generated from sunlight to remove pollutants in water without requiring additional energy input. Since the interaction between polluted water and a catalyst is crucial in water treatment, an emerging technology involves the combination of porous materials and light-sensitive materials. In this study, $BaTiO_3$ nanoparticles are loaded into a Zeolitic Imidazolate Framework (ZIF-8) to create $BaTiO_3$ @ZIF-8 nanocomposites for the photocatalytic degradation of methylene blue (MB) under solar irradiation. To facilitate the smooth transfer of charge carriers between $BaTiO_3$ and ZIF-8, ZIF-8 has been synthesized in the presence of $BaTiO_3$, allowing ZIF-8 to grow on the surface of $BaTiO_3$. The concentration of $BaTiO_3$ is adjusted during synthesis to optimize the photocatalytic performance. Among the different compositions, 25 wt% $BaTiO_3$ @ZIF-8 demonstrates the highest photocatalytic activity. This composite efficiently degrades 93 % of MB dye in 180 min and completely degrades the Congo Red dye in just 75 min under solar irradiation. Furthermore, the photocatalyst exhibits good cyclability over four cycles, maintaining its excellent performance. These results suggest that the current study contributes to the synthesis of highly effective photocatalysts for the breakdown of dyes in aqueous media under sunlight exposure.

Figure:



References and Notes:

1. Li, Y., Xu, H., Ouyang, S. and Ye, J. *Physical Chemistry Chemical Physics* **2016** 18(11), pp.7563-7572.
2. Soliman, A.I., Abdel-Wahab, A.M.A. and Abdelhamid, H.N. *RSC advances* **2022** 12(12), pp.7075-7084.

Magnetically recyclable Poly(m-aminophenol)/Manganese ferrite composite with enhanced visible-light-driven photocatalytic activity for dye degradation

Priyanka P. Mishra, Chirasmayee Mohanty, Ajaya K. Behera, and Nigamananda Das*

Department of Chemistry

(E-mail: priyankamishra1807@gmail.com)

Abstract: The massive development of the industrialized world and population in the modern era has resulted in alarming increases in pollution which have adverse consequences for living organisms and the environment. As a result, extensive research has assessed the best technique to eliminate this toxic contamination. Poly(m-aminophenol)/manganese ferrite nanocomposites were synthesized and applied as photocatalysts for the removal of aqueous cationic (malachite green) and anionic (Congo red) dyes with varying contact time, adsorbent amount, pH, and adsorbate concentration from contaminated waste under neutral conditions. The maximal adsorption capacities of the dyes MG and CR were 137 and 118 mg/g, respectively. In contrast, photocatalytic degradation of both the dyes was 92.96% (CR) and 93.95% (MG) after 120 minutes. The adsorption data correlated with Langmuir and Freundlich isotherm models followed by the pseudo-second-order kinetics. The nanocomposite before and after dye degradation are characterized and reported. The current study proved that polymer nanocomposite is an efficient and recyclable adsorbent for the decontamination of wastewater and for eliminating aqueous dyes.

References and Notes:

1. Mohanty, C., Das, N., Behera, A. K., & Tripathy, B. C. *Water Air and Soil Pollution*,2023, *234*(3), 204.
2. Somasundaram, A. J., Xiao, H., Pandiyarajan, S., Liao, A. H., Lydia, S., & Chuang, H. C. *Journal of Colloid and Interface Science*, 2023,*642*, 584-594.

Chiral Lanthanide-Acetate-Sulfite with Significant dielectric properties and Cryogenic Magnetic Refrigeration

Ranjay K. Tiwari and J. N. Behera*
School of Chemical Sciences, National Institute of Science Education and Research (NISER),
An OCC of Homi Bhabha National Institute (HBNI), Khordha, Bhubaneswar 752050, Odisha, India.
(E-mail: jnbehera@niser.ac.in)

Abstract:

The synthesis of chiral microporous materials is a great challenging work for their interesting application in pharmaceutical industry, agricultural, food biotechnological industry, asymmetric catalysis, enantioselective separation, adsorption, catalysis, dielectric materials, optical devices, chiroptical switching etc.[1] The chirality of microporous materials plays an imperative roles in biological evolution, chemical asymmetric catalysis. The chiral microporous materials can be prepared by addition of chiral component or configuration of chiral assembly occur from achiral structural unit. Our group has been involved in an exploring the sulfur based anionic open-framework materials, such as sulphide, sulfate, sulfite and thiosulfate as secondary building unit to generate open-framework materials.[2] The metal sulfite open framework are vastly not explore this is due to the easy oxidation of sulfite anions to sulfate anions in hydrothermal and acidic condition.[3] The choice of lanthanide metal is due to the availability of more coordination site, which can binds with sulfite and form hierarchy of structure. Here we present chiral lanthanide metal-sulfite frameworks having layered structure. In an effort to synthesize open-framework lanthanum sulfites, we have been able to synthesize chiral lanthanide metal sulfite with layered structures and formulated as $[Ln(SO_3)(CH_3COO)(H_2O)].(H_2O)$.

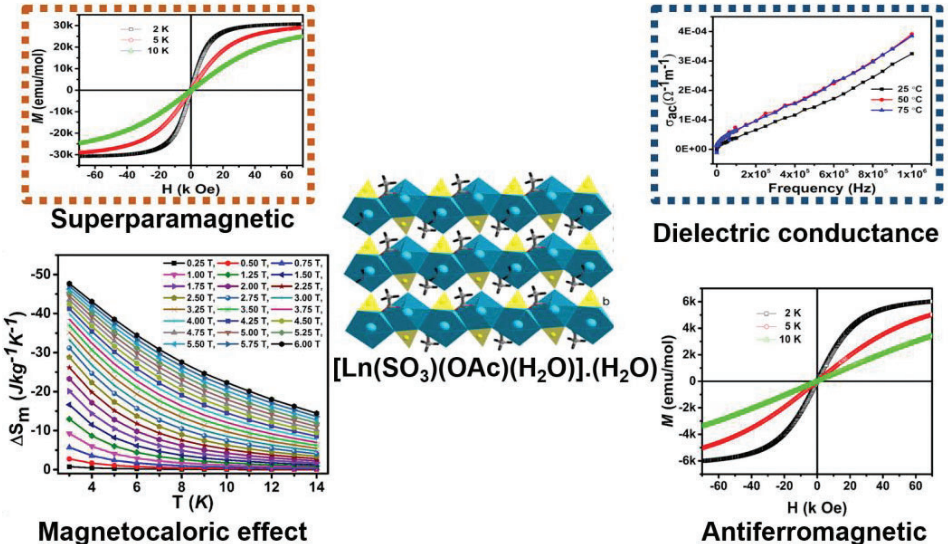


Figure: A polyhedral view of $[Ln(SO_3)(CH_3COO)(H_2O)].(H_2O)$ featuring layered structured (in center) showing magnetic, dielectric properies and change in magnetic enropy.

References:

1. Morris, R. E.; Bu, X., *Nat. Chem.* **2010,** 2, 353-361
2. Tiwari, R. K.; Kumar, J.; Behera, J. N., *Chem. Commun.* **2016,** 52, (6), 1282-1285.
3. Tiwari, R. K.; Behera, J. N., *Dalton Trans.* **2017,** 46, (18), 5911-5917.

Title: Organic-inorganic hybrid manganese phosphonate-derived metal oxides for miniaturized flexible in-plane micro-supercapacitors

Rupali Ipsita Mohanty[1,2], Piyali Bhanja[1]*, Bikash Kumar Jena[1,2]*
[1] *Materials Chemistry Department*
CSIR-Institute of Minerals and Materials Technology, Bhubaneswar-751013, India
[2] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India*
Corresponding author: piyalibhanja4@gmail.com, bikash@immt.res.in

Abstract:

Developing high-power supercapacitors is tremendously relevant to the current energy demand and implementation of renewable energy storage. The modernization towards the fabrication of flexible inter-digited micro-supercapacitors is overwhelming on-chip power sources for wearable electronic devices with no degradation of areal capacitance under various angles of bending state[1,2]. The template-free microporous manganese phosphonate (MnPIm) is synthesized using Iminodi(methylphosphonic acid) as an organo-phosphorous ligand under hydrothermal condition and their derivatives heteroatom doped manganese oxides (NP/$MnO_2$500, NP/$MnO_2$700, NP/$MnO_2$900) are obtained by the pyrolysis at different temperatures. Among these, NP/$MnO_2$700 electrode material displays the superior specific capacitance value of 1362 Fg^{-1} at 1 mV s^{-1} in three-electrode assembly with 99.6% retention of its initial capacitance up to the 2000th cycle. Due to the unique globular morphology with a hollow structure, high surface area, and the effect of heteroatoms doping, leading to extraordinary specific capacitance of the material. The NP/$MnO_2$700 material is used to fabricate a flexible asymmetric micro-supercapacitor device (MSC) with an areal capacitance of 32.8 mF cm^{-2} with 84.2% capacitance retention up to 5000th cycle.[3]

Figure:

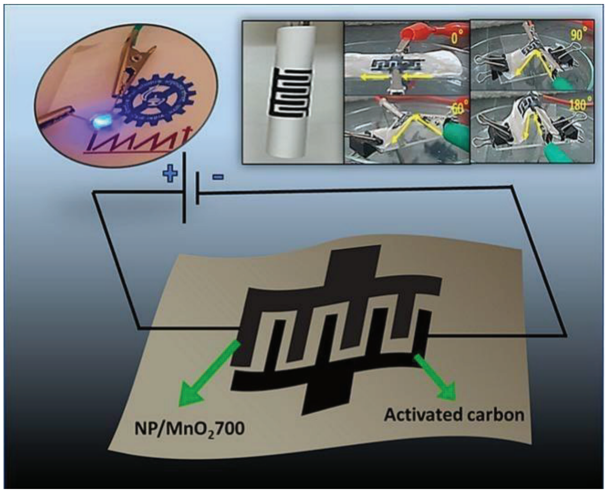


Figure 1: Fabricated flexible micro-supercapacitor device using $MnO_2$700.

Study of Dielectric Properties of TiO_2 embedded PMMA/Clay Nanocomposite for Electronic Applications

Sachit K Das[#], Debasrita Bharatiya, Sarat K Swain*

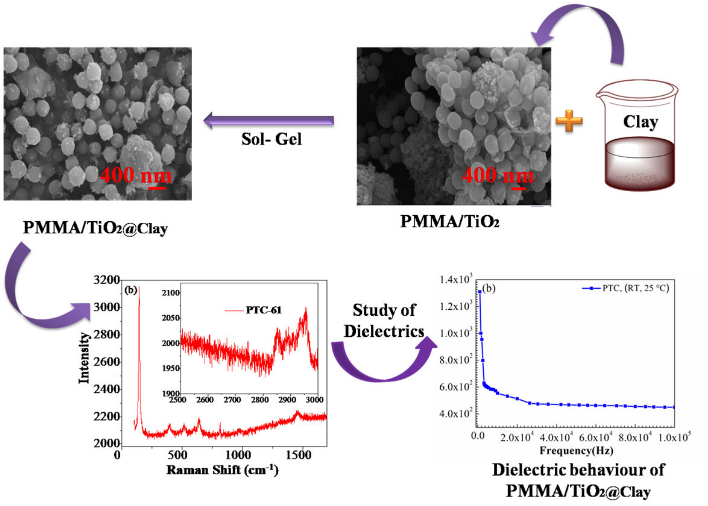
Department of Chemistry, Veer Surendra Sai University of Technology, Burla, Sambalpur, 768018, Odisha, India
*Corresponding Author; E-mail: skswain_chem@vssut.ac.in; [#]Presenting author

Abstract: Many inorganic based oxides (IOs) nanoparticles (NPs) have been synthesized and studied for dielectric behaviour for many decades [1]. It has gained popularity due to its cost-effectiveness, low toxicity and highly durable properties. Polymer-based materials are also easily found in nature and drag many researchers attention towards them for possessing good dielectric properties. This work aims to design and study of dielectric properties of Titanium dioxide nanoparticle embedded PMMA/Clay nanocomposite for electronic applications by sol-gel method. Important characterization techniques like XRD, TGA, DLS, Zeta, FESEM, Raman, UV-Vis and FTIR has been performed for designed materials to know about the properties including crystallinity, thermal stability, size, morphology, absorbance and chemical compositions respectively. The dielectric behaviour of Titanium dioxide nanoparticle embedded PMMA/Clay nanocomposite is studied at different ranges of frequency from 10^2 Hz to 4×10^6 Hz and at room temperature. The availability of permanent dipoles, interfacial polarization and atomic arrangements has enhanced the dielectric behaviour of the nanocomposites. The prepared nanocomposite showed a good dielectric behaviour and can be applied for charge storage uses [2].

Keywords: Charge; IOs; NPs; Storage; Dielectric.

Reference:

[1] C. Tamuly, I. Saikia, M. Hazarika, M.R. Das, 2014, Reduction of aromatic nitro compounds catalyzed by biogenic CuO nanoparticles, RSC Adv., (**2014**), 4, 53229
[2] B. Parhi, D. Bharatiya, S.K. Swain, Surfactant free green synthesis of GOSiMa hybridnanocomposite for charge storage application, Ceram. Int. (**2020**), 46, 27184.



Critical Optimization of Phosphorus Functionalized Carbon Nanomaterials for Metal-Free Solar fuel and chemical production

Subhajit Kar, Lopamudra Bishwal, Bramhaiah Kommula, and Santanu Bhattacharyya*

Indian Institute of Science Education and Research Berhampur, Berhampur, Odisha 760010, India

Email- subhajitk18@iiserbpr.ac.in, santanub@iiserbpr.ac.in

ABSTRACT:

Complete metal-free P-functionalized carbon nanomaterials are synthesized from a single molecular precursor, Phytic acid, for photocatalytic solar H_2 production and simultaneous organic transformation of 4-methyl benzyl alcohol to 4-methyl benzaldehyde by managing the complete redox cycle. Increasing the carbonization time, P-functionalized amorphous carbon dots convert to the highly defined 2D sheet-like nanostructure with optimum P-functionality and exhibit optimum photocatalytic efficiency. Finally, the highly defined sheet-like structure converts to a more defected aggregated form, resulting in the depletion of photocatalytic efficiency. The structural and elemental features are further correlated with the ongoing photo physics using steady-state and time-resolved fluorescence spectroscopy. Transient photocurrent responses and Mott-Scotty plots and detailed computational studies support the optimization of P-functionalized carbon nanostructure for efficient photocatalysis[1]. Overall, the in-depth structure–property correlation and critical optimization of the heteroatom functionalized carbon nanomaterials will open up new possibilities for further development of metal-free photocatalysts for solar-energy conversion devices.

Keywords: carbon nanomaterials, H_2 generation, organic transformation, phosphorous functionalization

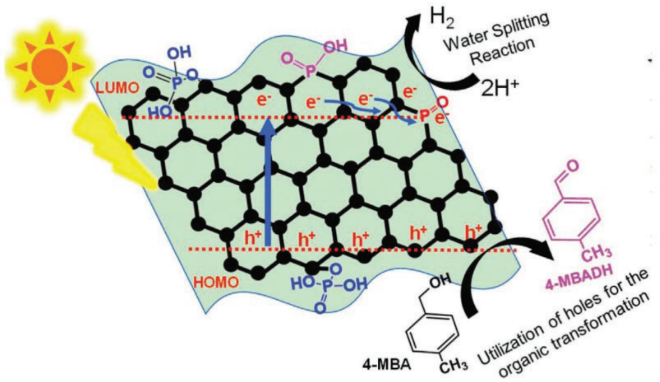


Fig. 1: **Plausible photocatalytic reaction mechanism of P-functionalized carbon nanostructures[1]**

References:

1. Kar, S.; Bishwal, L.; Kommula, B.; Bhattacharyya*. Critical Optimization of Phosphorus Functionalized Carbon Nanomaterials for Metal-Free Solar Hydrogen Production and Simultaneous Organic Transformation. *Adv. Optical Mater.* **2022**, 2102641.

Nanoflowers to Nanospheres Morphology Tuning of CuSe$_{1-x}$Te$_{1+x}$ via a Facile Microwave-assisted Method for Optoelectronic and Dielectric Applications

Subhashree Das *, Ramakanta Naik

Department of Engineering and Material Physics, Institute of Chemical Technology-Indian Oil Odisha Campus, India

(E-mail: phy20s.das@stuiocb.ictmumbai.edu.in)

Abstract: Transition metal chalcogenides have grabbed significant attention for their applications in various fields due to their elemental composition-dependent tunable properties. A facile microwave-assisted approach was used to synthesize different CuSeTe-based (CST) nanomaterials. The morphology was tuned from nanosheet-based flowers to nanospheres by varying Se and Te concentrations. With an increase in the value of the Te to Se content ratio, the material shows the transition from mixed nanosheets/nanospheres to pure nanospheres, where the average sheet thickness and sphere diameter are ~25 and 80 nm, respectively. The as-synthesized material shows high crystallinity with mixed phases of hexagonal Cu2Te and CuSe. The nano-crystallite size gradually increases with an increment in the Se to Te concentration ratio.[1] The chemical bonding of the material exhibits shifts of the spectra towards the lower binding energies with the decrease in the Se to Te ratio. The material exhibits a change in the absorption edge with a blue shift of the optical bandgap for the increase of Te content.[2] Fig.1(a) exhibits the enhanced optical bandgap of the CST nanomaterial. The increment in absorption made them eligible for solar cell application. This increase in the absorption ability of the material can serve as an absorbing layer for photovoltaic applications. The photoluminescence spectra of different CST samples show broad emission in the 550-950 nm range with peaks at ~700 nm. Such optical properties make CST materials for possible applications in optoelectronics devices.[3] The dielectric measurement of the sample exhibits an increase in the dielectric constant and loss with the temperature, whereas a decrease in both values is apparent for an increase in the frequency. Fig.1. (b) illustrates the variation between temperature and dielectric constant at various frequencies. The complex modulus of the studied material gradually increases with an increment in the frequency. [4,5] The dielectric study of the material reveals its potential application for energy storage. The Scheme 1 represents the schematic representation of the synthesis techniques of CST nanomaterial and the transformation in the morphology of the material.

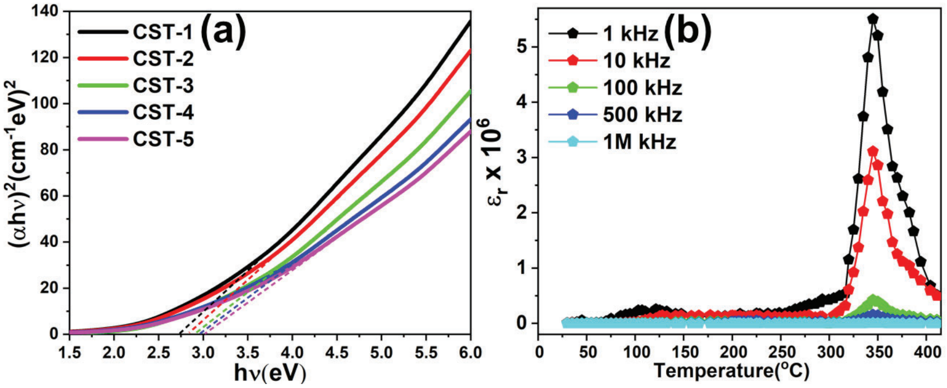


Figure.1.(a) Direct optical bandgap of the CST material, and (b) Temperature-dependent plot of the dielectric constant of the CST nanomaterial.

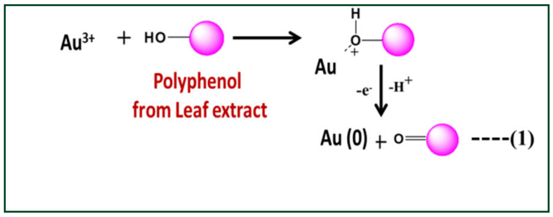
Green Synthesis of Gold Nano-particle and its Applications

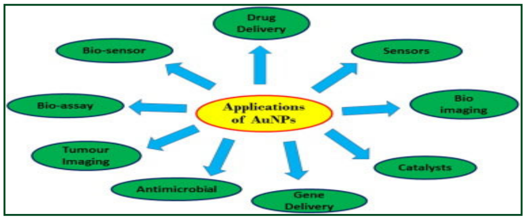
Adrushya Jyoti Pattanayak and Sarat K Swain*

Department of Chemistry, Veer Surendra Sai University of Technology, Sambalpur 768018, Odisha, India

Corresponding author E-mail:* ***swainsk2@yahoo.co.in* **; skswain_chem@vssut.ac.in** Phone: 91-9937082348, Fax: 0663-2430204

Abstract: Nanoparticles are particles that exist on a nanometre scale (i.e., below 100 nm in at least one dimension). These can possess properties such as uniformity, conductance or optical properties that make them desirable in materials science and biology. Green chemistry is the utilization of a set of principles that reduces or eliminates the use or generation of hazardous substances in the design, manufacture and application of chemical products. An *in situ* green synthesis of gold nanoparticles using Hirakud sand as source of gold solution and red tea infusion as a reducing and stabilizing agent and their applications have been presented. The size and shape of gold nanoparticles are modulated by varying the ratio of metal salt and tea leaf extract in the reaction medium. The nanoparticles obtained can be characterised by UV-vis, transmission electron microscopy (TEM) and X-ray diffraction (XRD) (continuing) A special attention to varying nano gold particle size, Tyndall effect and Target drug delivery have been presented in the form protocol.





References

1. H. Qian, L. A. Pretzer, J. C. Velazquez, Z. Zhao, M. S. Wong. J. Chem. Technol. Biotechnol. 2013, 88,735-41.
2. B.S. Bhau, S. Ghosh, S. Puri, B. Borah, D.K. Sarmah, R. Khan. Adv. Mater. Lett.2015, 6(1), 55-58.

The influence of EDLC and pseudocapacitor active quantum dots on graphene matrix towards enhancement of supercapacitor properties

Lingaraj Pradhan[1,2], Bishnupad Mohanty[1], Bikash Kumar Jena[1,2]*
[1]*Materials Chemistry Department, CSIR-Institute of Minerals and Materials Technology, Bhubaneswar, Odisha,751013, India*
[2]*Academy of Scientific and Innovative Research, Ghaziabad, 201002, India*
(E-mail: lingarajpradhan616@gmail.com)

Abstract:

The construction of composite electrode materials that exhibit superior energy and power densities has stirred rigorous research on supercapacitors. Herein, we have successfully designed nitrogen-doped carbon dots (CDs) and hematite dots (HtDs) functionalized reduced graphene (RG) hybrid ternary composites (RG@CDs/HtDs) by liquid exfoliation followed by the solvothermal method. The hybrid electrode material, RG@ CDs/HtDs, exhibits a high specific capacitance of 1566 F.g^{-1} at a scan rate of 2 mV.s^{-1} and excellent stability up to 10,000 cycles. The DFT calculations have been performed to investigate the capacitance enhancement in the hybrid structure. The enhanced quantum capacitance and intense electronic states near the Fermi level for the ternary structure RG@CDs/HtDs justify the superior charge storage. When HtDs and CDs are introduced into RG, charge transfers from the Fe 3d orbital to the C 2p orbital of RG occur. An asymmetric aqueous supercapacitor device has been fabricated using RG@CDs/HtDs as a cathode and Mn_3O_4/C as an anode. Remarkably, the assembled aqueous asymmetric supercapacitor operates in a stable and wide potential window of 2.5 V with an ultrahigh energy density (134 Wh.kg^{-1}) along with extraordinary rate capability and is stable at 10,000 cycles performance that was validated on powering of the red light-emitting diode (LED).

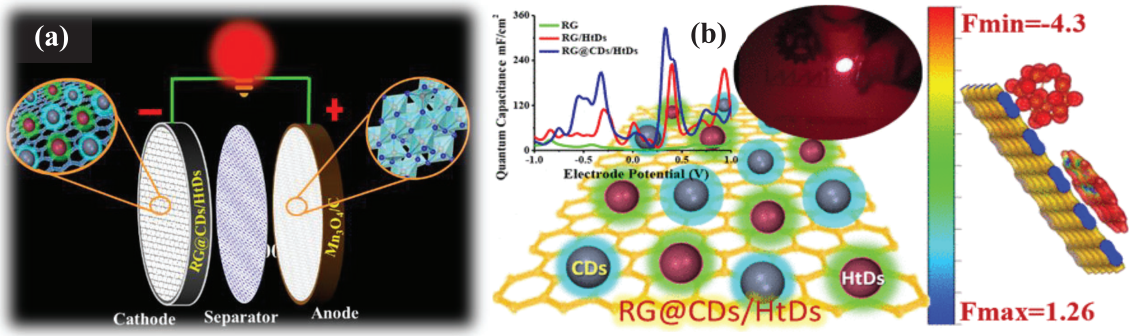


Figure 1: (a) Schematic presentation of the fabricated asymmetric supercapacitor, **(b)** Graphical abstract of the proposed work.

References and Notes:

Mohanty, B.#; Pradhan, L.#; Kandasamy, M.; Chakraborty, B.*; and Jena, B. K.*, *Energy & Fuels* **2023**, *37*, 7530-7538.

Green synthesis and characterization of cerium oxide nanoparticles

Lipsa Ray, Kaniz Fatma, Jasaswini Tripathy*

School of Applied Sciences (Chemistry),

KIIT Deemed to be University, Bhubaneswar, India

(E-mail: *jasaswinitripathy@gmail.com, jtripathyfch@kiit.ac.in*)

Abstract: Nanomaterials have a tremendous impact on human life owing to their numerous applications in material science, engineering, and medicine. Numerous health risks are associated with nanoparticles produced through chemical route. Recently, the green synthetic technique from plant extracts has attracted much attention to address this issue[1]. In addition to being a substitute for chemical synthesis, green synthesis is a method that is both economical and environmentally benign. The present study focuses on the synthesis of cerium oxide nanoparticles through a "green" synthetic approach using Impatiens Balsamina leaf extract, commonly known as rose balsam and comes under the Balsaminaceae family. Scanning electron microscopy (SEM), FTIR spectroscopy, UV-Visible spectroscopy, and X-ray diffraction (XRD) were used to characterize the green synthesized cerium oxide nanoparticles. The synthesized green nanoparticles can find uses in a wide range of antibacterial applications.

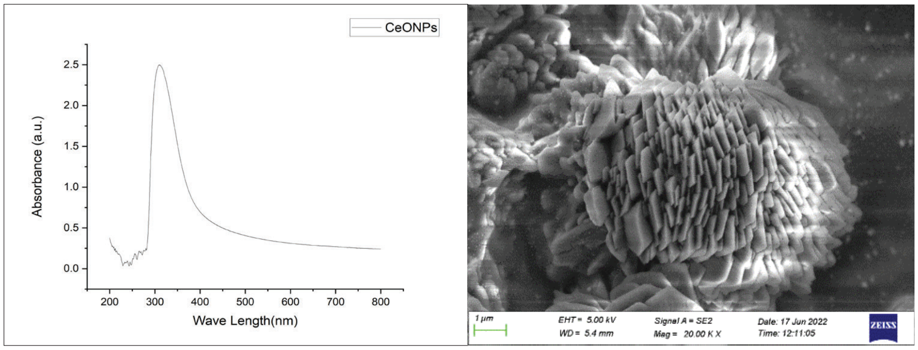


Figure: UV and FESEM of synthesized nanoparticles.

References:

1. Bordiwala, R. V.; *Results in Chemistry* **2023**, *5*, 100832.

Synthesis, Characterization of ZnO and ZnO-TiO_2 nanoparticles and Photocatalytic degradation of Malachite Green dye

Nibedita Nayak[1], Sasmita Sarangi[1], Tapas R. Sahoo[1*]

[1]Department of Chemistry, School of Applied Sciences, KIIT deemed to be University, Bhubaneswar 24, Odisha, India

Abstract: The swift advancement of human civilization through rapid industrialization has triggered detrimental consequences, notably the depletion of freshwater reserves, posing a grave threat to future generations due to an impending water crisis. Tackling this issue requires a decisive focus on preventing water pollution and eliminating pollutants. One such class of harmful pollutants is dyes, widely employed across industries like textiles, plastics, paper, leather, cosmetics, and food, thereby necessitating urgent intervention. In this current study, the primary objective revolved around evaluating the efficacy of photocatalytic techniques to eliminate malachite green dye from water systems. To achieve this, two distinct nanoparticles were employed as photocatalysts: ZnO and ZnO-TiO_2 nanoparticles. These nanoparticles, synthesized via microwave-assisted combustion and co-precipitation methods respectively, were minutely characterized using analytical tools such as XRD, FESEM, FTIR, TGA, and BET. The findings exhibited the superior photocatalytic capability of ZnO-TiO_2 nanoparticles compared to both ZnO and TiO_2 nanoparticles when subjected to sunlight irradiation. To further comprehend the variables, the study also investigated the impact of nanoparticle dose and pH levels. Remarkably, the highest degradation efficiency, reaching 92%, was achieved at pH 5.8 under sunlight radiation.

References:

1. 1. B. Priyadarshini, T. Patra, T. R. Sahoo, *J. Magnes*. Alloys. **2021**, *9*, 478-488.
2. 2. P. P. Rath, S. S. Behera, B. Priyadarshini, S. R. Panda, D. Mandal, T. Sahoo, S. Mishra, T. R. Sahoo, and P K Parhi, *Appl. Surf. Sci.* **2019**, *491*, 256-266.
3. 3. T. Patra, A. Mohanty, L. Singh, S. Muduli, P. K. Parhi, T. R. Sahoo, *Chemosphere* **2022**, *288*, 132472.
4. 4. S. Muduli, S. S. Behera, R. K. Mohapatra, P. K. Parhi, T. R. Sahoo, *Mater. Sci. Eng.* B **2023**, *290*, 116275.

Superior Electrochemical Supercapacitor Performance of Boron-doped Diamond Films due to Nitrogen Addition

Shradha Suman,1,2 Kamatchi Jothiramalingam Sankaran, 1,2* Benadict Rakesh,1,2
Ramasamy Sakthivel1,2

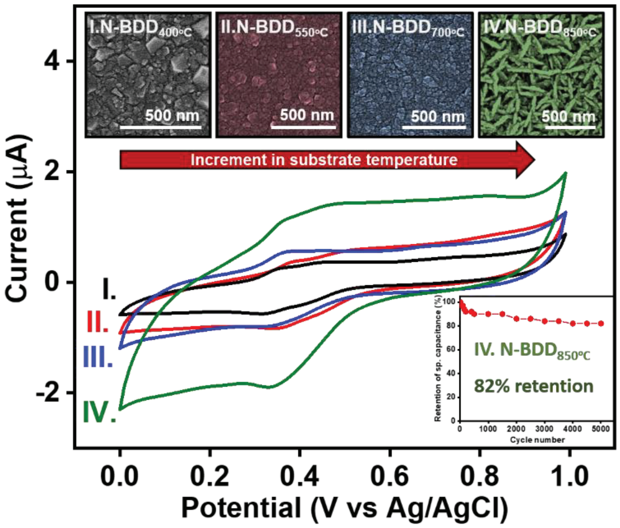
[1]*CSIR-Institute of Minerals and Materials Technology, Bhubaneswar 751013, India.*

[2]*Academy of Scientific and Innovative Research (AcSIR), CSIR-HRDC Campus, Ghaziabad 201002, India.*

(E-mail: kjsankaran@immt.res.in)

Abstract:
Diamond thin films have gained popularity as energy storage device materials due to their robust mechanical and chemical properties, as well as their extended lifetime stability. Numerous investigations have been conducted on supercapacitors made of boron-doped diamond (BDD) with varying diamond morphologies. Nevertheless, the impact of diamond grain size and structure on electrochemical performance has yet to be comprehensively understood. In the present work, BDD films of 4 different morphologies, obtained via varying the growth temperature (400^0, 550^0, 700^0 and 850^0 C), have been studied and compared. The increase in substrate temperature during the growth of diamond film varies from faceted structures (400^{0}C) to nanowire-like structures (850^{0}C). The variation in grain structure has a direct impact on the electrochemical behaviour of supercapacitors. For the nanowire diamond, the specific capacitance (C_s) is 412 μF/cm^2 at a current density of 2.55 μA/cm^2 in 1M Na_2SO_4, which is the maximum. The loss in specific capacitance for the 400^{0}C sample is found to be 30%, whereas the loss decreases with an increase in growth temperature and is 19% for the 850^{0}C sample. Such efficient nature of the material can be attributed to the nanowire-like structure, boron doping and induction of sp^2-graphitic grain boundaries, which enhance the electrical conduction and the interaction area, in turn enhancing the EDLC value and the lifetime stability of the ES system. These results indicate that the nanostructured BDD materials will pave a pathway for the next-generation electrochemical supercapacitors.

Figure:



Heterojunction-derived Ternary Metal Sulphides For Photocatalytic Degradation and Hybrid Supercapacitors Applications

Subhashree Mohapatra[1], Himadri Tanaya Das[2], Bankim Chandra Tripathy[3], NigamanandaDas[1]*

[1]*Department of Chemistry, Utkal University, Bhubaneswar, 751004, Odisha*

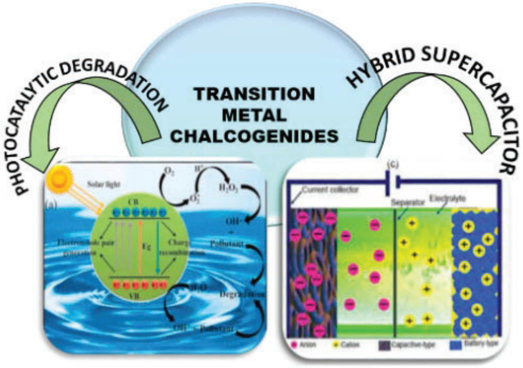
[2]*Centre of Advanced Materials and Applications, Utkal University, Bhubaneswar, 751004,Odisha*

[3] *Department of Hydro and Electro Metallurgy, CSIR-IMMT, Bhubaneswar 751013, India*

Email: chemnou@gmail.com: subhashree.mohapatra12@gmail.com

Abstract: Energy exhaustion and environmental pollution have been the biggest concern in recent years, requiring a sustainable approach to address these issues. Photocatalysis remediation of harmful contaminants from wastewater and generation of green energy by developing energy storage devices are some of the viable solutions for the emerging future crisis. In this context, transition metal chalcogenides including sulphides and selenides act as promising photocatalysts and electrode materials for supercapacitors owing to their distinguishing features [1]. However, the limiting performance of single-metal-based chalcogenides could be improved by designing a heterojunction-like architecture, which effectively delayed the charge carriers recombination during the photocatalysis. Further, the electrochemical performance was boosted due to rich redox reactions and high active sites [2, 3]. In view of this, the present work focuses on the study of nanostructured ternary metal sulphides as a potential material for both photocatalytic and energy storage applications.

A facile two-step hydrothermal approach has been employed to synthesize ternary $Co_3S_4/NiS_2/Cu_2S$ nanocomposites with different compositional ratios followed by physical and electrochemical characterizations. The synthesized material was used as an efficient photocatalyst for the degradation of toxic and carcinogenic Congo red dye under visible light irradiation. Its electrochemical performance was also investigated and implemented as battery electrodes in hybrid energy storage devices to power electronics. The synergistic properties of this ternary system as an effective photocatalyst and supercapacitor electrode material suggest a new route for applications in the environment and energy domain.



References:

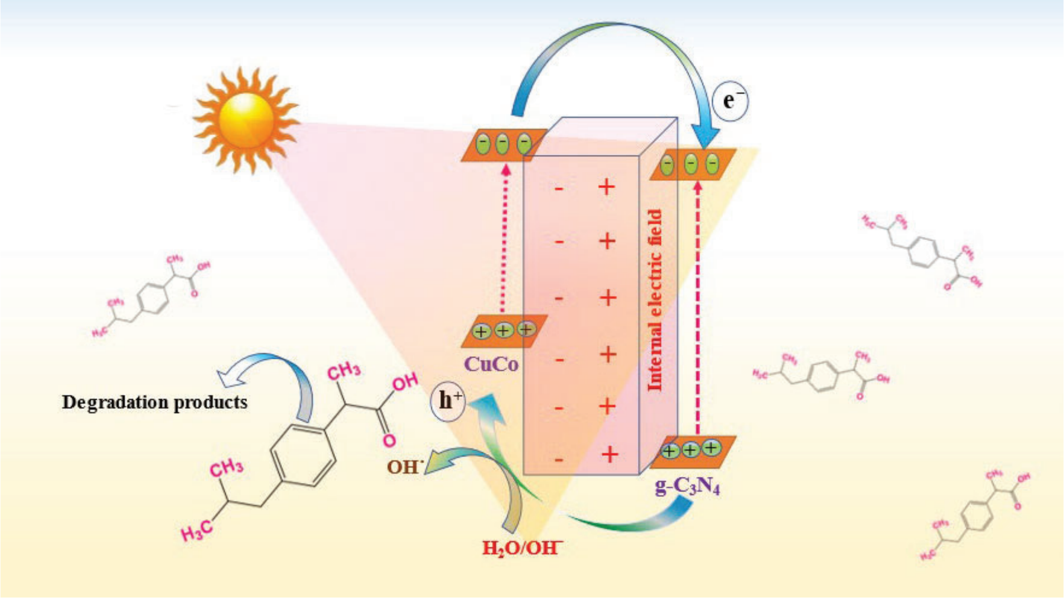
1. Yadav, S.; Yashas, S. R.; Shivaraju, H. P., *Environ Chem Lett 2021*
2. Ayodhya, D.; Veerabhadram, G., *Mater. Today Energy* 2018
3. Li, Y.; Zhang, J.; Chen, Q.; Xia, X.; Chen, M., *Adv. Mater.* 2021

"Exploring the Antibacterial Potential and Mechanism of Action of a Novel Biogenic Silver Nanoparticle as an Antibacterial Agent: Assessment of Biocompatibility with Mammalian Cells"

Swati Singh

Abstract: A dramatic increase in infectious illnesses, as well as a surge in drug-resistant pathogenic microbes, are regarded as serious public health concerns. As a result, the development of alternative treatment processes such as nanoparticle-based therapy is attracting a lot of attention these days. Based on this, we explored the antibacterial effectiveness of Ag NPs in the current study. For the production of Ag NPs, a green synthesis technique was developed. Andrographis paniculata plant extracts was used to effectively synthesize Ag NPs. The nanoparticles' morphology is studied using a Transmission Electron Microscope (TEM) and found to be cubic and spherical. The presence of Ag elements in nanoparticles was discovered using an EDAX investigation. The Dynamic Light Scattering (DLS) technique is used to characterize the size distribution of nanoparticles. The synthesized nanoparticle demonstrated antibacterial activity against *Staphylococcus aureus* at 100 and 200 µg/mL of Ag NPs. The formation of reactive oxygen species (ROS) by nanoparticles leads in antibacterial action. The NPs' antibacterial efficacy and toxicity against 3T3 primary murine fibroblast cells were validated by cytotoxicity testing. The obtained results show that synthesized nanoparticles might be used effectively in a variety of biological applications.

Scheme:



References and Notes:

1. Zhang, P.; Liu, H.; and Li, X., *Appl. Surf. Sci* **2021**, *559*, 149865.
2. Zhang, P.; Liu, H.; and Li, X., *ACS Sustain. Chem. Eng* **2020**, *8*, 17979.
3. Bulut, A.; Yurderi, M.; Ertas, I.E.; Celebi, M.; Kaya, M.; and Zahmakiran, M., *Appl. Catal. B* **2016**, *180*, 121.
4. Zhang, P.; Zeng, G.; Song, T.; Huang, S.; Wang, T.; and Zeng, H., *Appl. Catal. B* **2019**, *242*, 389

Surface engineering of sulphur defect in Ni doped ReS_2 nanostructure for efficient oxygen evolution reaction

Tapan Ping[1,2], Bikash Kumar Jena[1,2*]
[1] *Materials Chemistry Department, CSIR-Institute of Minerals and Materials Technology, Bhubaneswar, Odisha, 751013, India*
[2] *Academy of Scientific & Innovative Research, Ghaziabad, 201002, India*
(E-mail: tapanping99@gmail.com)

Abstract:

In 21th century, global energy demands increasing day by day. The search for renewable energies to replace our dwindling supply of fossil fuels is a key challenge that confronts humanity. To resolve the above-aforementioned problem shifting towards new sustainable energy technology is necessary. A green way to hydrogen generation, an alternative energy source by electrochemical water splitting, is a promising pathway for energy conversion. water splitting consists of two half-cell, Hydrogen evolution reaction (HER) at cathode and Oxygen evolution reaction (OER) at anode. However, the efficiency of this process is greatly limited by the slow kinetics of the anodic oxygen evolution reaction. Creating a cost-effective and highly efficient electrocatalyst to drive sluggish OER is one of the most critical issues for efficient water splitting. A one-step hydrothermal reaction is developed to synthesize a Ni-doped ReS_2 nanostructure with sulphur defects. Based on XRD, HRTEM, XPS and EPR characterization analysis deduced the physiochemical properties of the material. The material exhibited excellent OER activity with a current density of 10 mA cm^{-2} at an overpotential of 270 mV, a low Tafel slope of 31 mV dec^{-1}, and good long-term durability of 10 h in 1 M KOH. It shows high faradaic efficiency of 96%, benefiting from the rapid charge transfer caused by the concerted effect of Ni-in and S-out on the ReS_2 nanostructure.

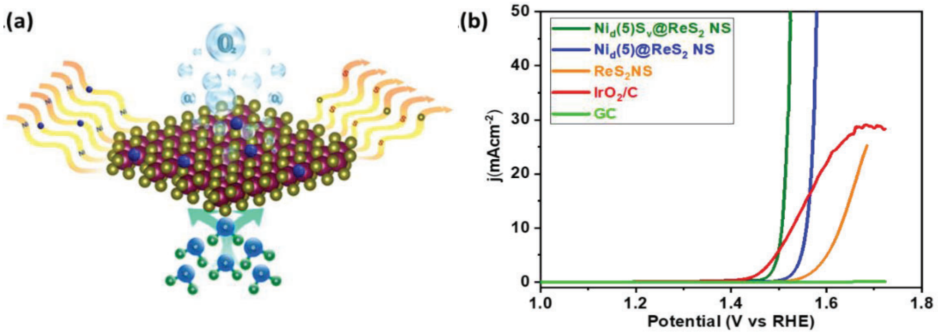


Figure:1(a) Scheme showing the concerted effect of Ni-in and S-out on ReS_2 nanostructures towards the OER, 1(b) The OER LSV polarization plots of the materials

Table 1. From this data $Ni_d(5)S_v@ReS_2$ NS show good OER as well as Tafel slope.

Catalyst	OER (η_{10}) mV	Tafel slope(mV/dec)
$Ni_d(5)S_v@ReS_2$ NS	**270**	**31**
$Ni_d(5)@ReS_2$ NS	327	38
ReS_2 NS	398	53.5
IrO_2/C	297	65

References and Notes:

[1] Das, T.K.; Ping, T.; Mohapatra, M.; Anwar, S.; Gopinath, C. S.; and Jena, B. K., *Chem. Commun.* **2022**, *58*, 3689-3692

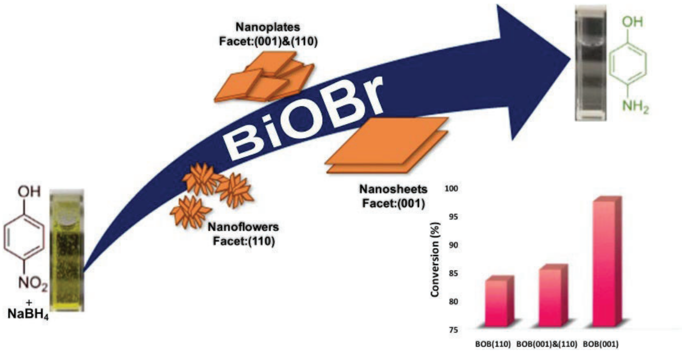
Understanding the role of dominant crystal facets on heterogeneous catalytic activity of BiOBr nanomaterials: Boosting catalytic efficiency through Fe (III)/Fe(II) incorporation

Vinay Kumar Sriramadasu,[a] Santanu Bhattacharyya [a]*

Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER)
Berhampur, Odisha 760010, India

(E-mail: svkumar@iiserbpr.ac.in)

Abstract: We have synthesized three different types of BiOBr nanomaterials (nanosheets, nanoplates and nanoflowers) by simply varying the pH of the solvent medium. Results suggest that the nanosheets show (001) facets as the major exposed surface. On the other hand, nanoflowers possess mainly (110) plane as the major exposed facet. However, nanoplates show both the facets (001) & (110). Detailed morphological and elemental studies quantitatively unveil the variation of positively charged oxygen vacancies with varying the nature of the crystal facets. Furthermore, the relative extent of oxygen vacancies and tunable crystal facets are further correlated with the overall surface area and the porosity of the as synthesized nanomaterials. Finally, all these three different types of nanomaterials with tunable crystal facets have been utilized for the catalytic reduction of para-nitrophenol to para-aminophenol as a model system through mild reducing agent $NaBH_4$. A possible mechanism has been proposed to explain the facet dependent catalytic activities of different BiOBr nanomaterials. Finally, we have incorporated Fe (III)/ Fe (II) ions in different types of BiOBr nanomaterials. The iron ions incorporation has been further correlated with the detail structural, elemental and optoelectronic features. A huge enhancement has been observed for overall catalytic efficiency upon incorporation of Fe (III)/Fe (II) ions. A plausible mechanism has been proposed to explain the effect of Fe (III)/Fe (II) incorporation for highly efficient catalysis process on the surface of BiOBr nanomaterials.



References:

1. Sriramadasu, V. K.; Kommula, B.; Prabhakar Bhardwaj; and Bhattacharyya, S., *J. Alloys and Compounds* 2023, 967, 171814.
2. (2) Chen, H.; Yang, M.; Tao, S.; and Chen, G., *Applied Catalysis B: Environmental* 2017, 209, 648-656.

CuCo Alloy Bimetallic Nanoparticle Supported on Graphitic Carbon Nitride for Efficient Photocatalytic Degradation of Ibuprofen and Hydrogen Gas Evolution by Water Splitting

Vishal Rout[1], Priyabrat Dash[2*]

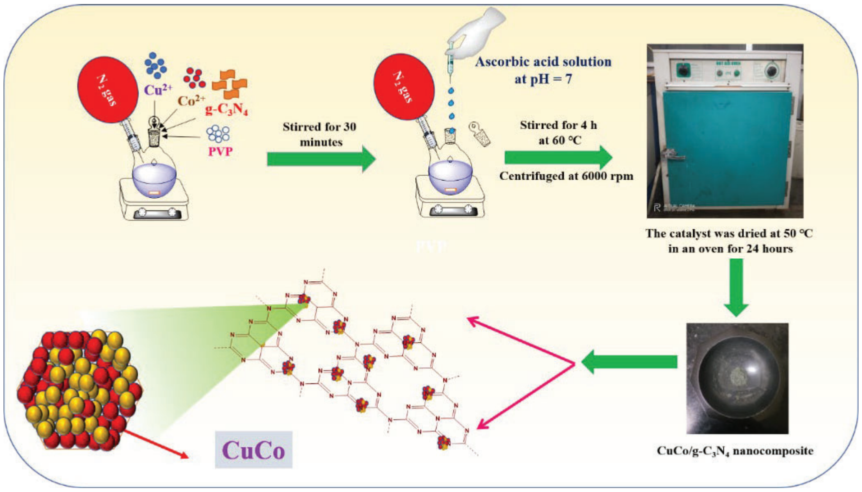
Department of Chemistry

National Institute of Technology, Rourkela, 769008, Odisha, India

(E-mail: 520cy3015@nitrkl.ac.in, dashp@nitrkl.ac.in)

Abstract: Metal nanoparticles (MNPs) have been usually applied for photocatalytic applications as they show enhanced physical and chemical properties. Bimetallic nanoparticles, composed of two different metals have drawn a greater interest than the monometallic nanoparticles as they possess abundant active sites and high surface energy because of the numerous defects. However, bimetallic Nanoparticles lose their catalytic behaviour due to their aggregation. To overcome this issue support material like graphitic nitride (g-C_3N_4) has been found as suitablematerial. g-C_3N_4 possesses a narrow band gap (about 2.7 eV) that endows it with superior lightabsorption capacity. Besides, it shows unique electronic structure, high thermal and chemical stability as well as less toxicity. Highlighting this, in this work we report a non-noble CuCo bimetallic nanoparticle supported on g-C_3N_4 as efficient nanocatalyst for the photocatalytic degradation of Ibuprofen. In addition, its efficiency for H_2 evolution by water splitting has alsobeen evaluated. The structural confirmation of the synthesized nanocatalyst was characterized by using sophisticated techniques like Powder X-ray diffraction (PXRD), Fourier Transform Infrared Spectroscopy (FTIR), Raman spectroscopy, UV-visible spectroscopy (UV-Vis), X-ray photoelectron spectroscopy (XPS), Transmission electron microscopy (TEM), Scanning electron microscopy (SEM), photoluminescence study and N_2 adsorption-desorption analysis. Our study revealed that CuCo supported on g-C_3N_4 showed the photocatalytic degradation of Ibuprofen of about 97%. It also showed H_2-evolution amount of 4638.4 μmol g^{-1} h^{-1}. The enhanced photocatalytic activity may be due to CuCo bimetallic nanoparticles that convert theenergy of the sunlight into surface plasmon resonance oscillations and transfers the plasmonicenergy to the electron-hole pair.

Figure:



Green synthesis and characterization of cerium oxide nanoparticles

Lipsa Ray, Kaniz Fatma, Jasaswini Tripathy*

School of Applied Sciences (Chemistry),
KIIT Deemed to be University, Bhubaneswar, India
(E-mail: *jasaswinitripathy@gmail.com, jtripathyfch@kiit.ac.in*)

Abstract:

Nanomaterials have a tremendous impact on human life owing to their numerous applications in material science, engineering, and medicine. Numerous health risks are associated with nanoparticles produced through chemical route. Recently, the green synthetic technique from plant extracts has attracted much attention to address this issue[1]. In addition to being a substitute for chemical synthesis, green synthesis is a method that is both economical and environmentally benign. The present study focuses on the synthesis of cerium oxide nanoparticles through a "green" synthetic approach using Impatiens Balsamina leaf extract, commonly known as rose balsam and comes under the Balsaminaceae family. Scanning electron microscopy (SEM), FTIR spectroscopy, UV-Visible spectroscopy, and X-ray diffraction (XRD) were used to characterize the green synthesized cerium oxide nanoparticles. The synthesized green nanoparticles can find uses in a wide range of antibacterial applications.

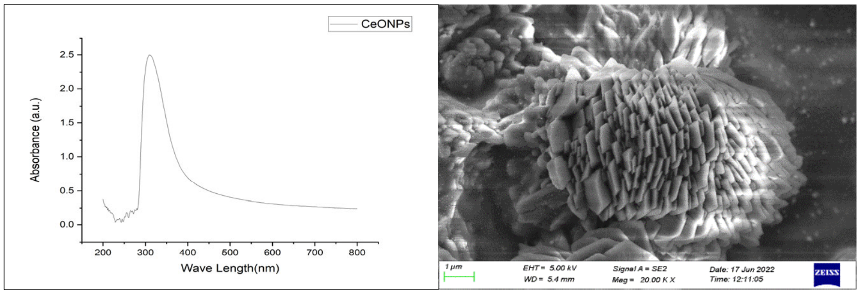


Figure: UV and FESEM of synthesized nanoparticles.

References:

Bordiwala, R. V.; *Results in Chemistry* **2023**, *5*, 100832.

Synthesis of Pure and Fe-doped CeO2 nanoparticles and their catalytic activity towards CO oxidation and soot combustion

Tapas Ranjan Sahoo

Department of Chemistry, School of Applied Sciences, KIIT deemed to be University, Bhubaneswar 24, Odisha, India

E-mail: trsahoofch@kiit.ac.in

Abstract: Pure CeO_2 and two samples of Fe-doped CeO_2 containing either 3 or 6 at.% Fe were obtained by microwave assisted combustion synthesis. The powders were extensively characterized by several techniques and tested as catalysts for both CO oxidation and soot combustion. As-synthesized CeO_2 nanoparticles have a mostly squared shape and size well below 100 nm; they are characterized by the presence of surface Ce^{3+} species likely due to the occurrence of very defective ceria crystalline phases, as revealed by HR-TEM. Oxidation at 400 ◦C leads to the formation of a hydroxyls-rich surface, with several types of OH groups related to both Ce^{4+} and Ce^{3+} species; reduction in H_2 at mild temperature (200 ◦C) leads both to reduction of surface Ce^{4+} to Ce^{3+} and formation of new OH groups. With respect to CeO_2 nanoparticles, Fe-doped ones have, as a whole, a larger size and less abundant surface OH species. A core-shell structure is inferred where Fe is mostly present in the shell, both in a secondary phase ($CeFeO_3$) and as a dopant, finally lowering the band gap of the material. The presence of Fe improved samples reducibility, as shown by the lowering of the onset of temperature programmed reduction. Catalytic tests of CO oxidation showed that surface Fe species significantly improve the catalytic performance of the samples, by lowering the onset of CO conversion to CO_2 especially at low Fe content (i.e. 3 at.%), whereas at 6 at.% Fe loading, the preferential formation of the secondary phase $CeFeO_3$ occurs, finally lowering the CO conversion with respect to the sample containing 3 at.% Fe. Conversely, the soot combustion activity was higher for pure CeO2 nanoparticles, likely due to their smaller size, which increases the amount of solid–solid contact points between soot and the catalyst. However, a positive effect of the presence of surface Fe species on the catalytic activity towards soot combustion was observed, as well.

Polymer Chemistry

Nitrogen rich porous organic polymer derived porous carbon: facile for electrochemical oxygen reduction reaction

Biswajit Nayak[1,2], Piyali Bhanja[1]*, Bikash Kumar Jena[1,2]*
[1]*Materials Chemistry Department, CSIR-Institute of Minerals and Materials Technology, Bhubaneswar, Odisha, 751013, India*
[2]*Academy of Scientific & Innovative Research, Ghaziabad, 201002, India*
(E-mail: biswajitnayak023@gmail.com)

Abstract:

Advanced electrochemical technologies, such as fuel cells and metal-air batteries, are promising alternative in the field of energy conversion and storage technology that plays a crucial role in the development of human civilization by reducing the use of carbonaceous fuel and related environmental issues. The efficiency of these large-scale clean energy devices is strongly limited by sluggish oxygen reduction reaction (ORR), which can be overcome by development of low-cost, durable, and effective electrocatalysts. In this regard, a newly designed porous organic polymer (POPQ) has been synthesized using two organic monomers, i.e., 2,6-diaminoanthraquinone and cyanuric chloride, under reflux conditions for 48 h in an inert atmosphere. The triazine containing porous organic polymers undergoes pyrolysis, which produces two nitrogen-doped porous carbon materials, N/POPQ600 and N/POPQ800, at 600 °C and 800 °C temperatures, respectively. Since the resultant N-doped porous materials have a higher surface area than the parent porous organic polymer and the materials have a synergistic effect due to the enriched nitrogen content throughout the matrix, the metal-free N/POPQ600 and N/POPQ800 materials exhibit good electrocatalytic activity towards oxygen reduction reaction (ORR). Among these, N/POPQ800 material shows excellent ORR activity with a nearly 4-electron oxygen reduction pathway where the half-wave potential is estimated to be 0.728 V vs RHE, comparable with commercially available Pt/C catalyst. Most interestingly, the N/POPQ800 catalyst displays outstanding long-lasting stability. It shows a better methanol tolerance capability than Pt/C, which can be attributed to the high specific surface area and N-doped well-defined crystalline porous structure.

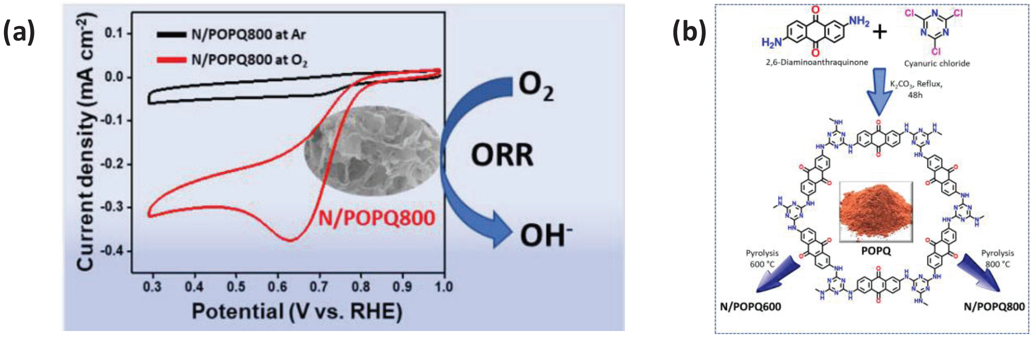


Figure 1 **(a)** Cyclic voltammograms of N/POPQ800 in Ar and O_2 saturated 0.1 M KOH solution confirming the activity towards ORR. **(b)** Scheme showing the formation of triazine-based porous polymer (POPQ) and their derivatives N/POPQ600 and N/POPQ800 at two different temperatures.

References and Notes:

[1] Nayak, B.; Mukherjee, A.; Basu, S.; Bhanja, P.*; Jena, B.K.*, *ACS Appl. Energy Mater.* **2022**, *5*, 15899–15908

Fabrication and Characterization of Graphene Oxide Reinforced Bio-Nanocomposite Films with Antibacterial Properties

Kaniz Fatma, Mamata Das, Jasaswini Tripathy*

School of Applied Sciences (Chemistry), KIIT Deemed to be University, Bhubaneswar, India

(E-mail: *jasaswinitripathy@gmail.com, jtripathyfch@kiit.ac.in*)

Abstract: The development of GO-based antimicrobial polymer nanocomposites has garnered considerable interest due to graphene oxide's (GO) antibacterial properties[1]. Polymer nanocomposites with GO-integrated polyvinylpyrrolidone (PVP) and carboxymethyl cellulose (CMC) blends were developed for antibacterial applications. The successful synthesis of GO is confirmed by transmission electron microscopy while the fabrication of CMC/PVP blend and CMC/PVP/GO is confirmed through FT-IR spectroscopy and X-ray diffraction (XRD) analysis. The morphological characteristics of polymer nanocomposites are studied using scanning electron microscopy. The films are also characterized using energy dispersive spectroscopy (EDX) which reveals the successful inclusion of the GO sheets in the polymeric matrix. Escherichia coli is used to investigate the antibacterial effectiveness of a polymeric nanocomposite. The growth of bacterial cells was inhibited by the CMC/PVP/GO nanocomposites.

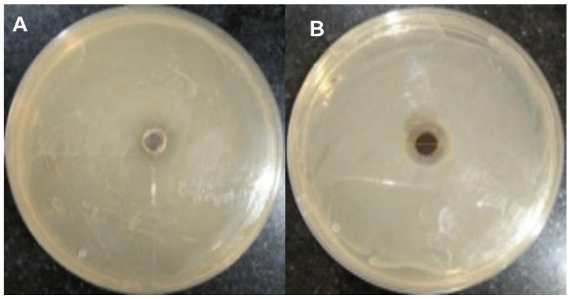


Figure: A*ntibacterial activity of (A) CMC/ PVP and (B) CMC/PVP/GO against E-coli bacteria*

References:

1. Díez-Pascual, A.M.; Luceño-Sánchez, J.A. *Polymers* **2021**, *13*, 2105

Geopolymer technology-recent trends

Manisha Dash[1], Barada Prasanna Sahoo[3], Diptikanta Dash[2,*], Prasanta Rath[1,*]

[1]*School of Applied Sciences (Chemistry) KIIT Deemed to be University, Bhubaneswar, India*

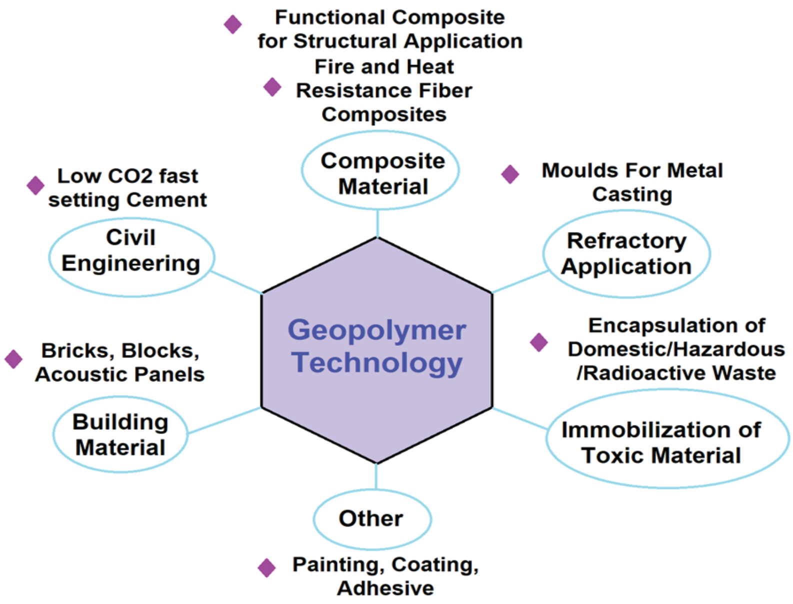
[2]*School of Mechanical Engineering KIIT Deemed to be University, Bhubaneswar, India*

[3]*KIIT-Technology Business Incubator, Bhubaneswar, India*

(E-mail: Prathfch@kiit.ac.in , dkdasfme@kiit.ac.in)

Abstract: In recent years, the field of geopolymer technology has experienced notable progress, prompting a compelling exploration of its latest trends. This abstract offers a comprehensive overview of these burgeoning advancements. Geopolymer technology, characterized by the alkali activation of aluminosilicates, presents an environmentally conscious alternative to conventional cement-based materials. Importantly, geopolymer composites exhibit heightened sustainability compared to their cement counterparts due to lower energy demands during production and reduced carbon emissions. Unlike traditional cement-based materials, the dominant hydration products in geopolymer systems comprise calcium aluminosilicate hydrate (C-A-S-H) and sodium aluminosilicate hydrate (N-A-S-H) gels, bypassing reliance on calcium silicate hydrate (C-S-H) formation for strength development. Consequently, meticulous chemical analysis of diverse aluminosilicate precursors and their corresponding geopolymerization behavior become pivotal for successful commercial integration. Recent research endeavors have extended the spectrum of viable raw materials, encompassing metakaolin, fly ash, slag, ferrochrome ash, mine tailings, rice husk ash, and red mud. These augmentations serve to amplify the efficacy and sustainability of geopolymeric products. Noteworthy innovations in binder compositions and activator formulations have heralded the emergence of environmentally friendly alkaline and acidic activators. This novel range of activators empowers tailoring of geopolymer characteristics, thus expanding the horizon of potential applications. Moreover, the integration of fiber reinforcements (both short and long fibers) into geopolymer composites has garnered significant attention due to its capacity to enhance mechanical properties and retain overall durability. A notable advantage of the geopolymer matrix employed in these composites is its ability to confer a finite period of durability even under elevated temperatures, all while inhibiting emission of toxic gases into the surrounding environment. This innovation paves a promising path toward structural applications, reinforcing the technology's practicality. However, the lack of standardized guidelines for geopolymer mixture design is limiting its industry acceptance. Developing a standard mix design code for geopolymer is complex due to its chemical activation and varied parameters. Current design studies focus on critical factors affecting compressive strength and workability, often using regression analysis. However, the absence of consensus on design parameters and categorization, especially with differing raw material properties, hinders the standardization of procedures.

Figure:



References:

1. Farhan, K. Z., Johari, M. A. M., &Demirboğa, R. (2020). Assessment of important parameters involved in the synthesis of geopolymer composites: A review. Construction and Building Materials, 264, 120276
2. Krishna, R. S., Mishra, J., Zribi, M., Adeniyi, F., Saha, S., Baklouti, S., ... & Gökçe, H. S. (2021). A review on developments of environmentally friendly geopolymer technology. Materialia, 20, 101212
3. Duxson, P., Fernández-Jiménez, A., Provis, J. L., Lukey, G. C., Palomo, A., & van Deventer, J. S. (2007). Geopolymer technology: the current state of the art. Journal of materials science, 42, 2917-2933

Selective Adsorption of Dyes by Epichlorohydrin Grafted Nanopolyaniline

Sai Sushree Rath, Braja N. Patra *

Department of Chemistry

Utkal University, Bhubaneswar- 751004

(E-mail: brajapatra@gmail.com)

Abstract: Dyes having their recalcitrance nature and mutagenic, embryotoxic, carcinogenic effect on terrestrial animals emerges as a potent pollutant of water today. Out of all developing method to treat contaminated water adsorption remain propitious due to its advantages like natural process, low cost, easiness, eco-friendly, reusability. Herein the adsorbent Epichlorohydrin grafting Nanopolyaniline (PANI-g-EC) was synthesised by ring opening reaction of epichlorohydrin by polyaniline acting as a nucleophile. The structural properties of the synthesised adsorbent were determined by using techniques like Scanning Electronic Microscopy (SEM), Fourier Transformation Infrared (FTIR), Thermo Gravimetric Analysis(TGA), X-Ray Diffraction (XRD). The synthesised adsorbent shows both cationic and anionic dye adsorption at two different pH. The adsorption parameters like dosages of adsorbent, initial dye concentration, pH, Temperature, thermodynamic parameters (ΔGo, ΔHo, ΔSo) of the adsorption process were extensively studied for potential application. The adsorption process follows pseudo second order reaction kinetics and Langmuir adsorption isotherm.

Keywords: dye: adsorption; nanopolyaniline; pH

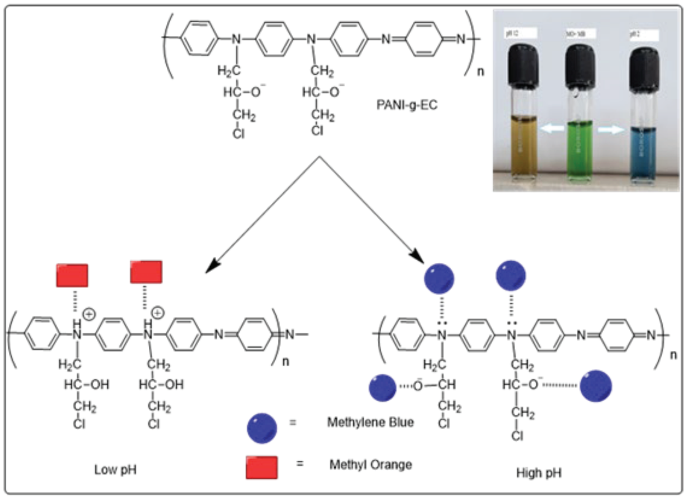


Figure: Removal of dyes by PANI-g-EC

References and Notes:

1. Huang, J.; Virji, S.; Weiller, B. H.; Kaner, R. B., J. Am. Chem. Soc. **2003**, 125, 314–315
2. Majhi, D.; Patra, B. N. *J. Chem. Eng. Data* **2018**, *63*, 3427–3437.

Exploring MXene/RGO Hybrid Nanofillers in Enhancing PVDF/PANI Conducting Polymer Nanocomposites for Electrochemical Devices and Electromagnetic Interference Shielding

Pooja Mohapatra, Lipsa Shubhadarshinee, Aruna Kumar Barick*

**Corresponding Author E-mail: akbarick_chem@vssut.ac.in; Contact No.: +91-9937069518*

Department of Chemistry, Veer Surendra Sai University of Technology, Burla, Sambalpur, 768018, Odisha, India

Abstract:

The exploration of 2D MXenes has been continuously growing due to their distinctive structure, remarkable conductivity, and exceptional mechanical characteristics. Surface-modified reduced graphene oxide (rGO) hybrids find application in diverse electrochemical devices as high-performance electrode materials for energy storage systems. Particularly, the MXene/rGO nanohybrid effectively hinders the self-stacking between graphene and MXene layers, leading to increased accessible specific surface area, accelerated diffusion of electrolyte ions, and enhanced material properties. This hybrid demonstrates substantial volume capacitance, elevated energy and power density, and extended cycling stability, making it suitable for advanced energy storage applications. Despite these promising advancements, further enhancements are needed for both mass capacitors and area capacitors. Electrically conductive blends of polymers have garnered significant attention as dielectric materials. However, achieving uniform behaviour, stable electrical characteristics, and minimal current leakage remains a persistent challenge. In this context, we have synthesized a conductive polymer blend comprising Polyaniline (PANI) and Poly (vinylidene fluoride) (PVDF), exhibiting relatively high dielectric permittivity (ε′) coupled with a low band gap. The synthesis and practical application of MXene, rGO, PVDF, and PANI, along with their composites, can be substantiated through the utilization of advanced analytical tools such as X-ray diffraction (XRD), small-angle neutron scattering (SANS), X-ray absorption spectroscopy (XAS), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS), transmission electron microscopy (TEM), pair distribution function analysis, atomic force microscopy (AFM), nuclear magnetic resonance (NMR), Raman spectroscopy, dynamic light scattering (DLS), UV-Visible spectroscopy (UV), Fourier transform infrared spectroscopy (FTIR). Additionally, the thermal, dielectric, and sensing properties can be examined using techniques such as thermogravimetry-differential scanning calorimetry (TG-DSC), LCR meter, and UV-Vis instrumentation. A pivotal aspect of our study centres on ensuring the safety of all living organisms and maintaining environmental friendliness.

Keywords: *Mxene; Reduced graphene oxide;* Poly (vinylidene fluoride)*; Polyaniline; Nanocomposites; Thermal, Dielectric and Sensing Properties*

References and Notes:

1. Liu, Y.; Yu, J.; Guo, D.; Li, Z.; and Su, Y., *Journal of Alloys and Compounds* **2020**, *815*, p.152403.
2. Meher, D.; N. Karna; and B. P. Sahoo., *Polymer* **2019**, 181, p.121759.

Fabrication of TPU/PPy/rGO and TPU/PPy/MWCNT for Electromagnetic shielding application in X band.

Swatee Acharya, Bibhu Prasad Sahoo*

Department of Chemistry, School of Applied Sciences

KIIT Deemed to be University

E-Mail: bibhuprasadfch@kiit.ac.in

Abstract: Electromagnetic radiation pollution is a serious concern in today's environment, causing problems not just for technological gadgets but also for humans. Researchers and engineers are both interested in solving this challenge. The goal of this research is to fabricate a thermoplastic polyurethane (TPU) and Polypyrrole(PPy) based blend nanocomposites using a simple solvent casting method at such a low concentration of rGO and MWCNT(0.3,0.4,0.5 php) (parts per polymer), for electromagnetic interference shielding applications. The chemical interaction morphology of the nanocomposites is characterized by Raman spectroscopy, X-ray diffraction (XRD) and Field emission scanning electron microscopy (FESEM) techniques. The material properties, such as dielectric and magnetic, are analyzed in X band frequency (8.2-12.4 GHz). The total shielding effectiveness of (SE_{Tot}) 0.5 rGO composites is found to be 25 dB, whereas, for corresponding MWCNT composites, it is 24 dB. Interestingly, in 0.5 rGO nanocomposites, absorption shielding effectiveness (SE_{Abs}) is approximately 23 dB, and reflection shielding effectiveness (SE_{Ref}) is less than 2 dB. As a result, it indicates more than 60% of the electromagnetic wave is absorbed, and the rest gets reflected.

keywords – Polymer nanocomposite, EMI shielding, rGO, X band

ORGANIC CHEMISTRY

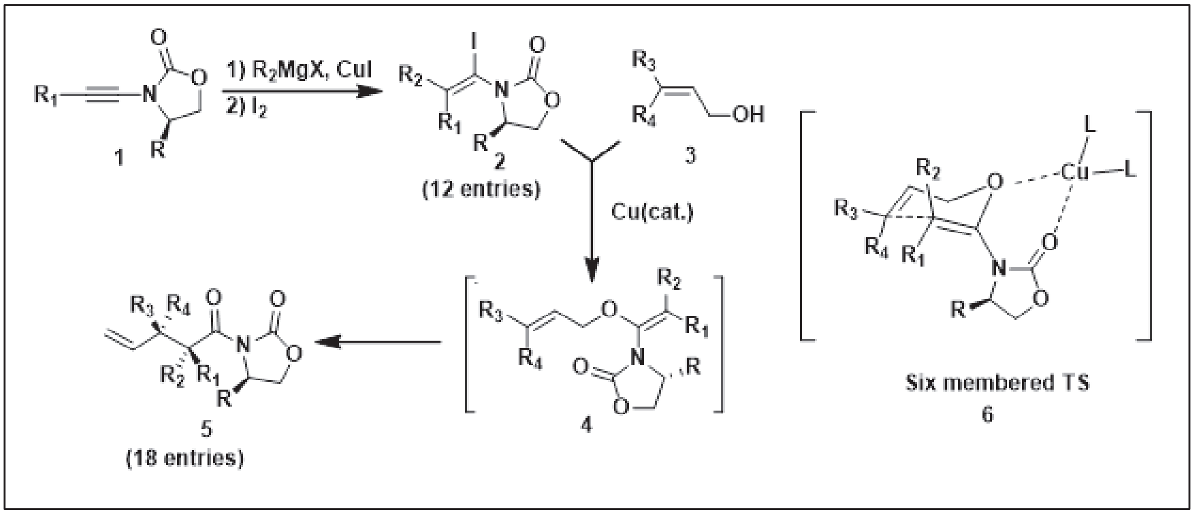
Organic synthesis and catalysis

A Cu-(I) Catalyzed Stereoselective Claisen Rearrangement Process: Construction of *vic*-All-C quaternary and Tertiary Stereocenter in Acyclic System

Subhransu Sekhar Pati and Jaya Prakash Das*

Department Of Chemistry, Ravenshaw University, Cuttack, 753003

Abstract: The Claisen rearrangement is considered one of the most efficient methods for the construction of C-C single bond along with the formation of γ, δ- unsaturated carbonyl compounds. This reaction proceeds through a six-membered (Zimmermann-Traxler) transition state which itself provides diastereoselectivity. Furthermore, the construction of all carbon quaternary stereogenic centers along with contiguous stereo centres in acyclic system is still a challenge to achieve. This work focuses on the design of a novel domino process that consists of a metal-catalyzed C-O bond coupling and a subsequent Claisen Rearrangement with diastereo- & enantioselectivity, which leads to the construction of two adjacent stereocenters along with the desired all-carbon quaternary stereocenter.



References:

1. Chechik-Lankin, H.; Marek, I. *Synthesis*. **2005**, *19*, 3311–3318. (b) Chechik-Lankin, H.; Marek, I. *Org. Lett*. **2003**, *5*, 5097-5089. (c) Das, J. P.; Marek, I. *Chem. Soc. Chem. Commun*. **2011**, *47*, 4593-4623.
2. Nordman, G.; Buchwald. S. L. *J. Am. Chem. Soc*. **2003**, *125*, 4978.
3. Uyeda, C.; Jacobsen, E. N. *J. Am. Chem. Soc*. **2008**, *130*, 9228.

Cobalt Catalyzed Chemoselective Reduction of Nitroarenes: Hydrosilylation under Thermal and Photochemical Reaction Conditions

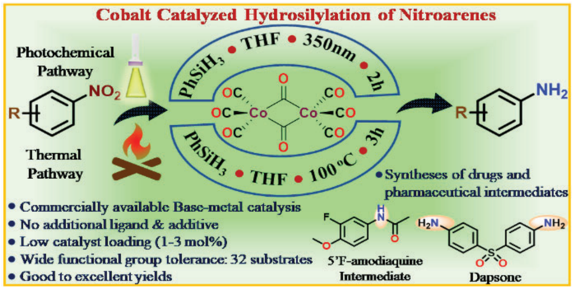
Surajit Panda, Amareshwar Nanda, Rakesh R Behera, Rahul Ghosh, Bidraha Bagh *

Department of Chemistry,
National Institute of Science Education and Research (NISER), Bhubaneswar 752050 Odisha, India.

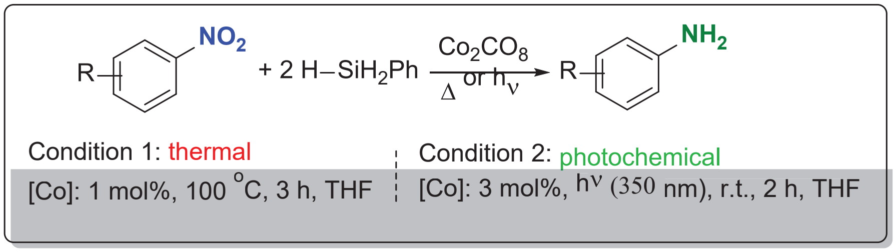
(E-mail: surajit.panda@niser.ac.in)

Abstract: Commercially available $Co_2(CO)_8$ was used as an effective catalyst for the hydrosilylation of nitroarenes under both thermal and photochemical conditions. A wide variety of nitroarenes with various functionalities were selectively reduced to aromatic amines. Syntheses of drug molecules expands the potential utility of this protocol. Experimental evidences suggested radical pathway.

Figure:



Scheme:



References and Notes:

1. Panda, S.; Nanda, A.; Behera, R. R.; Ghosh, R.; Bagh, B. *Chem. Commun.*, **2023**, *59*, 4527.
2. Wu, J.; Tongdee, S.; Ammaiyappan, Y.; Darcel, C. *Adv. Synth. Catal.* **2021**, *363*, 3859.
3. Vijaykumar, G.; Mandal, S. K. *Dalton Trans.* **2016**, *45*, 7421.

Carboamination and olefination: *ortho* C–H functionalization of phenoxyacetamide

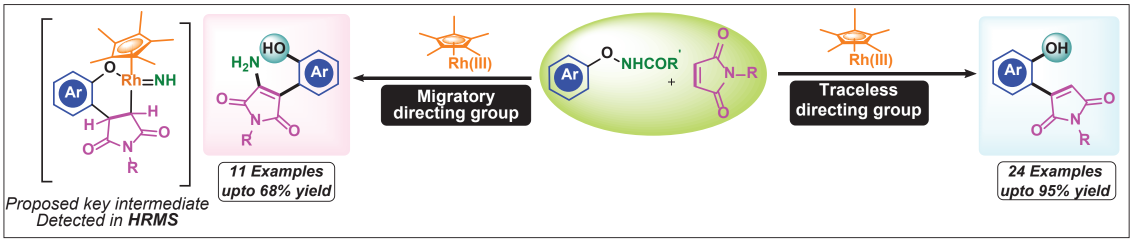
Tanmayee Nanda,[ab] Shubham Kumar Dhal,[ab] Gopal Krushna Das Adhikari,[ab] Namrata Prusty[ab] and
Ponneri C. Ravikumar [*ab]

[a] *School of Chemical Sciences, National Institute of Science Education and Research (NISER),*
Bhubaneswar, Odisha 752050, India. E-mail: pcr@niser.ac.in

[b] *Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai 400094, India*

shubhamdhal45@niser.ac.in pcr@niser.ac.in

Abstract: we have demonstrated a rhodium-catalyzed carboamination of olefin with the double bond intact. For the first time, deacylative carboamination of the maleimide has been achieved wherein phenoxyacetamide has behaved as the aminating source. In addition to carboamination, we have also disclosed the C–H olefination protocol, where the maleimide group has been installed successfully in the *ortho*-position of phenoxyacetamide. In this protocol, phenoxyacetamide behaved as a traceless directing group with the *in-situ* release of acetamide. The base-assisted E2-elimination is the key to the success of the olefination reaction.



References and Notes:

1. 1. Nanda, T.; Dhal, S. K.; Adhikari, G. K. D.; Prusty, N.; and Ravikumar, P. C., *Chem. Commun* **2023**, *59*, 8818-8821.

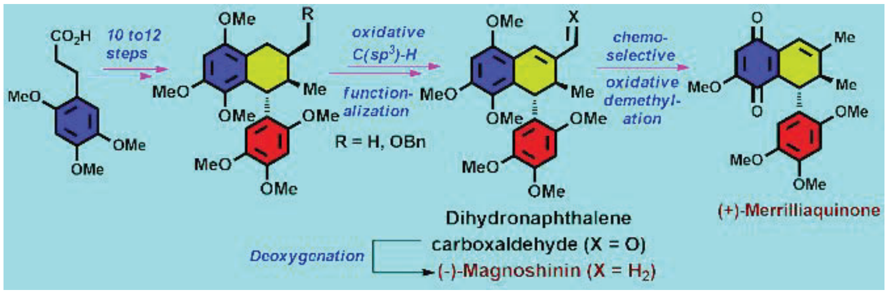
Asymmetric Total Synthesis of (-)-Magnoshinin and (+)-Merrilliaquinone: Application of an Organocatalyzed Late-Stage C(sp^3)-H Functionalization Logic

Chandrakanta Sahoo[†] and Tabrez Khan*
Organic Synthesis Laboratory, School of Basic Sciences
Indian Institute of Technology Bhubaneswar
(E-mail[‡]: s23cy09003@iitbbs.ac.in)

Abstract:

Cyclolignans with the dihydronaphthalene scaffold represent one of the distinct and structurally interesting classes of lignans natural products. Magnoshinin and merrilliaquinone are two -examples of this family.[1] Through the present poster, a unified approach for the first asymmetric total synthesis of (-)-magnoshinin and (+)-merrilliaquinone will be presented. The key feature of the synthesis is the DDQ-assisted chemoselective late-stage oxidative functionalization of the polyoxygenated chiral tetralin core accessed by utilizing the relayed asymmetric induction strategy. Then, the follow-up of chemoselective redox chemistry[2] facilitates the synthesis of (-)-magnoshinin (28.2% overall yield) and (+)-merrilliaquinone (20.6% overall yield) along the shortest route, starting from the known 3-(2,4,5-trimethoxyphenyl)propanoic acid.[3]

Scheme:



References and Notes:

1. D. Kumar, O. Das, M. S. Kaurav, T. Khan, *RSC Adv.* **2017**, 7, 36844–36851.
2. D. Kumar, A. Salam, T. K. Sahu, S. S. Sahoo, Tabrez Khan, *J. Org. Chem.* **2021,** *86,* 15096-15116.
3. A. Salam, D. Kumar, T. K. Sahu, R. Khan, T. Khan, *Eur. J. Org. Chem.* **2022**, e202101452 (1-8).

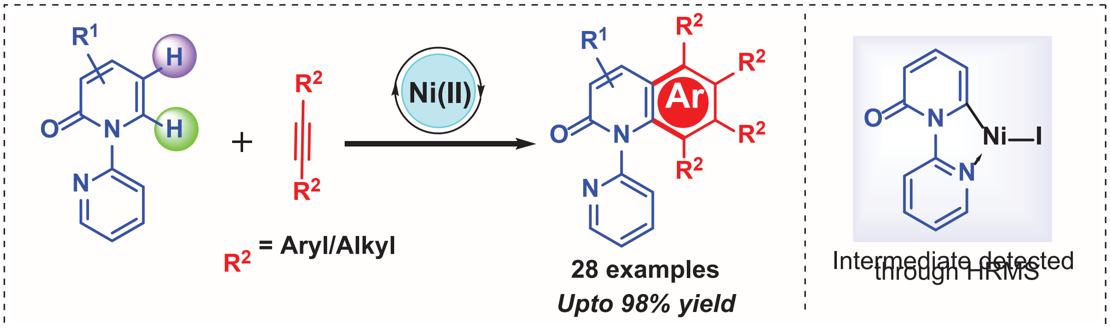
Switching the Reactivity of Nickel Catalyzed reaction of 2-Pyridones with Alkynes: Easy Access to Poly-Aryl/Alkyl Quinolinones

Namrata Prusty, Smruti Ranjan Mohanty, Shyam kumar Banjare, Tanmayee Nanda, and Ponneri C. Ravikumar*

Department of Chemistry, National Institute of Science Education and Research (NISER), Bhubaneswar

(E-mail: namrata.prusty@niser.ac.in and pcr@niser.ac.in)

Abstract: Catalytic C-H functionalization (activation) offers the promise of atom economical introduction of functionality into organic molecules by direct transformation of C -H bonds to C-C, C-N, or C-O bonds. Compared to more traditional approaches that involve functional group manipulations, the direct utilization of C-H bonds in synthesis can minimize chemical steps, economic cost, and environmental impact. In these regards, the use of 1st row transition metal catalyst has received much more attention as compared to 2nd & 3rd row transition metal atom because of their low cost, unique reactivity profiles, and easy availability. Among these metals, nickel (Ni) catalysts have drawn considerable attention from the scientific community. Herein, we have discussed, Ni-catalyzed C6- followed by C5 cascade C-H activation/[2+2+2] annulation of 2-pyridone with alkynes which afford Poly-Aryl/Alkyl Quinolinones. A change in the reaction pathway was achieved by tuning the reaction condition and incorporation of the directing group.



● Cascade C-H activation ● Nickel-catalyst ● Access to quinolinone molecule

Figure.1: Schematic representation for nickel catalyzed double C-H bond activation of pyridylpyridones.

References and Notes:

1. Prusty, N.; Mohanty, S. R.; Banjare, S. K.; Nanda, T.; and Ravikumar, P. C. ***Org. lett.*** **2022**, *24*, 6122–6127.

Metal-free Approaches Towards C-N Bond Formation

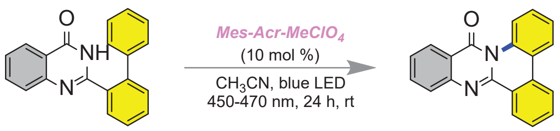
Rosalin Bhanja,‡ Shyamal Kanti Bera‡ and Prasenjit Mal*

NISER, An OCC of HBNI, Jatni, Khurda, Odisha 752050, India

(E-mail: rosalin.bhanja@niser.ac.in)

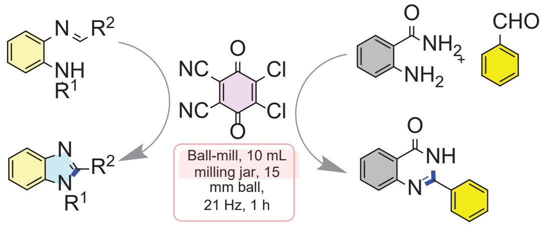
Abstract: The demand for sustainable energy sources and mild metal-free reaction techniques in synthetic organic chemistry have surged due to growing environmental concerns and global warming. To combat with issues associated with metal catalysed reactions like poor atom economy, extreme sensitivity for moisture and air, difficulties in purifications etc., metal free strategies have emerged as alternatives. Visible light photocatalysis is the most pronounced one which can selectively transform substrates by avoiding the use of high thermal energy and stochiometric amount of reagent. Similarly, solvent-free mechanochemical procedures are another greener alternative that can make the world more sustainable by following the “Twelve Principles of Green Chemistry”.[1]

Scheme 1.



Bhanja, R.; Bera, S. K.; Mal, P., *Chem. Commun.* **2023,** *59*, 4458

Scheme 2.



Bera, S. K.; **Bhanja, R.**; Mal, P., *Beilstein J. Org. Chem.* **2022,** *18*, 646

Here, a straightforward photocatalytic regioselective intramolecular C-N coupling reaction is illustrated for the construction of 14*H*-quinazolino[3,2-f]phenanthridin-14-one employing the Mes-Acr-MeClO$_4$ (9-mesityl-10-methylacridinium perchlorate) as a visible light organoredox photocatalyst (Scheme 1).[2] In addition to that 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) mediated oxidative C-N coupling toward the synthesis of 1,2-disubstituted benzimidazoles and substituted quinazolin-4(3*H*)-one derivatives under the solvent-free mechanochemical (ball milling) condition is also discussed (Scheme 2).[3]

References and Notes:

1. Ardila-Fierro, K. J.; Hernandez, J. G., *ChemSusChem* **2021,** *14* (10), 2145-2162.
2. Bhanja, R.; Bera, S. K.; Mal, P., *Chem. Commun.* **2023,** *59* (30), 4455-4458.
3. Bera, S. K.; Bhanja, R.; Mal, P., *Beilstein J. Org. Chem.* **2022,** *18*, 639-646.

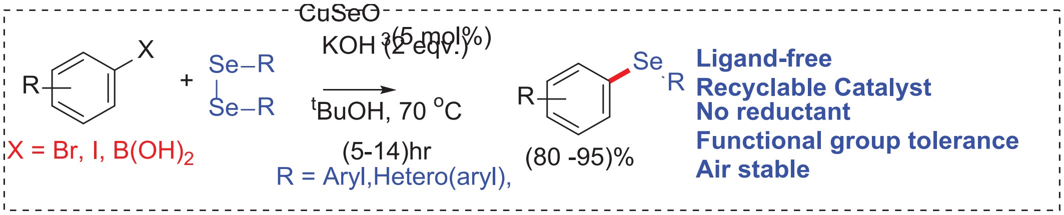
Bimetallic $CuSeO_3$ Catalyst: A Sustainable Approach to *Csp2-Se* Bond Formation

Amit Kumar pradhan and Dr. Laxmidhar Rout*

Department of Chemistry, Berhampur university

(E-mail: kumaramitpradhan455@gmail.com, ldr.chem@buodisha.edu.in)

Abstract: A remarkable progress achieved in the realm of *Csp2-Se* cross-coupling, showcasing its pivotal role in contemporary organic synthesis.[1] We have noticed a scarcity of instances in the existing literature concerning the formation of carbon-selenium bonds through *Csp2-Se* cross-coupling using diaryl diselenides [2] and arylhalides. In this study, we present $CuSeO_3.2H_2O$ as an effective catalyst for facilitating the direct *Csp2-Se* cross-coupling between diaryldiselenides and aryl iodides, bromides, as well as aryl boronic acids.[3] Notably, this reaction takes place at a relatively low temperature (70 °C) and is conducted in a sustainable *tert*-butanol solvent without ligand.[4-5] It's noteworthy that arylboronic acids also exhibited higher reactivity compared to both aryliodides and bromides.



Scheme - 1 : Reaction of diarylselenide with arylhalide

References and Notes:

1. Ramana, T.; Punniyamurthy, T.; Eur. J. Org. Chem. 2011, 2011, 4757.
2. Ding, Y.-N.; Huang, Y.-C.; Liang, Y.-M.; et al., Org. Lett. 2021, 23, 564
3. Pradhan, A.K.; Rout, L.; et al. Chemistry Select. 2023, 2023, 8, e202300378 .
4. Sahoo, S. K.; Behera, P.K.; Rout, L. et al., New . J. Chem. 2022, 46, 1650.
5. Choudhury, P.; Pradhan, A.K.; Rout, L. et al., Eur. J. Org. Chem. 2022, e202201194

Acknowledgement :

Dr. Rout is thankful to Director Professor A K Ganguli, IISER Berhampur, Odisha, India for providing NMR and HRMS spectroscopy facilities. This work was supported by Council of Scientific and Industrial Research CSIR/02(0393)/21/EMR-II. Dr Rout acknowledges Science and Engineering Research Board, SERB, New Delhi SERB/CRG/2022/001544. New Delhi, India, Science and Technology department, Govt. of Odisha, (no. S&T/2587/2023) for Funding. Dr. Rout is also thankful to Berhampur University and University Grants Commission (UGC) for providing infrastructure facilities.

Bimetallic heterogeneous catalyst for *Csp2-S* cross-coupling in sustainable aqueous solvent

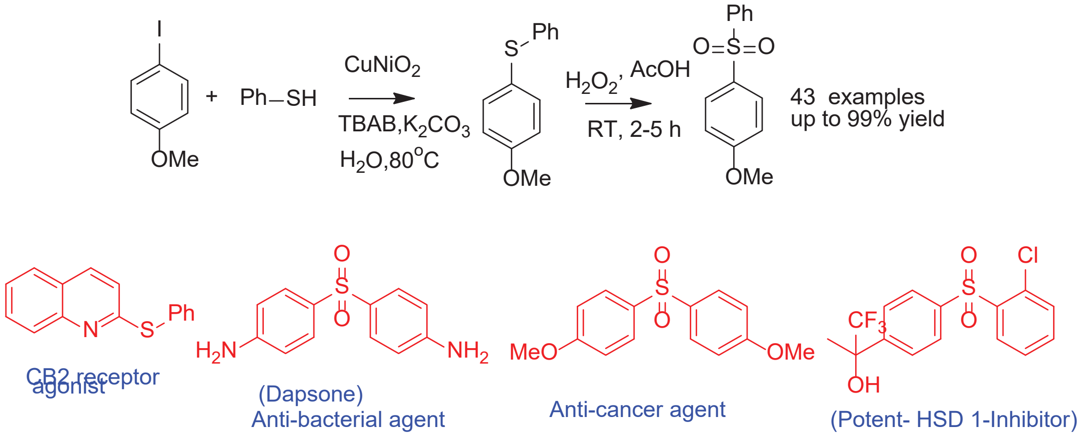
Amlan Swain[a], and Laxmidhar Rout[b]*

[a]*Department of Chemistry, Berhampur University, https://ldrout.in/*

Email:amlanswain15@gmail.com; ldr.chem@buodisha.edu.in

Abstract:

Sulfur compounds demonstrate tunable biological activity, and the *Csp2-S* motif is found in many natural compounds.[1] Transition metals were frequently used for above cross-coupling reaction. Among the various solvents used for this purpose, water have attracted notable interest in recent years due to its properties such as nontoxicity, non-flammability, renewability, and widely availability compared with other solvents. Herein, we have developed a new bimetallic heterogenous catalyst which profoundly performed the *Csp2-S* cross-coupling in water. The protocol is ligand free, scalable and tolerates to a wide range of heteroaromatic halide and thiols. The protocol allows synthesis of bioactive thioether.



Scheme 1: Synthesis of bioactive sulfone derivatives.

References and Notes:

1. P. Ertl, E. Altmann, and J. M. McKenna; *J. Med. Chem.*, **2020**, *63*, 15, 8408-8418.
2. L. Rout;T. Punniyamurty; *Angew. Chem. Int. Ed*, **2007**, *46,* 5583-5586.
3. S. Jamini; L. Rout; T. Punniyamurty et al.; *Tetrahedron Lett.*, **2008**, *49*, 1484-1487.
4. R. Panigrahi; L. Rout et al.; *Chem. Eur. J.*, **2020**, *26*, 620-624.
5. S. Panda; L. Rout et al.; *New. J. Chem*., **2020**, *44*, 2500-2504.
6. P. K. Behera; A. Swain; L. Rout et al.; *Chemistry Select*, **2022**, *7*, e202202919.
7. P. Choudhury, A. Swain, L. Rout et al.; *Eur. J. Org. Chem*., **2022**, *2022*, 48, e202201194.
8. **A. K. Pradhan, A. Swain, L. Rout et al.; *Chemistry Select*, 2023, *2023*, 8, e202300378.**

Acknowledgement :

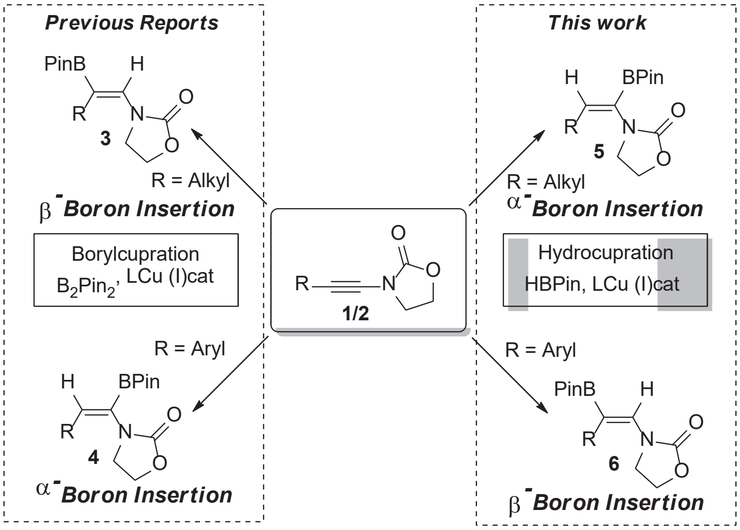
Dr. Rout is thankful to Director Professor A K Ganguli, IISER Berhampur, Odisha, India for providing NMR and HRMS spectroscopy facilities. This work was supported by Council of Scientific and Industrial Research CSIR/02(0393)/21/EMR-II. Dr Rout acknowledges Science and Engineering Research Board, SERB, New Delhi SERB/CRG/2022/001544. New Delhi, India, Science and Technology department, Govt. of Odisha, (no. S&T/2587/2023) for Funding. Dr. Rout is also thankful to Berhampur University and University Grants Commission (UGC) for providing infrastructure facilities.

Cu^I Catalyzed Regio- and Stereo-selective Hydroboration of Ynamides: α- and β-Borylation via Hydro-Cupration and Borylation

Archana Mishra, Subhra Roy, Subhransu sekhar Pati, Minati Behera, Jaya Prakash Das*

Dept. of Chemistry, Ravenshaw University ,Cuttack-753003

Abstract:- A Cu^I-catalyzed hydrocupration and borylation protocol for the region- and stereoselective borylation of ynamides utilizing pinacolatoborane (HBpin) as the borylating agent has been developed.The reaction features mild conditions, good substrate scope and functional group tolerance-representing a highly efficient and practical method for the synthesis of region- and stereoselective tri-substituted alkenylboronates from readily available ynamides.The regioselectivity is controlled by altering substituents on the ynamides (alkyl vs aryl) and utilizing a catalytic species [LCuH] generated in situ from HBpin and [LCuX].Suzuki coupling and other transformations highlight the synthetic utility of the method.



References and Notes:

1. P.V Ramachandra, H. C. Brown, Recent Advances in Borane Chemistry. In Organoboranes for Synthesis; ACS Symposium Series 783; *American Chemical Society:* Washington, DC, **2001**.
2. N. Miyaura, A. Suzuki, *Chem. Rev.* **1995**, *95*, 2457-2483.
3. R. Barbeyron, E. Benedetti, J. Cossy, J. J. Vasseur, S. Arseniyadis, M. Smietana, *Tetrahedron* **2014**, *70*, 8431-8452.
4. G.A. Molander, N. M. Ellis, *J. Org. Chem*. **2008**, *73*, 6841-6844.
5. H. Y. Jung, X. Feng, H. Kim, J. Yun, *Tetrahedron* **2012**, *68*, 3444-3449.

Homogeneous and Heterogeneous Photocatalyst in Chemodivergent Functionalisation of Aryl Alkynoates or *N*-Methylalkanamides

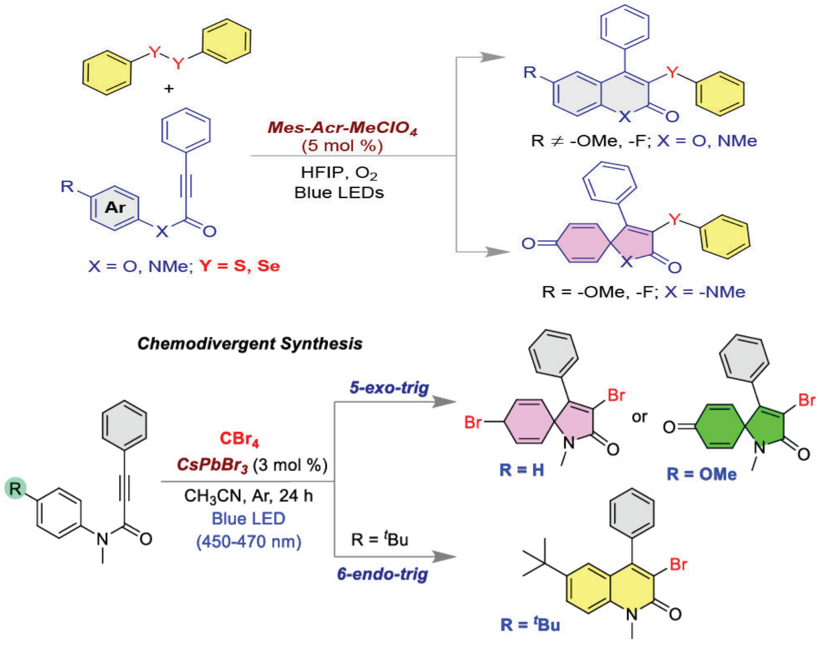
Buddhadeb Pal, and Prasenjit Mal*

Department of Chemistry, NISER Bhubaneswar

(E-mail: buddhadeb.pal@niser.ac.in)

Abstract: Visible light photocatalysis Plays an important role in organic synthesis. Metal catalysis utilizing $Ru(bpy)_3^{2+}$, $Ir(ppy)_3$ and metal-free catalysis employing organic dye molecules like Eosin-Y, Eosin-B, Rose Bengal, and Mes-Acr-$MeClO_4$ have both shown tremendous growth over the past 20 years. The use of nanomaterials that can function as visible light photocatalysts in organic synthesis is now being investigated by researchers. Additionally, employing CBr_4 and $CsPbBr_3$ perovskite as photocatalysts, we recently reported on the chemo-divergent functionalization of N-Methylalkanamides. Furthermore we are also able to disclosed the visible-light induced 9-mesityl-10-methylacridinium perchlorate catalyzed cascade chalcogenation of aryl alkynoates or N-arylpropynamides to afford either 3-sulfenylated/selenylated coumarins or spiro [4,5] trienones in one pot. The substitution controlled and radical-driven sulfenylation or selenylation reaction goes through either 6-endo-trig or 5-exo-trig mood of cyclization, affording a multiple C-S, C-Se, C-C and C=O bond forming reaction in one step.

Scheme:



References and Notes:

1. Pal, B.; Mathuri, A.; Manna, A.; and Mal, P., *Org. Lett.* **2023**, *25*, 4075-4079.
2. Mathuri, A.; Pal, B.; Pramanik, M.; and Mal, P., *J. Org. Chem.* **2023**, *88*, 10096-10110

Mechanistic Evaluation of Benzoin Catalysis Enabled by NHC-Triazolium: Application in the Preparation of Benzil and Heterocycles

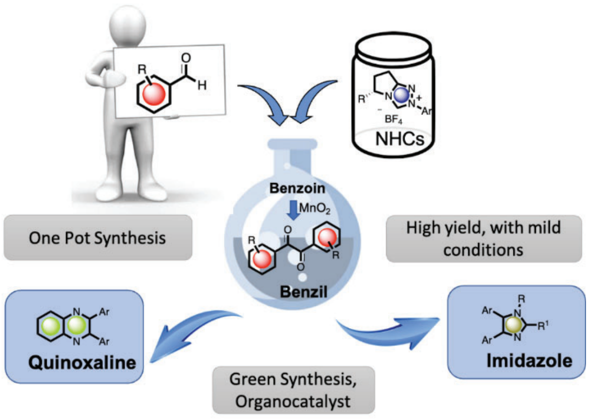
Deepika Sharma[a†], Chitrarasu Manikandan[b†], Vasudevan Dhayalan[b]* and Rambabu Dandela[a]*

[a]*Department of Industrial and Engineering Chemistry Institute of Chemical Technology, Indian oil Odisha Campus, IIT Kharagpur extension Centre, Mouza Samantpuri, Bhubaneswar-751013, Odisha, India*

[b]*Department of Chemistry, National Institute of Technology Puducherry, Karaikal-609609, Union Territory Puducherry, India*

(E-mail: r.dandela@iocb.ictmumbai.edu.in, dhaya.chem@nitpy.ac.in)

Abstract: A library of functionalized pyrrolidine-based NHC triazolium salts containing a BF_4 counterions have been prepared from readily accessible 2-pyrolidinone *via* one-pot reaction protocol. By separating imine-ether intermediates, a detailed mechanistic pathway has been investigated. Studied mechanistic investigation improved the synthetic process, resulting in higher yields for pyrrolidine-based triazolium NHC structures and the large-scale synthesis of chiral NHCs pre-catalyst with free OH-group. The presence of a hydroxyl functional group on the NHCs has the potential for further functionalization and for non-covalent control over catalytic reactions in which the NHCs can serve as organocatalysts or donor ligands for organometallic catalysis. This benzoin catalytic system was investigated by testing different solvents and aldehydes, NHC-catalysts loading and time variation effects to prepare a broad range of functionalized benzoin compounds with high yields. The highly reactive pyrrolidine-based triazolium salts (TAC_{F5}) showed significant potential application of organocatalysts in benzoin condensation-oxidation. EDG and EWG substituted α-hydroxy ketone derivatives were directly converted to corresponding benzil scaffolds from an aldehyde through one-pot reaction condition with MnO_2 acting as an oxidating reagent in open-air atmosphere. Selective heterocycles, quinoxaline, imidazole and pyrazine precursor were achieved from simple benzil under green conditions.



Title: One Pot synthesis of hierarchically formed radial [2], [3] and [4] catenane using Co(III) metal templated protocol and well defined CuAAC strategies

Mana Bhanjan Podh, Radhakanta Ratha and C. S. Purohit*

Department of Chemistry, NISER, OCC of HBNI, Bhubaneswar, Odisha, India 752050

(E-mail: mana.podh@niser.ac.in)

Abstract: Herein, we report, one pot synthesis of radial metalla[n]catenanes (n=2-4), which collectively formed using click reaction. The mandatory preorganization is obtained through preferred orthogonal geometry, achieved by cumulative addition of hard trivalent Co(III) metal template extracted from low-valent Co(II) and tridentate anionic ligand, is adopted to synthesis metalla[n]catenanes(n=2-4). The pseudorotaxane with bis(alkyne) functionalized groups coupled with bis(azide)functionalized counterparts by CuAAC strategies resulted in radial metalla[n]catenanes. For Intermolecular macrocyclisation, CuAAC strategy has advantageous as It utilizes heterogeneous functionalized(alkyne) and (azide) ligand and also yield is relatively high. The fascinating and challenging molecule. quantitative synthesis relatively impossible, is obtained in abundance. All metalla[n]catenanes (n=2-4) are fully characterized by both nuclear magnetic resonance spectroscopy and electron spray mass spectrometry.

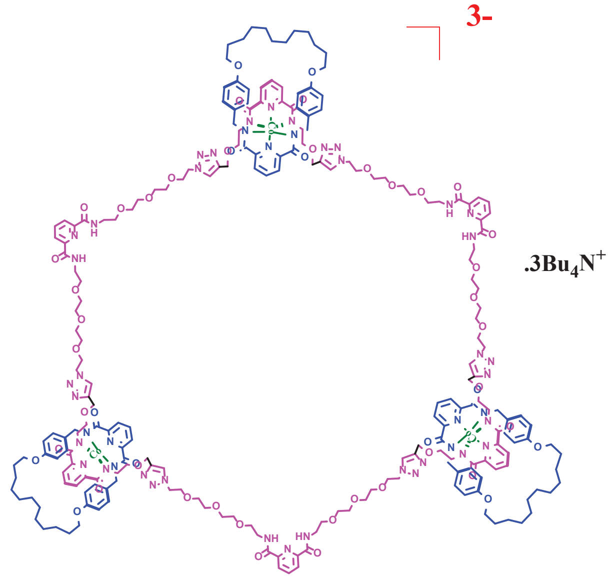


Figure 1. Structure of radial [4]catenane characterized by ^{1}H nmr and ESI-MS spectroscopy

References and Notes:

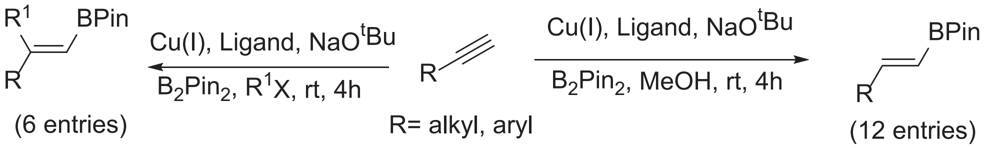
1. Amabilino, D.; Ashton P.; and Stoddart J.F., *Angew.Che. Int Ed Engl* **1994**, *4*, 33.
2. Wu, G.; Zhu, H.; Pan, F., Lu. Z. *Front. Chev.* **2021**, *117*, 3102−3137.
3. Nguyen, M.; Ferris D.P.; Pezzato, C.;Stoddart, J. F., *Chem.* **2018**, *4*, 1-16.

Cu-(I) Catalyzed Selective Hydroboration And Carboboration of Alkyne Enabling Synthesis of Allyl-Vinyl Ethers

Minati Behera and Jaya Prakash Das*

Dept. of Chemistry, Ravenshaw University, Cuttack-753003

Abstract: Alkynes are common functional existing reagents structurally diverse, shelf- stable and readily available, consequently converting them to the borylation reaction which play an important role in different settings.Realizing the well-recognized borylation reaction, the chemical space of alkyne to vinyl boronic ester transformation possible via vinyl cuprate intermediate due to kinetic inertness of alkyne to strongly reducing diboron reagent bis-(pinacolato)diboron. However, copper (Cu) is a catalyst for this transformation to grow the area of research, promoted by a catalytic amount of ligand 1,10-phenanthroline. We are well grounded that both borylation (hydroborylation and carboborylation) would require the presence of an electrophile and a base to reveal the stepwise formation of vinylboronic ester, inspire and encourage more invoking to the synthesis of allyl vinyl ether to 3,3-sigmatropic Claisen rearrangement.



Reference:

1. A. Suzuki and H.C. Brown, *Organic Synthesis via Boranes Aldrich*, Milwaukee, WI, **2003**. Vol. 3.
2. H.C . Brown, B.C.S, Rao*, J.Am. Chem. Soc***. 1956**, 78, 2582-2588.
3. D. Manning, H. Noth*, Angew. Chem., Int. Ed. Engl* **1985**,24,878.
4. T. Ishiyana, N. Matsuda, N. Miyaura, A.Suzuki, *J. AM. Chem. Soc* .**1993**, 115, 11018
5. M. Suginome, H. Nakamura, Y. Ito, *Chem. Common*. **1996**, 2777.
6. Uncatalyzed allylboration using triallylborane : B.M. Mikhailov, Yu. N. Bubnov, *Tetrahedron let***. 1971**, 12, 2127
7. D.Hall, in Boronic acid, ed. D. Hall, *Wiley, Weinheim***, 2005**, p.1.
8. N.A Petasis and I. Akritopoulou, *Tetrahedron let***. 1993**, 34, 583

Palladium Free;*Csp-Csp*^{2} Sonogashira cross-coupling using an oxygen-bridged bimetallic [Cu–O–Se] catalyst

Papita Behera,[a]Santosh K. Sahu,[a] and Dr. Laxmidhar Rout[a]*

Department of ChemistryBerhampur University, Bhanja Bihar, Odisha-760007

(E-mail: pb.rs.chem@buodisha.edu.in, ldr.chem@buodisha.edu.in)

Abstract: C-H activation has emerged as a powerful tool in organic synthesis, allowing for the direct functionalization of C-H bonds without the need for pre-functionalized starting materials. Among the various C-H activation reactions, Sonogashira cross-coupling stands out as a versatile method for the synthesis of C-C bonds. However, this cross-coupling needs Pd-metal catalyst to facilitate the formation of *Csp–Csp*^{2} bond between terminal alkyne and aryl halide. So, the development of efficient and selective Pd-free catalyst for ligand-free C-H activation is crucial for such organic transformations. Herein, we report a cheap and commercially available oxygen-bridged $CuSeO_3.2H_2O$ catalyst for Sonogashira cross-coupling between terminal alkyne and aryl halide (Figure 1), which enhances performance in terms of activity, selectivity, and stability compared to traditional catalysts for this transformation (Scheme 1). The catalyst is palladium free up to 0.02ppm.

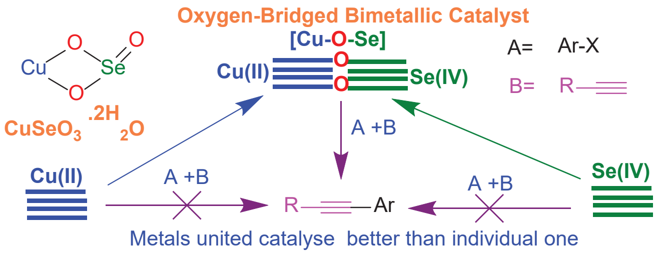
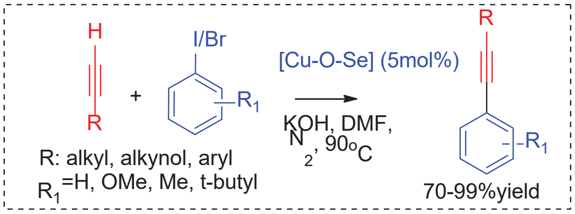


Figure1: Concept of an oxygen-bridged bimetallic catalyst.



Palladium free
Ligand Free
Functional Group Compatibility
No Reductant
Under Mild Condition

Scheme1: Cu-O-Se catalyzed *Csp-Csp*^{2} Sonogashira cross-coupling reaction.

References and Notes:

1. L. Rout et al; *Eur. J. Org. Chem.***2022,** e202201194.
2. L. Rout et al; *New. J. Chem.,* **2021,** *45,* 5775–5779.
3. L. Rout et al; *Asian J. Org. Chem.,* **2021,** *10,* 1117-1122.
4. L. Rout et al; *Chem. Eur. J.,* **2020**, *26*, 620-624.
5. L. Rout et al; *New. J. Chem*., **2020**, *44*, 2500-2504.

Acknowledgement:

Dr. Rout is thankful to Director Prof. A K Ganguli, IISER Berhampur, Odisha, India for providing NMR and HRMS spectroscopy facilities. This work was supported by Council of Scientific and Industrial Research CSIR/02(0393)/21/EMR-II. Dr Rout acknowledges Science and Engineering Research Board, SERB, New Delhi SERB/CRG/2022/001544. New Delhi, India, Science and Technology department, Govt. of Odisha, (no. S&T/2587/2023) for Funding. Papita thanks OURIIP, OSHEC Govt. of Odisha for fellowship. Dr. Rout is also thankful to Berhampur University and University Grants Commission (UGC) for providing infrastructure facilities.

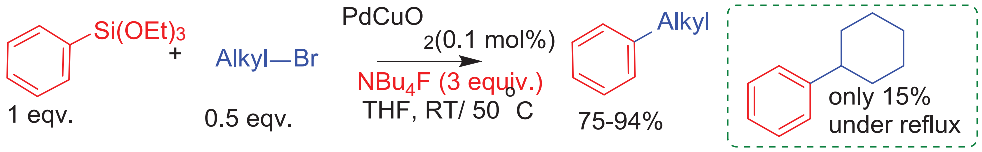
Green Synthesis of Hiyama Coupling: Exploiting Recyclable $PdCuO_2$ Nanoparticles

Pradyota Kumar Behera and Dr. Laxmidhar Rout*

Department of Chemistry, Berhampur University

(E-mail: pkb.rs.chem@buodisha.edu.in, ldr.chem@buodisha.edu.in)

Abstract: Organosilicon compounds offer many advantages over other cross-coupling protocols due to their stability, non-toxicity, and natural abundance. The development of several extremely efficient palladium catalysts, primarily for the silicon-based technique, owes a great deal to the development of organosilicon reagents that successfully undergo trans metalation, a crucial step in the silicon-based cross-coupling reaction. [1-2] In this regard we developed bimetallic heterogeneous PdCuO2 nanoparticle which worked efficiently to a number of substrate, ligand free and mild reaction protocol. [3-4] The catalyst recyclability, unique composition and compatibility with diverse substrates enhance the product formation. The products has very good potential for crop protections.



Scheme -1 : cross-coupling of alkyl halide with arylsilane using CuO_2Pd nano-particle

References and Notes:

1. Nakao ,Y.; Hiyama, T., *Chem. Soc. Rev.* **2011**, *40*, 48932.
2. Noor, R.; et al , *Molecules* **2022**, 27, 5654.
3. Sahoo, S. K.; Behera, P.K.; Rout, L. et al., *New . J. Chem.* **2022,** *46*, 1650.
4. Behera, P. K.: Choudhury, P.: Rout, L. et al., *A. J. Org. Chem.* **2021,** *10*, 1117.

Acknowledgement :

Dr. Rout is thankful to Director Professor A K Ganguli, IISER Berhampur, Odisha, India for providing NMR and HRMS spectroscopy facilities. This work was supported by Council of Scientific and Industrial Research CSIR/02(0393)/21/EMR-II. Dr Rout acknowledges Science and Engineering Research Board, SERB, New Delhi SERB/CRG/2022/001544. New Delhi, India, Science and Technology department, Govt. of Odisha, (no. S&T/2587/2023) for Funding.. Dr. Rout is also thankful to Berhampur University and University Grants Commission (UGC) for providing infrastructure facilities.

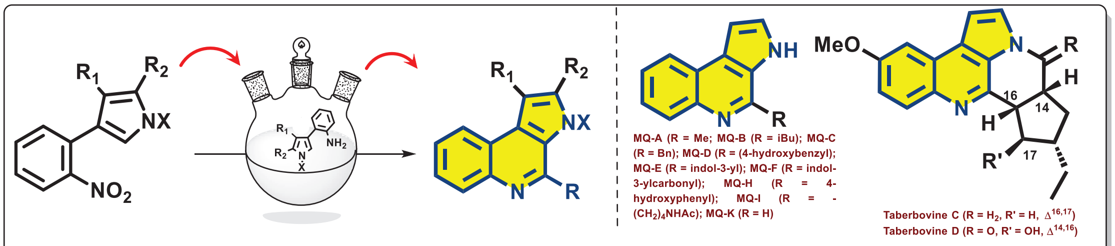
Repurposing Heteroarenes for Polyheteroarenes: A Regioselective One-Carbon Annulation Strategy

Rahimuddin Khan†, Dipun Kumar Penthi and Tabrez Khan*
Organic Synthesis Laboratory, School of Basic Sciences
Indian Institute of Technology Bhubaneswar
(E-mail‡: a21cy09008@iitbbs.ac.in)

Abstract:

Aza-heterocycles are widely distributed in nature and vital for life in a number of ways. Furo-/thieno-/pyrrolo fused quinolines constitute one of the very important fused polyheteroaromatic skeletons that are found in pharmaceutical drugs, natural products and other functional molecules, which come under the class of quinolines.[1] Therefore, with our ongoing interest in the development of metal-free strategies for carbo-/heterocycles [2-5], a new one-pot metal-, acid-/base-free synthesis of pyrrolo[2,3-c]quinolines has been developed through the repurposing of the 3-aryl pyrrole motifs/pyrrolnitrin derivatives available through the in-house protocol [5]. A detailed discussion of the adopted strategy, substrate scope, mechanistic studies, and application to access some natural alkaloids will be presented in the poster.

Scheme:



MQ-A (R = Me; MQ-B (R = iBu); MQ-C (R = Bn); MQ-D (R = (4-hydroxybenzyl); MQ-E (R = indol-3-yl); MQ-F (R = indol-3-ylcarbonyl); MQ-H (R = 4-hydroxyphenyl); MQ-I (R = -$(CH_2)_4NHAc$); MQ-K (R = H)

Taberbovine C (R = H_2, R' = H, $\Delta^{16,17}$)
Taberbovine D (R = O, R' = OH, $\Delta^{14,16}$)

- one-pot domino for SM preparation
- one-pot 2-step strategy
- acid-, base-, oxidant-free
- Broad substrate scope
- Mechanistic probing studies
- access to natural alkaloids

References and Notes:

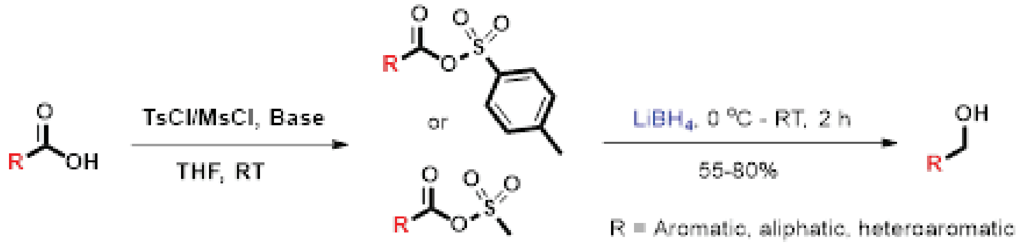
1) a) Teja, C., Khan, N. *Asian J. Org. Chem.* 2020, 9, 1889-1900; b) O.Ajani, K.T. Lyaye, O.T. Ademosun, *RSC Adv.* 2022,*12*, 18594-18614.
2) Salam, A., Kumar, D., Sahu, T.K., Khan, R. and Khan, T. *Eur. J. Org. Chem.* 2022, e202101452.
3) Kumar, D., Salam, A., Sahu, T.K., Sahoo, S. S. and Khan, T. *J. Org. Chem.* 2021, *86,* 15096-15116.
4) Kumar, V., Salam, A., Kumar, D. and Khan, T. , *ChemistrySelect* 2020, *5*, 14510-14514
5) Kumar, V., Awasthi, A., Metya, A. and Khan, T., *J. Org. Chem.* 2019, *84*, 11581-11595.

Tosyl chloride as an activator of carboxylic acid: Convenient one pot conversion of carboxylic acid to alcohol

Ranjan Kumar Panigrahi and Samaresh Jana *

Department of Chemistry, School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT)-Deemed to be University, Bhubaneswar-751024, Odisha, India

Abstract: A simple one pot conversion of carboxylic acid to alcohol is described. This transformation is achieved by using a mild reducing agent lithium borohydride under an ambient condition. In this methodology, carboxylic acid is activated using sulphonyl chloride (tosyl or mesyl chloride). The activated acid reacts with the hydride to form the alcohol in a convenient way. Aromatic, aliphatic and heteroaromatic acids were proved to be good substrates for this reaction. The product obtained from the reaction mixture does not require any purification on column chromatography.

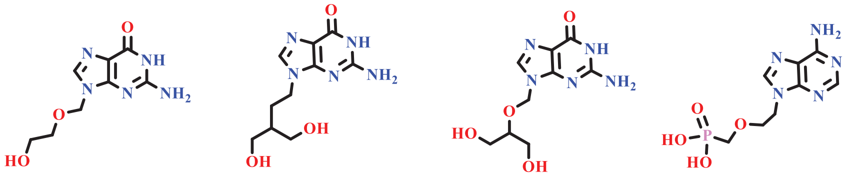


Synthesis and Antiviral Activity of Acylic Purine Nucleosides

Samir Kumar Mondal and Dr. Shantanu Pal*
School of Basic Sciences (Chemistry), Indian Institute of Technology Bhubaneswar
(E-mail: s21cy01002@iitbbs.ac.in, spal@iitbbs.ac.in)

Abstract:

Nucleoside analogues are widely used for the treatment of antiviral infections and anticancer chemotherapy. Towards this, a number of acyclic nucleosides have been synthesized, tested, and many of them have been approved by U.S. Food and Drug Administration (FDA) such as Acyclovir (I), Penciclovir (II) for herpes simplex virus (HSV I and HSV II), Ganciclovir (III) for human cytomegalovirus (HCMV) and Adefovir (PMEA) (IV) for hepatitis B virus (HBV) (Figure-1).



I Acyclovir
HSV, VZV

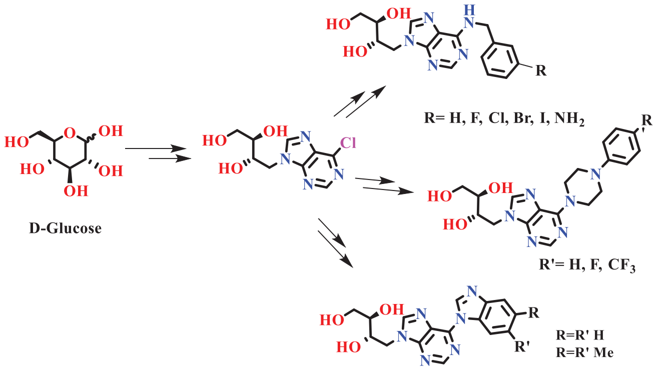
II Penciclovir
HSV, VZV

III Ganciclovir
HCMV

IV Adefovir
HBV

Figure-1 Example of Antiviral drug molecules

Considering their importance and rational, various modified acyclic purine nucleosides (Scheme-1) were synthesized from D-glucose. Further coupling reaction such as Suzuki coupling and C-N coupling on 6 Cl-purine acyclic nucleosides were explored to get corresponding acyclic nucleosides. Biological evolutions of the synthesized nucleosides have shown that iodobenzylamine nucloside is the most potent against dengue serotype-II in human liver cell.



Scheme-1

References:

1) Clercq, E. D.; Holy, A. *Nat. Rev. Drug Discov*, **2005**, *4*, 928–940.
2) Hao, E. J.; Li, G. X.; Liang, Y, R.; Xie, M, S.; Wang, D. C.; Jiang, X. H.; Cheng, J. Y.; Shi, Z. X.; Wang, Y.; Guo, H. M. *J. Med. Chem*. **2021**, *64*, 2077-2109.

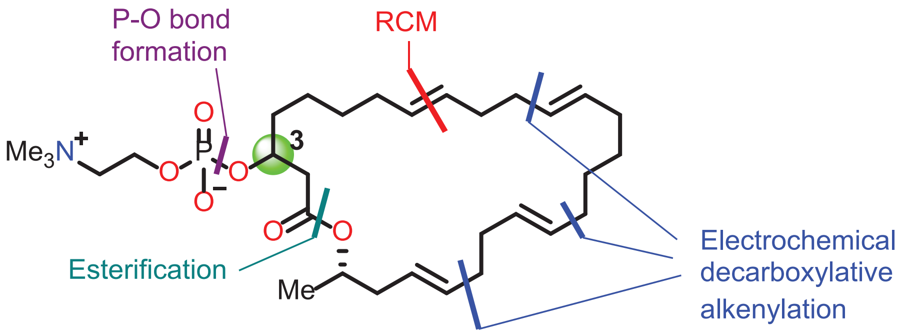
Total Synthesis and Absolute Configuration Determination of 26-Membered Macrolactone Colletotrichumolide

Sudip Mandal, Barla Thirupathi *

Department of Chemical Sciences, IISER Berhampur, India

(E-mail: sudipm@iiserbpr.ac.in)

Abstract: Macrocycles are a class of structurally complex and biologically important natural products that trigger, or at least inspire, investigations relating to drug discovery. In total, 67 macrocycles have been approved as drug by the U.S. Food and Drug Administration.[1] In 2022, Berlinck and co-workers identified a new 26-membered macrolactone colletotrichumolide (**1**) from *Colletotrichum* spp. a fungal species.[2] Unfortunately, they were able to isolate minuscule amount, so that, it was difficult to conduct further investigation into their biological activity and mechanism of action. Also, the absolute configuration at C-3 could not be established by the isolation group due to the reactivity of the phosphate group under the methanolysis conditions. Organic chemist plays a crucial role in producing sufficient amount of these natural products through total synthesis. Our plan is to synthesize the 26-membered colletotrichumolide (**1**) by iterative electrochemical decarboxylative alkenylation, RCM and esterification reaction. Our synthesis will allow us to determine the absolute configuration of C-3. We are also planning to evaluate biological activity in future.



Colletotrichumolide (**1**)

References and Notes:

1. U.S. Food and Drug Administration: Approved Drugs; https://www.Accessdata.Fda.Gov/Scripts/Cder/Daf/Index.Cfm (accessed Sept 1, 2022).
2. Takaki, M.; Williams, D. E.; Freire, V. F.; Sartori, S. B.; Lira, S. P.; Bizarria, R., Jr.; Rodrigues, A.; Gonçalves da Costa, D. R.; Amorim, M. R.; Ferreira, A. G.; Andersen, R. J.; Linington, R. G.; Berlinck, R. G. S., *Org. Lett.* **2022,** *24*, 9381-9385.

Synthesis of highly substituted 1, 2, 4-triazole based 3-nitro-2*H*-chromanes through aza-Michael addition reaction under catalyst and base free condition

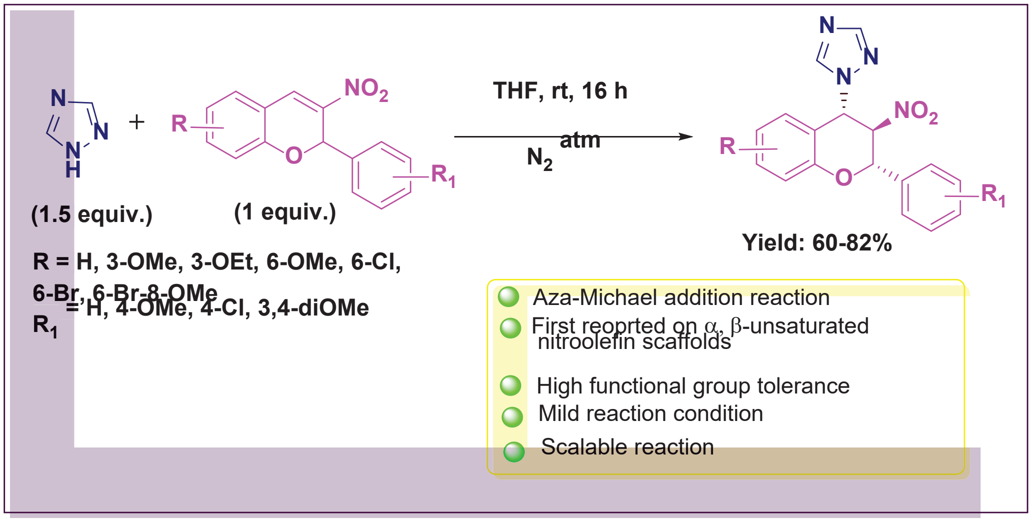
Tapaswini Das[1] | Seetaram Mohapatra[1]

Department of Chemistry, Ravenshaw University, Cuttack-753003, Odisha, India

E-mail: dastapaswini70@gmail.com

Abstract: Among the most significant sub-families of 3-nitro-2*H*-benzopyrans, the benzopyrans comprising chromanes bearing diverse *N*-functionalities at the C4-position i.e. 4-amino-3-nitro-2*H*-chromanes[1] have attracted much attention of scientific community because of their wide range of therapeutic applications.[2] In this regards, A simple and efficient aza-Michael addition reaction of 1, 2, 4-triazoles to functionalized 2-aryl-3-nitro-2*H*-chromenes have been demonstrated under catalyst and base free condition. In this transformation, one intermolecular C-N bond formation has been achieved at room temperature. A series of highly-substituted 1, 2, 4-triazole based 3-nitro-2*H*-chromanes were produced in good to excellent yield up to 86%. The relative configuration of the Michael adduct was confirmed by X-ray crystallographic analysis. In addition, several advantages are involved with this protocol such as operational simplicity, high yield, easy accessibility, wide variety of functional group tolerance are the key features of this aza-Michael addition reaction.

Scheme 1: Aza-Michael addition reaction of 1,2,4-triazole to 3-nitro-2*H*-chromenes for the synthesis of poly substituted 4-amino-3-nitro-2H-benzopyrans



References:

1. Das, T.; Mohapatra, S.; Pradhan, A. K.; Nayak, S. *ChemistrySelect*, 2023, *8*, e202300477.
2. Das, T.; Mohapatra, S.; Mishra, N. P.; Nayak, S. Tetrahedron Lett. 2022, 96, 153762.

Acknowledgement: I wish to express my sincere gratitude to Dr. Seetaram Mohapatra for his valuable guidance & support throughout my research work. I am also thankful to INSPIRE, New Delhi for providing me financial supports.

Modern Trends in Chemical Sciences (MTCS 2023)
Department of Chemistry, SAS, KIIT Bhubaneswar

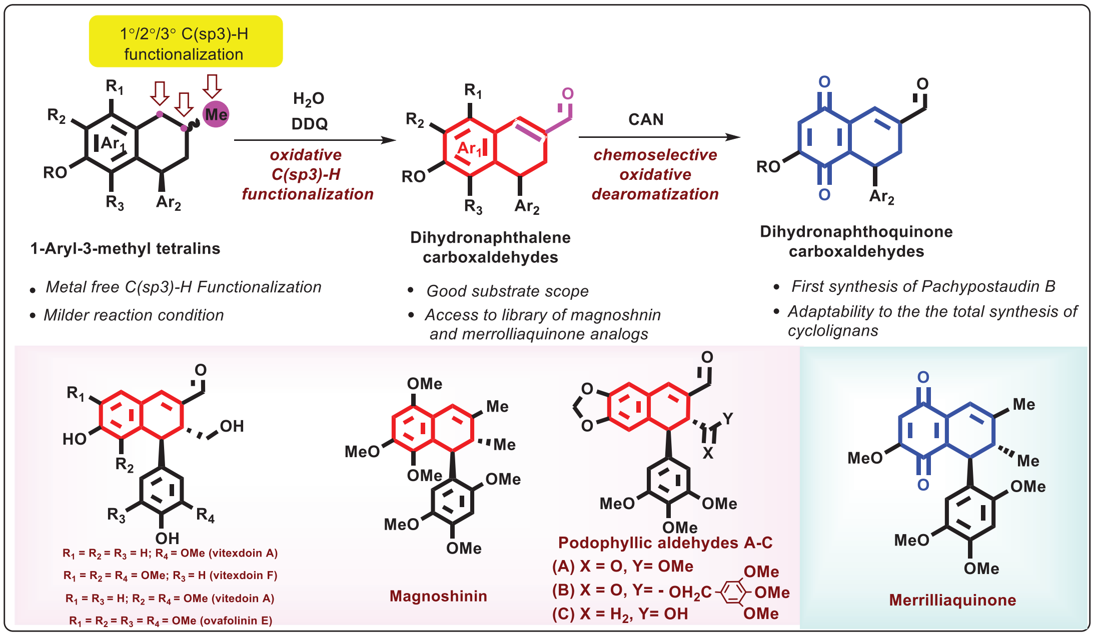
DDQ-Catalyzed Oxidative C (sp^3)–H Functionalization of Aryltetralins and Subsequent Chemoselective Oxidative Demethylation to Access Dihydronaphthalenes and Dihydronaphthoquinones

Abhaykumar R. Vishwakarma[†] and Tabrez Khan*
Organic Synthesis Laboratory, School of Basic Sciences
Indian Institute of Technology Bhubaneswar
(E-mail[‡]: a22cy09005@iitbbs.ac.in)

Abstract:

The dihydronaphthalene scaffold has a noteworthy presence in numerous biologically potent natural products and pharmaceutically active molecules. In addition, the dihydronaphthoquinone core's distinctiveness in the natural product repertoire, as well as its application in pharmaceutics stimulated our interest in developing a simple and effective synthesis method.[1-2] Through the present poster, C(sp^3)–H functionalization approach for efficient access to diverse oxygenated dihydronaphthalene scaffolds will be presented. Then the use of dihydronaphthalene scaffolds as linchpin to arrive at the rarely observed dihydronaphthoquinone core will be showcased. Also, the application of the strategy for the synthesis of some natural products will be presented in the poster.

Scheme:



- *Metal free C(sp3)-H Functionalization*
- *Milder reaction condition*

- *Good substrate scope*
- *Access to library of magnoshnin and merrolliaquinone analogs*

- *First synthesis of Pachypostaudin B*
- *Adaptability to the the total synthesis of cyclolignans*

References and Notes:

1) Salam, A., Kumar, D., Sahu, T.K., Khan, R. and Khan, T. *Eur. J. Org. Chem.* 2022, e202101452.
2) Kumar, D., Salam, A., Sahu, T. K., Sahoo, S. S. and Khan, T. *J. Org. Chem.* 2021, *86,* 15096-15116.

Palladium-Catalyzed C-C Bond Activation and Stereo-Selective Alkenylation Between Cyclopropanol and 1,3-Diyne: One-Step Synthesis of Diverse 1,3-Enynes

Bedadyuti Vedvyas Pati,[ab] Asit Ghosh,[ab] Komal Yadav,[ab] Shyam Kumar Banjare,[ab] Shalini pandey,[ab] Upakarasamy Lourderaj *[ab] and P. C. Ravikumar *[ab]

[a] *School of Chemical Sciences, National Institute of Science Education and Research (NISER), Bhubaneswar, Odisha, 752050, India,*

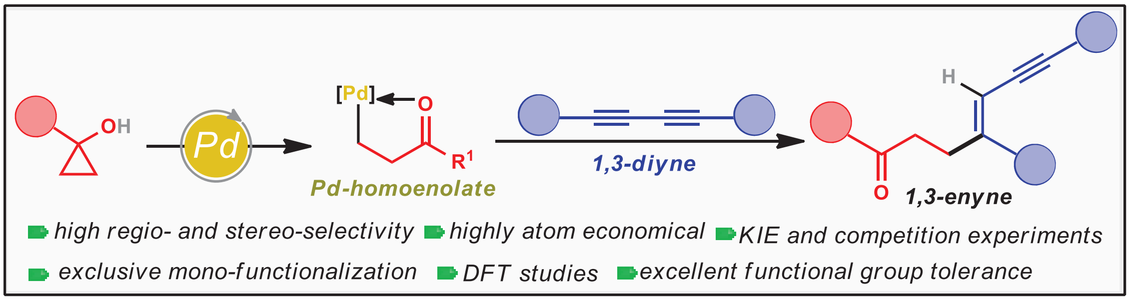
[b] *Homi Bhabha National Institute,Training School Complex, Anushaktinagar, Mumbai, 400094, India*

(E-mail: bedadyuti.pati@niser.ac.in)

Abstract:

Transition metal-catalyzed C–H and C–C bond functionalization have received immense attention in the last two decades owing to their potential applications in organic synthesis. Although extensive studies have been made on C–H bond activation, strategies involving C–C bond activation remain limited. We have reported the first example of the use of 1,3-dialkynes in C-C bond activation. The regio- and stereo-selective synthesis of 1,3-enynes from 1,3-diynes is demonstrated by the palladium-catalyzed C–C bond activation of cyclopropanol. Exclusive formation of mono-alkenylated adduct was achieved by eliminating the possibility of di-functionalization with high regio- and stereo-selectivity. Indeed, this protocol worked very well with electronically and sterically diverse substrates. Several mechanistic studies, including deuterium labeling experiments, kinetic isotope effect intermolecular competitive experiments, and experiments with radical scavengers were carried out to understand the mechanism. The atomic-level mechanism followed in the catalytic process was also validated using DFT calculations, and the rate-controlling states in the catalytic cycle were identified.

Figure:



Palladium-catalyzed C-C activation of cyclopropanol and alkenylation with 1,3-diynes.

References and Notes:

Pati, B. V.; Ghosh,A.; Yadav,K.; Banjare,S. K.; Pandey,S.;Lourderaj,U.; Ravikumar,P. C., *Chem. Sci.* **2022**, *13*, 2692-2700.

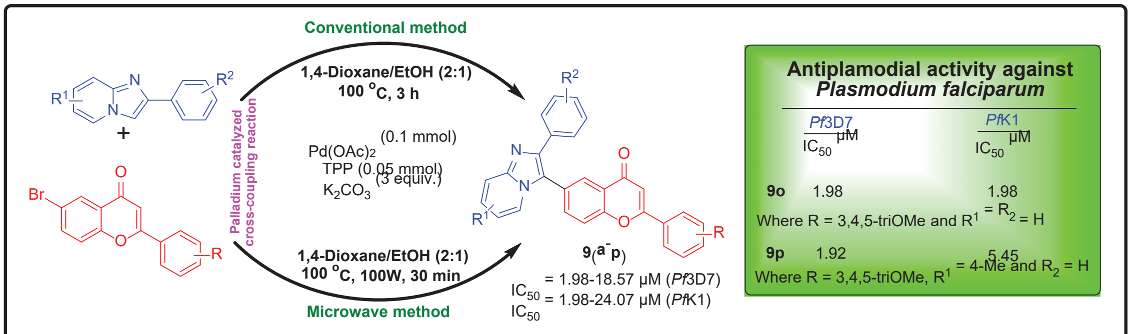
Palladium-catalyzed facile synthesis of imidazo[1,2-a]pyridine-flavone hybrids and evaluation of their antiplasmodial activity

Jasmine Panda,[a] Bishnu Prasad Raiguru,[a] Seetaram Mohapatra,[a*] Sabita Nayak[a]

[a]*Organic Synthesis Laboratory, Department of Chemistry, Ravenshaw University, Cuttack-753003, Odisha, India*

(E-mail: jasmine.chem@ravenshawuniversity.ac.in)

Abstract: An efficient cross-coupling reaction between imidazo[1,2-*a*]pyridine derivatives and 6-bromoflavones has been well established. This reaction proceeds through a Palladium-catalyzed cross-coupling reaction to provide imidazo[1,2-*a*]pyridine-flavone hybrids in good to excellent yield. Short reaction time, high yield, and wide substrate scope are the major advantages of this method. Using SYBR Green I assay, these hybrid molecules were examined for anti-plasmodial activity against Chloroquine-sensitive 3D7 and Chloroquine-resistant K1 strains of *Plasmodium falciparum*. The compounds **9o** {IC_{50}s (µM) 1.98^{3D7}, 1.98^{K1}} and **9p** {IC_{50}s (µM) 1.92^{3D7}, 5.45^{K1}} were found to be the most potent anti-plasmodial compounds in the series. Also, all these compounds were found to be non-cytotoxic towards Vero cells with their CC_{50}s > 100 µM. We have conducted microscopic examination experiments on compounds **9o** and **9p**, which resulted in a drastic impact on parasite growth of the malaria parasite. The interaction of these two potent hybrids was also examined in the binding site of wild-type *Pf*-DHFR-TS (*Plasmodium falciparum* dihydrofolate reductase-thymidylate synthase) using molecular docking studies. The computational ADME studies of the hybrid compounds confirmed their significant physicochemical, pharmacokinetic, and drug-likeness properties confirming these hybrids as a new oral antimalarial agent. As a result, these new hybrid compounds could be valuable in the creation of future antimalarial drugs.



- Short reaction time
- Broad substrate scope with good to high yield
- Potent antiplasmodial agent
- Excellent resistant index values
- Good in silico docking interactions within *Pf*DHFR enzyme
- Good pharmacokinetic behavior showed by ADMET predictions

Scheme 1: Synthesis of imidazo[1,2-*a*]pyridine-flavone hybrids and evaluation of their antiplasmodial activity

References and Notes:

1. Raiguru, B. P.; Mohapatra, S.; Nayak, S.; Sahal, D.; Yadav, M.; and Acharya, B. N., *Eur. J. Med. Chem. Rep.* **2022,** *4*, 100029.

Palladium-Catalyzed C–C Bond Activation: Achieving Regio/Stereo-Selective Alkenylation of Cyclopropanol and 1-(Phenylethynyl)cyclobutanol

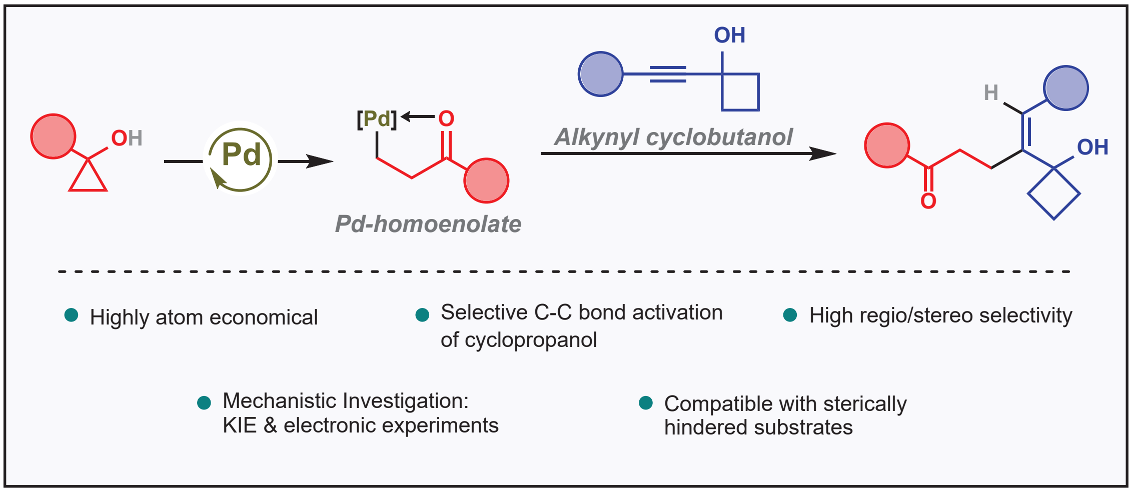
Bedadyuti Vedvyas Pati [ab], **Lamphiza O Najiar** [ab], Gopal K. D. Adhikari [ab], Tanmayee Nanda [ab] and Ponneri C. Ravikumar *[ab]. (Manuscript under preparation)

[a] *School of Chemical Science, National Institute of Science Education and Research (NISER), Bhubaneswar, Odisha, 752050, India*

[b] *Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai, 400094, India*

(E-mail: lamphiza.najiar@niser.ac.in)

Abstract: The regio- and stereo-selective synthesis of γ, δ-unsaturated ketones has been demonstrated. This achievement has been realized through palladium-catalyzed C–C bond activation of cyclopropanol, coupled with its selective hydroalkylation with alkynyl cyclobutanol. The developed protocol enables selective C–C bond activation of the cyclopropanol ring while keeping the cyclobutanol ring intact. This protocol is highly atom-economic, offering high regio- and stereo-control. The demonstrated methodology proves effective for a range of electronically and sterically diverse cyclopropanols and cyclobutanols. Several mechanistic studies, including competition experiments and deuterium labeling, were conducted to gain insight into the reaction mechanism. Preliminary mechanistic findings using radical scavengers indicate the non-involvement of radical pathways in the transformation.



- Highly atom economical
- Selective C-C bond activation of cyclopropanol
- High regio/stereo selectivity
- Mechanistic Investigation: KIE & electronic experiments
- Compatible with sterically hindered substrates

Figure: Palladium-catalyzed C–C bond activation and alkenylation between cyclopropanol and 1-(phenylethynyl)cyclobutanol.

References and Notes:

1. Pati, B. P.; Najiar, L. O.; Adhikari, G. K. D.; Nanda, T.; Ravikumar, P. C. (Manuscript under preparation)

Expanding the Boundary of C-H Activation: Weak Chelation-Assisted Cobalt-Catalyzed Synthesis of Indole C(4)-acrylophenone *via* C-O Bond Cleavage of Propargyl Alcohol Derivative

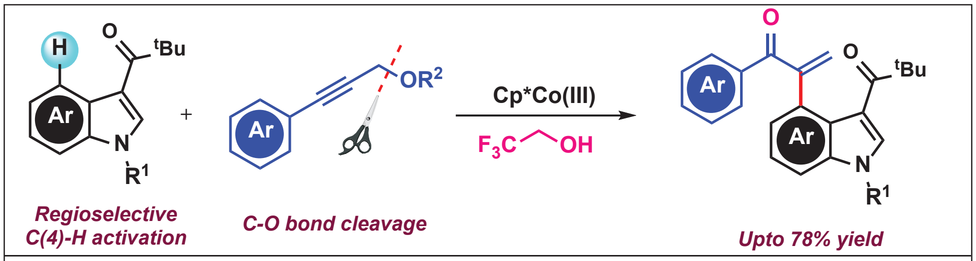
Pranav Shridhar Mahulkar,[ab] Sofaya Joshi,[ab] Shyam Kumar Banjare,[ab] and Ponneri C. Ravikumar *[ab]

[a] *School of Chemical Sciences, National Institute of Science Education and Research (NISER), Bhubaneswar, Odisha 752050, India.*

[b] *Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai 400094, India*

(Email: pranav.mahulkar@niser.ac.in, pcr@niser.ac.in)

Abstract: Herein, we have reported the facile synthesis of indole C(4)-acrylophenone using a C-H bond activation strategy. For this conversion, an unsymmetrical alkyne (phenylethynyl ether) in presence of cobalt(III)-catalyst works efficiently. In this process, alkyne gets oxidized in the presence of *in-situ* generated water, which is the key step for this method, for which trifluoroethanol is the water source. The pivaloyl directing group chelates effectively to generate the cobaltacycle intermediate, which has been detected through high-resolution mass spectrometry (HRMS). Also, reaction with radical scavengers implies non-involvement of radical pathway and kinetic isotope experiment suggests that the C-H metalation step is not the rate-limiting step. In addition, the applicability of obtained indole C(4)-acrylophenone product has been demonstrated for the synthesis of indanone derivative.



● One-step access to acrylophenone ● TFE as the sole water source ● 3d TM, weak chelation

References:

1. Mahulkar, P. S.; Joshi, S.; Banjare, S. K.; Ravikumar, P. C. *(manuscript under preparation)*

Cobalt(III)-catalyzed regioselective hydro-arylation of 1,6-diyne via weak-chelation assisted C-H bond activation

Kumar Banjare,[a,b] **Saista Afreen**,[a,b] Pranav Shridhar Mahulkar,[a,b] Annapurna Saxena[a,b] and Ponneri C. Ravikumar*[a,b]

[a]*School of Chemical Sciences, National Institute of Science Education and Research (NISER), Bhubaneswar 752050 Odisha, India.*

[b]*Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, India.*

Abstract: The 3d transition metal-catalyzed C-H bond activation using weakly coordinating directing groups such as aldehyde, ketone, esters and substituted amide are emerging and sustainable area.[1,2] In this regard, we have developed various C-H bond functionalization utilizing earth-abundant cobalt catalysts and weak chelation.[3,4] Herein, we have report cobalt(III)-catalyzed hydro-arylative functionalization of 1,6-diyne, which was never explored before. The *N*-aryl *γ*-lactam is the prime substrate that undergoes sp^2 C-H bond activation in a weakly coordinating manner. The reaction mechanism reveals the in-situ formation of a six-membered cobaltacycle which undergoes further functionalization with 1,6 diyne to give substituted enyne.

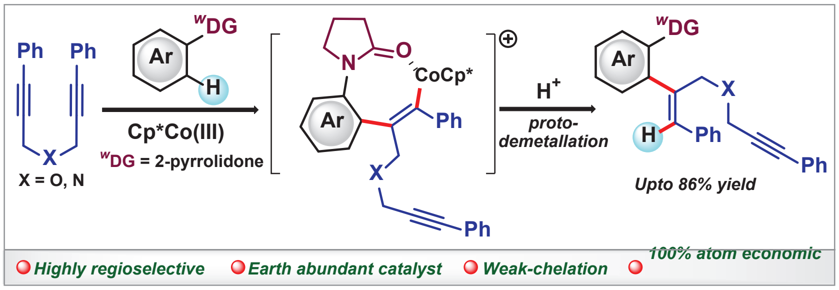


Figure: *Synthesis of enyne through cobalt-catalyzed regioselective hydroarylation of 1,6-diyne.*

Also, we have detected a six-membered cobaltacycle intermediate through high-resolution mass spectrometry (HRMS), which supports our proposed catalytic cycle. The radical scavengers' experiments suggest the non-involvement of the radical pathway for this transformation. In addition, the protocol worked well with the various substrate in good yield and high regioselectivity.

References:

1. Dalton, T.; Faber, T.; Glorius, F. C-H Activation: Toward Sustainability and Applications. *ACS Cent. Sci.* **2021**, *7*, 245−261.
2. Banjare S. K.; Nanda T.; Pati B.V.; Biswal P.; Ravikumar P.C. O-Directed C–H functionalization via cobaltacycles: a sustainable approach for C–C and C–heteroatom bond formations. *Chem. Commun*. **2021**, *57*, 3630−3647.
3. Banjare, S. K.; Nanda, T.; Pati, B. V.; Adhikari, G. K. D.; Dutta, J.; Ravikumar, P. C. Breaking the Trend: Insight into Unforeseen Reactivity of Al-kynes in Cobalt-Catalyzed Weak Chelation-Assisted Regiose-lective C(4)−H Functionalization of 3-Pivaloyl Indole. *ACS Catal.* **2021**, *11*, 11579−11587.
4. (a) Banjare, S. K.; Chebolu, R.; Ravikumar, P. C. Cobalt Catalyzed Hydroarylation of Michael Acceptors with Indolines Directed by a Weakly Coordinating Functional Group. *Org. Lett.* **2019**, *21*, 4049−4053. (c) Banjare, S. K.; Nanda, T.; Ravikumar, P.

Rapid Acsess of Benzimidazole Fused Poly-heterocycles *via* Cu-Catalyzed Dehydrogenative C-N Coupling: Synthetic Versatility and Photophysical Studies

Sakshi Singh and Shantanu Pal*
School of Basic Sciences (Chemistry), Indian Institute of Technology Bhubaneswar
(E-mail: ss122@iitbbs.ac.in, spal@iitbbs.ac.in)

Abstract:

Benzimidazole and pyrazole scaffolds are intriguing classes of frameworks due to their specific chemical reactivity and application in diverse fields such as medicinal, agricultural, and material sciences. The benzimidazole was annulated by a number of heterocyclic scaffolds, producing a range of benzimidazole-fused heterocycles with various biological (Figure 1) and photoelectronic properties.[1]

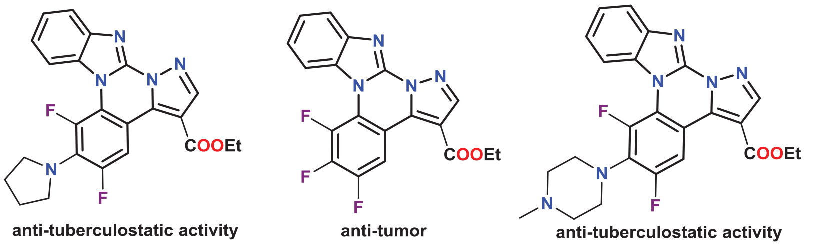
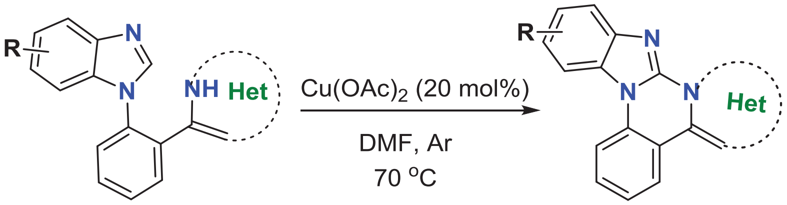


Figure 1 Examples of biologically active benzimidazole fused heterocyclic derivatives.

In the past few years, Cu-catalysed approaches have stimulated ongoing research in the field of synthetic organic chemistry.[2] Towards this, a simplified synthetic method to synthesize benzimidazole-fused poly-heterocycles via intramolecular C-N coupling reactions without using ligand, base, additives and solely using Cu-catalysts was explored (Scheme 1). The versatility of the approach is demonstrated by the synthesis of diverse fused compounds and mechanistic as well as photophysical studies.



Scheme 1

References and Notes:

1. Sahoo, S.; Pal, S. *J. Org. Chem.* **2021**, *86*, 4081−4097.

2. (a) Guo, X. X.; Gu, D. W.; Wu, Z.; Zhang, W. *Chem. Rev.* **2015**, *115*, 1622–1651; (b) Pal, T.; Lahiri, G. K.; Maiti, D. *Eur. J. Org. Chem.* **2020**, *44*, 6859–6869.

Towards synthesis of molecular capsule with purine moiety

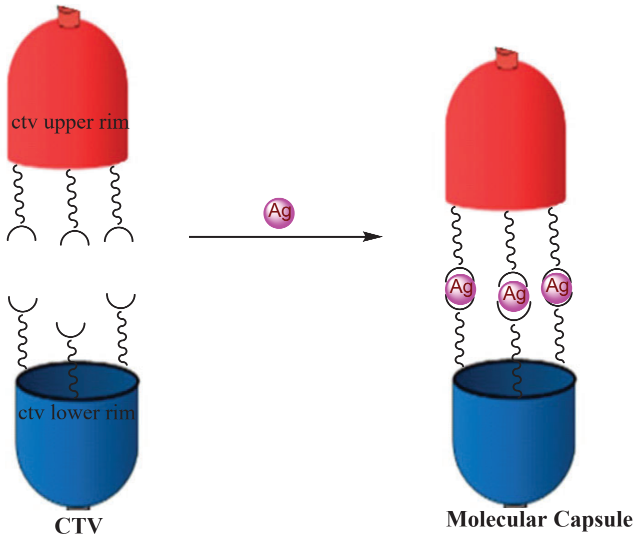
Sanjaya Kumar Moharana, Dr.C.S.Purohit*

School Of Chemical Sciences , NISER, BBSR

(E-mail: sanjaya.moharana@niser.ac.in)

Abstract: Cyclotriveratrylene (CTV) are host molecules with a crown-like conformation and electron-rich molecular cavities. Appropriately functionalized CTV derivatives can self-assemble into nano-scale cage-like assemblies through metal–ligand interactions or hydrogen bonding.[1] The crown conformation of CTV has a distinctive open-bowl pyramidal shape, and it can be easily envisaged that capsules or cage-type molecular structures will result from the divergent linking together of CTV's through their upper rims.[2] CTV is capable of binding alkali metal cations and Ag(I) to form complexes. Silver is widely used for its antimicrobial properties and low toxicity to mammalian cells. Silver(I) can exhibit many coordination environment such as linear, trigonal planar and tetrahedral.[3] The purine bases such as adenine and guanine are essential molecular components of living organisms and are incorporated within macromolecules (nucleic acids) and small molecules (enzyme cofactors). We have synthesized the CTV derivative having purine group as the coordinating sites and tried to incorporate silver metal which will self-assemble to create a silver mediated molecular capsule.

Figure:



References and Notes:

1. Chakrabarty, R: Mukherjee, P.S: P J Stang, P.J., *Chem. Rev*. **2011**, *111*, 6810–6918
2. Crowley,J.D., *Inorg. Chem.* **2011**, *50*, 1123–1134
3. Gipson, J.T: Beobide ,G: O Castillo,O ; *CrystEngComm*, **2011**, *13*, 3301

Cascade Nucleophilic Addition-Cyclic Michael Addition of Arynes, Indoles Bearing Michael Acceptor: A Strategy To Construct Pyrroloacridines, and Study of Their Physicochemical Properties

Sayantan Kundu,[†] Gurupada Hazra,[†], and Barla Thirupathi*

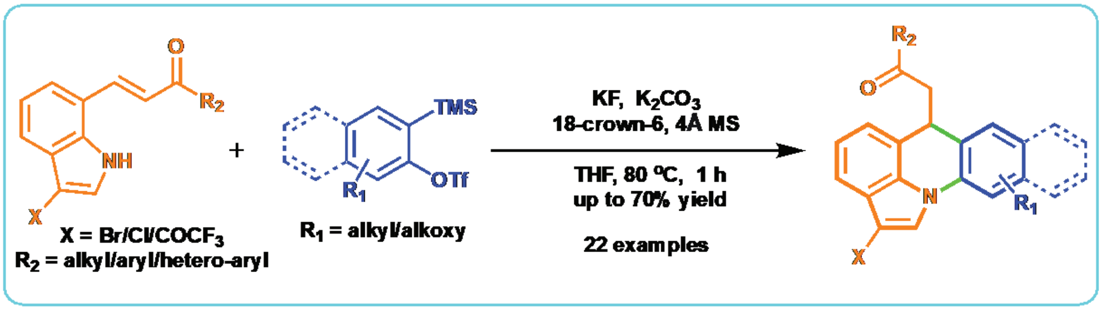
Department of Chemical Sciences,

Indian Institute of Science Education and Research Berhampur, Transit Campus, Govt. ITI Building,
NH 59, Engineering School Road, Ganjam-District, Berhampur 760 010, Odisha, India;

Email: sayantank20@iiserbpr.ac.in

Abstract: In connection with our ongoing research interest in developing novel and efficient methodologies by using aryne intermediates,[1] we were attracted to utilize substituted indoles having a suitable Michael acceptor to form a six-membered ring after the reaction with aryne. Accordingly, the Cascade N-nucleophilic addition followed by a cyclic Michael addition of reaction of arynes and indoles substituted with suitable Michael acceptors provided 6H-pyrrolo[3,2,1-de]acridines compounds under metal-free conditions. Additionally, photophysical studies of a few of the newly synthesized pyrroloacridine compounds indicated good fluorescence emission properties.[2]

Figure:



References and Notes:

1. Hazra, G[†].; Mishra, G[†].; Dandela, R.; Thirupathi, B. *The Journal of Organic Chemistry* **2022**, *87*, 11925-11938. († equal contribution)
2. Hazra, G[†].; **Kundu, S[†].;** Dandela, R.; Thirupathi, B. *The Journal of Organic Chemistry* **2023,** *88*, 8493–8504. († equal contribution)

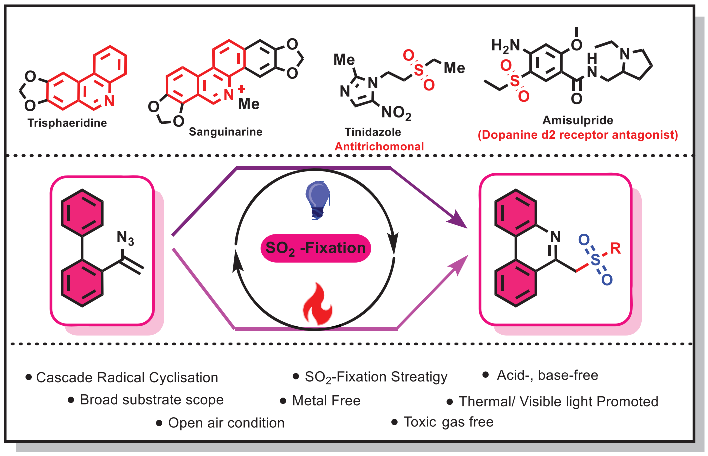
Sustainable Synthetic Method Toward the Synthesis of Benzo[c]phenanthridine Alkaloids

Tonish Kumar Sahu[†], Abhaykumar Rajkumar Vishwakarma and Tabrez Khan*
Organic Chemistry Laboratory, School of Basic Sciences
Indian Institute of Technology Bhubaneswar
(E-mail[‡]: s21cy09003@iitbbs.ac.in)

Abstract:

The presence of sulfur-based functionality such as sulfones, sulfoxide, sulfoximines, and 1,2-amino sulfonyl group in pharmaceuticals and agrochemicals has notably increased in the past decade. Traditional methods to introduce these S-based functionalities require the use of specifically designed substrates with multiple synthetic steps, suffer from limited compatibility to various functional groups, as well as require metal-based reagents and harsh reaction conditions which limits their application. On the other hand, phenanthridine derivatives manifest in several bioactive natural alkaloids and unnatural molecules of material interest. Therefore, with our ongoing interest in the development of metal-free strategies for carbo-/heterocycles[1-3] and the growing significance of visible-light-promoted photoredox catalysis,[4] we have developed both conventional thermally activated as well as photoredox catalyzed alkyl sulfonylative cascade cyclization.[5] The reaction optimization and the substrate scope studies along with the mechanistic probing studies will be presented through the poster.

Scheme:



References and Notes:

1. Salam, A.; Kumar, D.; Sahu, T. K; Khan, R.; Khan, T.; *Eur. J. Org. Chem*. **2022**, e202101452.
2. Kumar, D.; Salam, A; Sahu, T. K; Sahoo, S. S.; Khan, T.; *J. Org. Chem.* **2021**, 86, 21, 15096–15116
3. Kumar V.; Awasthi, A.; Salam, A.; Khan, T.; *J. Org. Chem.* **2019**, 84, 18, 11596–11603.
4. Nathan A.; David A.; Nicewicz; *Chem. Rev.* **2016**, 116, 10075−10166.
5. Manuscript Under Communication.

Bio-organic and medicinal chemistry

Binary to ternary drug-drug molecular adducts of antihypertensive drug, Ketanserin (KTS) with advanced physicochemical property

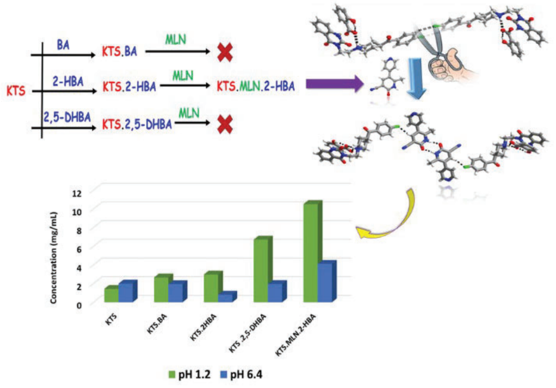
Smruti Rekha Rout and Rambabu Dandela*

Department of Chemistry, Institute of Chemical Technology-Indian Oil Campus

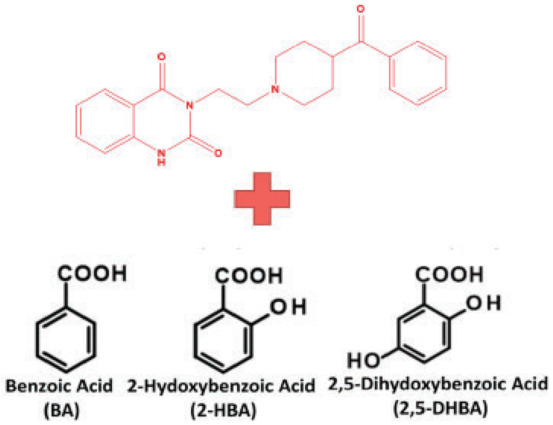
(E-mail: hiamsmruti@gmail.com)

Abstract: Focusing on a reliable supramolecular synthons approach, novel molecular salts of the antihypertensive medication ketanserin (KTS) with aromatic carboxylic acid derivatives (benzoic acid (BA), 2-hydoxybenzoic acid (2-HBA), 2,5-dihydroxybenzoic acid (2,5-DHBA)) are reported. Binary salts of KTS with respective salt former were obtained by solvent-assisted grinding followed by solution crystallization. Salt production was confirmed by crystal structure investigations that revealed proton transfer from the carboxylic acid group of salt formers to the piperidine nitrogen atom of KTS. A rigorous investigation of the crystal packing of novel binary salts of KTS inspired the construction of ternary adducts, and a ternary crystalline product was subsequently identified using Milrinone (MLN), another cardiotonic drug. According to our knowledge, this is the first instance of a dual-drug ternary co-crystal combining both antihypertensive drugs of KTS. In order to evaluate the impacts of co-crystallization on the in vitro release behaviours of binary and ternary adducts, solubility tests of the cocrystal were undertaken under a variety of physiological pH conditions. The results indicate that, in contrast to the parent drug and binary adducts, the ternary adducts solubility rate has significantly increased. Finally, the stability of the synthesised adduct was evaluated under a range of environments, including temperature (40 ± 1 °C); humidity (90% ± 5% RH, 25 °C) and various solvents media, and established that they have good stability. We anticipate that the present finding will work with a wide range of medication combinations, providing a potential new approach to create multi-drug systems for cardiovascular disease.

Figure:



Scheme:



References and Notes:

1. Tingey T, Shu J, Smuczek J, Pope J. *ARTHRITIS CARE \& Res*. 2013; 65: 1460–1471.
2. Janicek M, Grassi CJ, Meyerovitz M, Callahan MB, Sandor T, Whittemore A, mannick J, harrington DP, hollenberg NK. Invest Radiol. 1990; 25: 495–503.

Exploration of the first new solid variants of the anticancer medication Panobinostat (PNB), with improved physicochemical attributes

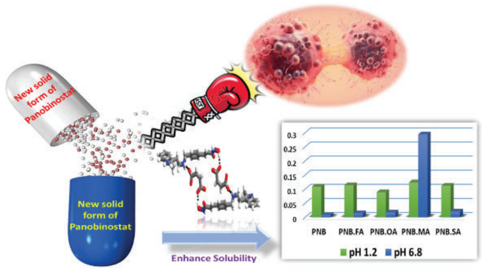
Gowtham Kenguva and Rambabu Dandela*

Department of Industrial and Engineering Chemistry, Institute of Chemical Technology, Indian Oil Bhubaneswar Campus, Bhubaneswar, India.

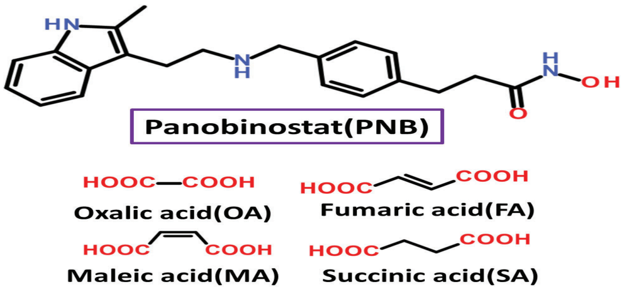
(E-mail: gautham.kenguva@gmail.com)

Abstract: Panobinostat (PNB), is a medication used for the treatment of multiple myeloma. It is a BCS Class II drug with strong permeability and poor solubility. It is therefore highly desirable to investigate novel PNB variants with improved physiochemical properties. In this regard, several solid forms of PNB have been produced employing mechanochemistry and solution crystallisation techniques using a variety of GRAS (Generally Recognized as Safe) salt formers, notably oxalic acid (OA), fumaric acid (FA), maleic acid (MA), and succinic acid (SA). Powder X-Ray Diffraction (PXRD), Single Crystal X-Ray Diffraction (SCXRD), and thermal analysis such as Thermogravimetric analysis (TGA) and Differential Scanning Calorimetry (DSC) were used to characterize all the synthesised molecular adducts. Hirshfeld surfaces and fingerprint plots demonstrate that the molecular entities are stabilized by O-H, C-H, C-C and H H intermolecular interactions. Moreover, the solubility of parent PNB and its molecular adducts in pH 1.2/pH 6.8 was evaluated at room temperature. In every instance, an increase in the solubility of molecular salts relative to the parent medication is seen, notably PNB.MA exhibits enhanced solubility of 0.294 mg/ml, a 73fold increase over the parent PNB. Furthermore, it is observed that this upsurge in solubility of all the forms is static at pH 1.2. A thorough analysis of the recovered residue after solubility showed that most of the molecular adducts were stable at pH 6.8 and did not display any phase change or dissociation (with the exception of PNB.MA), but at pH 1.2 they transferred into a new stable form and extensive analysis confirmed that it converted into PNB.Cl salt. To the best of our knowledge, this is the first report on novel solid forms of PNB with enhanced physicochemical properties which implies that the obtained PNB molecular adduct may help in the development of improved PNB formulations.

Figure:



Scheme:



Reference:

1. G. Bolla, A. Nangia, *Chem. Commun.*, *52* (54) (2016) 8342–8360, https://doi.org/10.1039/C6CC02943D
2. O. N. Kavanagh, D. M. Croker, G. M.Walker, M. J. Zaworotko, *Drug Discov. Today*, *24* (3) (2019), 796–804. https://doi.org/10.1016/j.drudis.2018.11.023.

Rational Design of Peptides Targeting the Complement Protein C5a

Manaswini Ghosh[1], Soumendra Rana[1]

[1]*Chemical Biology Laboratory, School of Basic Sciences, Indian Institute of Technology Bhubaneswar, Odisha, India.*

E-mail: ms40@iitbbs.ac.in

Abstract

The complement system is a concoction of several glycoproteins that aid in the proper functioning of the immune system. The human complement fragment 5a (C5a) is one such potent glycoprotein of the complement system that plays a critical role in complement-mediated inflammation. Excessive C5a in the plasma contributes to the pathophysiology of several inflammatory diseases,[1] including COVID19[2]. Thus, neutralization of excessive C5a has a great therapeutic value, and indeed, antibodies targeting C5 (Eculizumab, March 2007), the precursor of C5a, and the C5a (Vilobelimab, EUA April 2023) have been approved by FDA. In this context, small designer peptides targeting C5a appear to be a potential therapeutic alternative due to their smaller size, lower production cost, target specificity, and ability to penetrate membrane barriers. Our current study describes the binding of a pair of designer peptides to C5a, potentially mimicking the function of neutralizing polyclonal antibodies. The computational and experimental data strongly suggest both peptides bind to C5a with high affinity and form a stable complex. In addition, the peptides are thermostable free from aggregation, and relatively resistant to proteolysis with negligible toxicity toward mammalian cells like HEK and HeLa. The results indicate that the designer peptides have a strong potential to mimic the function of antibodies targeting C5a; however, further biological studies will be required to understand the function of the designer peptides properly.

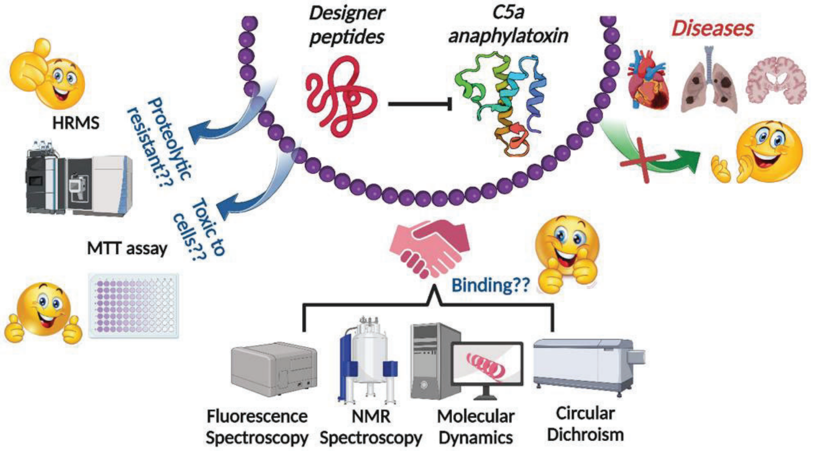


Figure 1: Schematic illustration of a peptide-based approach to neutralize the potent C5a protein.

References

1. Ghosh, M., Rana, S. The anaphylatoxin C5a: Structure, function, signaling, physiology, disease, and therapeutics. *Int. Immunopharmacol*., 2023, 118:110081.
2. Carvelli, J., et. al. Association of COVID-19 inflammation with activation of the C5a–C5aR1 axis. *Nature*, 2020, *588* (7836), 146-150.

Cu-Catalyzed Synthesis of Alkylaminotroponyl Sulfones as *Pseudomonas Aeruginosa* Quorum Sensing Inhibitors Targeting *lasI/R* QS Circuitry

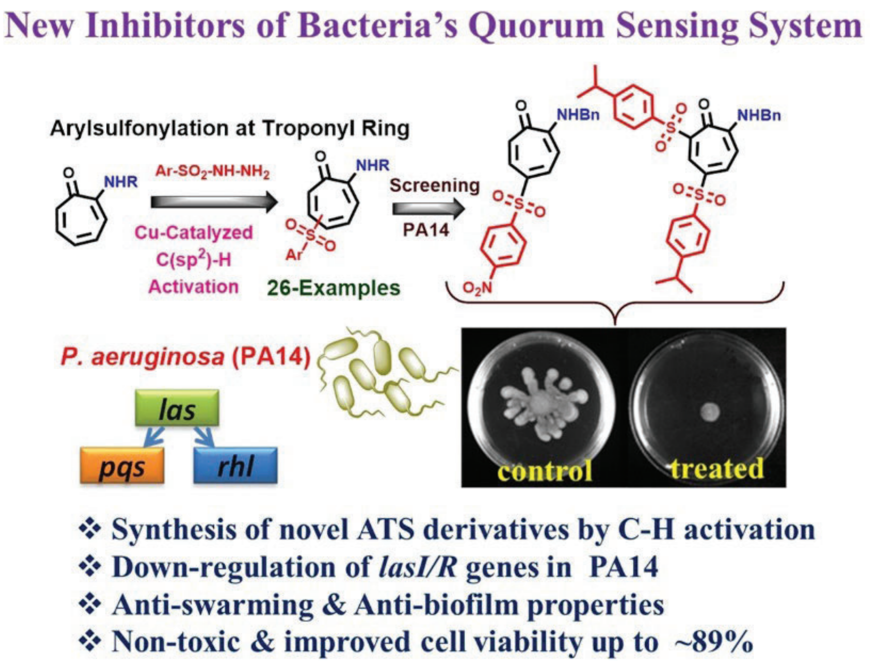
Dr. Sagarika Meher and Dr. Nagendra K. Sharma*

Department of Chemistry, School of Chemical Sciences, National Institute of Science Education and Research (NISER), Jatani-752050, Odisha, India.

(E-mail: sagarika.meher@niser.ac.in)

Abstract: The scarcity of novel bioactive molecules against multidrug-resistant (MDR) bacterial strains like *Pseudomonas aeruginosa* is alarming. This bacterial virulence is regulated via Quorum sensing (QS), a cell-cell communication process. Disabling QS circuits (*las*, *pqs*, *rhl*) with small molecules has been proposed as a potential strategy to prevent bacterial pathogenicity. This modern strategy focuses on interruption of bacterial virulence, rather than killing them to tackle the drug resistance problem. Herein, we have performed the synthesis of rationally designed Alklyamionotroponyl Sulfone (ATS) derivatives by Cu-catalyzed C(sp^2)−H functionalization at tropone ring and the screening of their anti-QS activity against *P. aeruginosa.* Importantly, two sulfones (~20 µM) remarkably exhibit the down regulation of the *lasI/R* QS genes. These molecules also inhibit swarming motility, biofilm formation and pyocyanin production, which reduce *P. aeruginosa* virulence in cells. Hence, ATS derivatives could be considered as potential therapeutic candidates for the treatment of *P. aeruginosa* infections.[1]

Figure:


New Inhibitors of Bacteria's Quorum Sensing System

- ❖ Synthesis of novel ATS derivatives by C-H activation
- ❖ Down-regulation of *lasI/R* genes in PA14
- ❖ Anti-swarming & Anti-biofilm properties
- ❖ Non-toxic & improved cell viability up to ~89%

References and Notes:

1. Meher, S.; Kumari, S.; Dixit, M.; Sharma, N. K. Cu-Catalyzed Synthesis of Alkylaminotroponyl Sulfones as *Pseudomonas aeruginosa* Quorum Sensing Inhibitors Targeting *lasI/R* QS Circuitry. *Chem. Asian J.* **2022**, *17* (23), e202200866

Exploration of impact of *in vitro* acetylation on the structure and function of *Mycobacterium tuberculosis* Hsp16.3 by using a chemical approach

Subhashree Barik[a,#] and Ashis Biswas[a,*]

[a]*School of Basic Sciences, Indian Institute of Technology Bhubaneswar, Bhubaneswar, India*

Email: #sb67@iitbbs.ac.in, *abiswas@iitbbs.ac.in

Abstract: The causative agent of tuberculosis is *Mycobacterium tuberculosis* which secretes a major immunodominant antigen Hsp16.3 throughout the course of infection. This protein belongs to small heat shock protein (sHsp) family. The molecular chaperone function of this protein plays a vital role in the growth and survival of *Mycobacterium tuberculosis* during the latency period of infection[1]. Inside this pathogen, Hsp16.3 undergoes a varied type of post-translational modifications and acetylation is considered as a pivotal one. Various lysine acetylated sites have been found in *Mycobacterium tuberculosis* Hsp16.3, but, the impact of lysine acetylation on the structure and chaperone function of Hsp16.3 still remains unclear. In order to execute the *in vitro* acetylation of a protein, researchers have been utilized different procedures. Those are (i) chemical modification procedure i.e. acetic anhydride modification, (ii) site-directed mutagenesis approach i.e. by creating acetyl-lysine mimic by replacing lysine residue with glutamine residue, (iii) site-directed mutagenesis approach followed by chemical modification i.e. by generating acetyl-lysine mimic by replacing lysine residue with cysteine firstly and then treating with methylthiocarbonyl-aziridine (MTCA). We executed a simple chemical modification approach and acetylated Hsp16.3 under *in vitro* condition by using acetic anhydride. Then, the extent of acetylation has been evaluated by fluorescamine assay and western blot analysis. This *in vitro* acetylation enhanced the chaperone function, altered the secondary structure, tertiary structure and tyrosine microenvironment which in turn lowered its thermostability. Such acetylation also enhanced the surface hydrophobicity and dissociated the oligomeric assembly of Hsp16.3. These two factors (surface hydrophobicity modulation and oligomeric assembly dissociation) are the key molecular basis behind the enhanced chaperone function of *in vitro* acetylated Hsp16.3. After this we performed the mass spectrometric analysis to identify the acetylation sites of *in vitro* acetylated Hsp16.3. From this analysis, it has been observed that except K136 all other lysine residues (K47, K64, K78, K85, K114, K119 and K132) along with the N-terminal end methionine got acetylated due to this *in vitro* acetylation. However, it has been observed that except K47 all the lysine residues got acetylated *in vivo*[2]. Nevertheless, we believe that acetylation of lysine residues of Hsp16.3 enhances its chaperone function, which may in turn help the *Mycobacterium tuberculosis* to survive more under hostile condition. Furthermore, our study opens up an important futuristic avenue where one can raise an acetylation mimic mutant using site-directed mutagenesis approach and compare its structure and chaperone function with unacetylated/wild-type Hsp16.3, so as to validate our findings.

References:

1. Panda, A. K.; Chakraborty, A.; Nandi, S. K.; Kaushik, A.; and Biswas, A. *The FEBS Journal* (**2017**), 284, 277-300.
2. Liu, F.; Mingkun Y.; Xude W.; Shanshan Y.; Jing G.; Jie Z.; Xian-En Z.; Jiaoyu D.; and Feng G. *Molecular & cellular proteomics* (2014), 13, 3352-3366.

Exploration and investigation of various solid forms of an antiglaucoma drug - Dichlorphenamide

Ananya Kar, Rambabu Dandela*

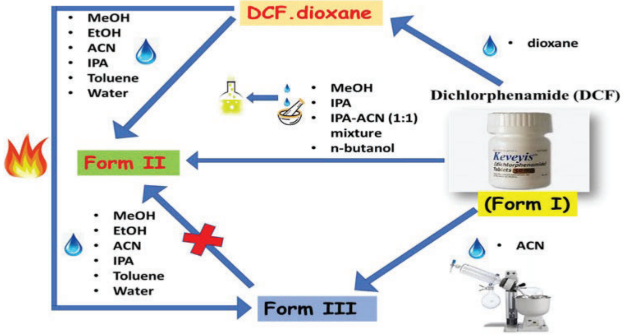
Department of Industrial and Engineering Chemistry

Institute of Chemical Technology - Indian Oil Odisha Campus, Bhubaneswar, India

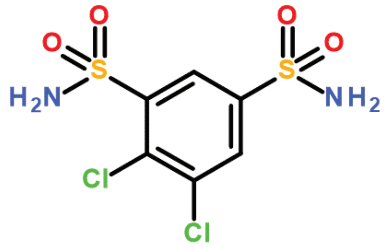
(E-mail: che22a.kar@stuiocb.ictmumbai.edu.in, r.dandela@iocb.ictmumbai.edu.in)

Abstract: Diclofenamide (or dichlorphenamide (DCF)) is a sulfonamide and a carbonic anhydrase inhibitor of the meta-disulfamoylbenzene class. It is used for the treatment of acute angle closure glaucoma. However, its weak solubility and slow rate of dissolution restrict its therapeutic applicability. A complete solid-state screening experiment was carried out in order to discover some new forms with useful physicochemical properties. As a result, two polymorphic (Form II and III) and one dioxane solvated structures (DCF.dioxane) were obtained under different crystallisation conditions. These solid forms were characterized by Powder X-Ray Diffraction (PXRD), Single Crystal X-ray Diffraction (SCXRD), Field Emission Scanning Electron Microscope (FE-SEM), Thermogravimetric analysis (TGA) and Differential Scanning Calorimetry (DSC). Variable temperature PXRD (VT-PXRD) and various solvent media were used to test the relative stability of the newly produced solid forms. Most of the forms remained stable at higher temperatures, but DCF. dioxane changed to Form III. A similar trend was also seen in various solvent environments but in this case DCF. dioxane transferred to Form II. Additionally, the physicochemical characteristics of these three polymorphs were extensively described, and the solubility was assessed in pH 1.2 and pH 6.4 media. All of the forms exhibited greater water solubility as compared to parent DCF. Thus, we anticipate that the current findings will provide some insight to consider prior to the formulation of the DCF drug.

Figure:



Scheme: Chemical structure of DCF.



References and Notes:

3. Kar, A., Giri, L., Kenguva, G., Rout, S.R., and Dandela, R. (2023) Exploration and investigation of various solid forms of an anti-glaucoma drug – dichlorphenamide. *CrystEngComm*, **25** (13), 1874–1883.

Solar-assisted Green Synthesis, Antimicrobial Activity and Cytotoxicity of Symmetrical N, N'-Alkylidene Bisamides

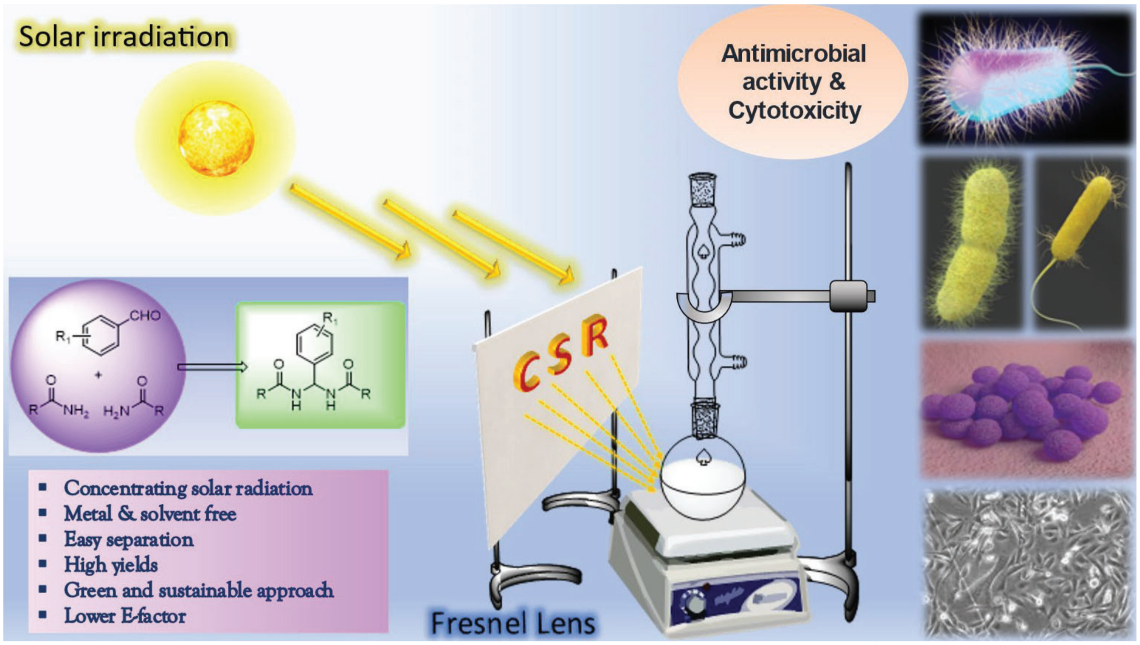
Omkar S. Kamble, [a] Rana Chatterjee, [a] Shubhada Gad, [b] Samarath Kansara, [c] Sonal Ayakar[b] Amit K. Pandey, [c] and Rambabu Dandela[a]*

[a]*Department of Industrial and Engineering Chemistry, Institute of Chemical Technology, Indian Oil Odisha Campus, Bhubaneswar, 751013, India.*

[b]*Department of Biotechnology, Institute of Chemical Technology, Indian Oil Odisha Campus Bhubaneswar, 751013, India.*

[c]*Amity Institute of Biotechnology (AIB), Amity University, Gurgaon, Haryana, India.*

Abstract: In current advanced chemistry, various developing approaches have emerged to satisfy the clean, renewable, and environmentally benign techniques. A useful approach has been developed for the green synthesis of N, N'-alkylidene bisamides with concentrating solar radiation (CSR) assistance. The one-pot reaction of aldehydes and amides efficiently produced the symmetrical bisamides in the presence of any conventional catalyst under solvent-free conditions. The simple filtration process obtained all the products, and no column chromatography is needed. The present method provides a good yield of the bisamides and applies for large-scale synthesis. Besides, a promising antimicrobial study and cytotoxicity of the synthesized derivatives have been evaluated. A molecular docking study was also done with proteins and ligands. Eventually, the present technique offers several advantages: metal-and solvent-free, clean conditions, high yields, and easy separation technique.



1st KIIT-CRSI SEMINAR on Modern Trends in Chemical Sciences

5th September, 2023

KALINGA INSTITUTE OF INDUSTRIAL TECHNOLOGY
(KIIT)
Patia, Bhubaneswar, Odisha, India 751024