

Prof. Narayan Pradhan

Prof. Narayan Pradhan did his PhD from IIT Kharagpur in 2001 and continued his post doc in Israel and USA till 2006. In 2007 he joined the Indian Association for the Cultivation of Science and is currently working there as senior professor. Prof Pradhan received DST Swarnajayanti Fellowship, DST Nanomission Young Career award and also he is a fellow of Indian Academy of Science. His research area is on Semiconductor Nanomaterials.



IL-1

Light Emitting Inorganic Semiconductor Nanocrystals: From Designing in Reaction Flask to Watching under Electron Microscope

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Solution dispersed light emitting inorganic nanocrystals are emerged as one of the most efficient optical materials for photovoltaics and light emitting devices. From chalcogenides to perovskites, these inorganic nanocrystals are prepared in reaction flasks and with size/compositions variations, these show color tunable emissions. In recent past, highly emitting perovskite nanocrystals were surfaced where all three important visible colors (RGC) could be obtained with halide composition variations having near unity photoluminescence quantum yields. These materials are dominated with ionic characters and do not follow the classical mechanism of crystal growth. Hence, chemistry of architecture of these nanocrystals, their facets tuning and designing new structures indeed became difficult. This talk will present the facet chemistry of these important materials as this part was less explored in the field. Excitements of seeing colors in reaction flask to watching those in electron microscope would be presented. Focus would be on cesium lead halide bromides; but the general chemistry with fundamentals of crystal growth in solution would be highlighted.

Dr. Himansu S. Biswal

Dr. Himansu S. Biswal was born in Bari, Odisha, India, in 1980. He received his B.Sc. and M.Sc. degree from the Department of Chemistry, Utkal University, in 2000 and 2002, respectively. He did his Ph.D. with Prof. Sanjay Wategaonkar from the Tata Institute of Fundamental Research (TIFR), Mumbai, India, in May 2009. Then he moved to Commissariat à l'Energie Atomique (CEA), Saclay, Paris, France, for his first postdoctoral research with CNRS postdoctoral fellowship and worked with Prof. Michel Mons. During his second postdoc, he worked on 2D Electronic spectroscopy of photosynthetic reaction center with Prof. Jennifer Ogilvie at the University of Michigan (UoM), Ann Arbor, the USA. He joined the School of Chemical Sciences (SCS) at NISER, Bhubaneswar, in April 2012. His fields of current interests include solvation and isomerization of peptides, conformational landscape of flexible biomolecules in jet cooled condition, sulfur/selenium/carbon center hydrogen bonds, and their role in the structure and function of biological compounds and inorganic complexes. Dr. Biswal involves in building scientific instruments. Recently, he and his colleagues at NISER set up a state of art ultrafast laser spectroscopy facility that includes supersonic –jet spectroscopy, fluorescence-up-conversion, fluorescence correlation spectroscopy (FCS) and transient absorption spectroscopy. Dr. Biswal is also interested in investigating ionic- liquid-biomolecules interactions in detail. Some of the research works on storing DNA and RNA at ambient temperature have been published in high-impact journals and highlighted in several newspapers. Presently, Dr. Biswal is an associate professor at SCS, NISER and holds the chairperson position of the school. In his recognition of his academic career and research, he has been received many awards, which includes the Best Student Award (Utkal University, 2002), Best Thesis Award (TAA-Zita Lobo Memorial Award (Honorable Mention), TIFR, 2010), Young Researcher Award (IRAMIS, SPAM, Commissariat à l'Énergie Atomique, Saclay, France. December 2010), Young Scientist Award (Dr. P. K. Bhattacharya Memorial Award, Indian Society for Radiation and Photochemical Sciences, BARC, 2011), and DST-INSPIRE Faculty Fellowship (DST, Govt. of India, 2012), and Affiliate Member of the Royal Society of Chemistry, UK.



IL-2

Carbon Bond, Carbon Centered Hydrogen Bond, and Carbo-hydrogen Bond: Notions about Hydrophobic Forces

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Abstract: The last decade has seen several discoveries of noncovalent supramolecular forces such as tetrel bonding, pnictogen bonding, chalcogen bonding, halogen bonding, and aerogen bonding, and last but not least, the hydrogen bonds with sulfur and selenium. These interactions are essential to understanding supramolecular chemistry and biomolecular structures. In this talk, I shall present recent developments and our contributions in this research area^{1,2}, explaining the existences and general consensus and counterintuition about carbon-bond (C-bond)³, Carbon-centered hydrogen bond (H-bond), and most recent carbo-hydrogen bond (C_H-bond)⁴ in proteins and nucleic acids.

A genre of noncovalent interactions such as C₅-hydrogen bond, halogen bond, and reciprocal carbonyl-carbonyl interactions involving carbonyl groups of proteins discovered in recent years is proved to be useful in de novo protein structure and function prediction. However, in proteins, the occurrence, strength, and importance of carbon bonds (C-bonds), the highly directional hydrophobic interactions between an electron-rich carbonyl-oxygen acceptor and an electron-deficient sp³-hybridized carbon σ -hole donor through n $\rightarrow\sigma^*$ electron delocalization are yet to be perceived. With the help of careful protein structure analysis, quantum calculations, nuclear magnetic resonance, and infrared spectroscopic methods, we discovered ubiquitous existences of C-bonds in proteins and determined C-bond energies precisely. We demonstrated the implications of C-bonds in explaining the photochemistry of oxygen-storage protein myoglobin and protein-DNA. It is highly anticipated that the inclusion of C-bonds in computational force fields would unravel many more implications of C-bonds in the structure, function and dynamics of proteins and protein-ligand/drug complexes.

Hydrogen bond (H-bond) without lone pair(s) of electrons and π -electrons is a concept developed two to three years ago. H-bonds involving less electronegative tetrahedral carbon are beyond the classical concepts on H-bonds. Careful protein structure analysis aided with several quantum chemical calculations suggests that these H-bonds are moderate in strength. These C-H \cdots C H-bonds are blue-shifted and are dispersive in nature. We developed an empirical equation to estimate the C-H \cdots C H-bond energy in proteins from the distances between the carbon and hydrogen atoms. In proteins, the binding energies range from -5.4 kJ/mol to -14.0 kJ/mol. The C-H \cdots C H-bonds assist the substrate binding in proteins. We also explored the potential role of these carbon-centered H-bonds in C-H bond activation through σ -bond metathesis. To our surprise, these H-bonds contribute almost of similar magnitude as C-H $\cdots\pi$ H-bonds for C-H bond activation.

In contrast to the conventional and non-conventional noncovalent interactions (NCIs) such as hydrogen bond, carbon bond, etc., a bidirectional NCI without π - and/ or lone pair(s) of electrons has

never been reckoned, until the recent report which confirms that this type of NCI can be possible with the involvement of only σ -electrons and this newly discovered NCI can be coined as Carbo-Hydrogen bond (C_H -bond) based on its resemblances with both C-bond and H-bond, and the logic behind the name of “dihydrogen bond” or $C^i:::H$ Hydrogen bond. A detailed crystal structure analysis of 5-cyano-1,3-dehydroadamantane, which contains inverted carbon atoms (C^i) and C^i-C^i σ -bond, gave us the opportunity to unveil the very first existence of $C^i:::H$ interaction. With the aid of several quantum chemical calculations, we concluded that molecules carrying C^i-C^i σ -bonds are capable of forming C_H -bond with main group hydrides through $\sigma_{C^i-C^i} \rightarrow \sigma^*_{X-H}$ (H-bond) and $\sigma_{X-H} \rightarrow \sigma^*_{C^i-C^i}$ (C-bond) orbital interactions. The interaction energy can be as much as -31.27 kJ/mol, which is comparable to that of water dimer. It is also one of the prominent attractive forces to hold the molecules together in the crystal structure, which can be responsible for the enzymatic activity of cytochrome P411-E10 and the formation of the noncovalent organic framework (NCOF) with trigonal and tetragonal C_H -bond connectors.

A brief overview of the experimental techniques and computational methods employed to understand such noncovalent interactions in gas, solution and solid-state will also be discussed. Our efforts to find such noncovalent interactions in biomolecules and their implications will be the highlights of the presentation.

References

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Award Presentations

AP-1

Prof. R. C. Tripathy Memorial Award (inside the state)

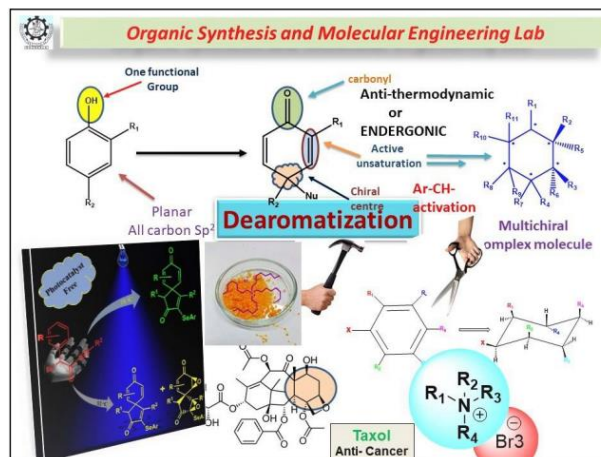
Dearomatisation - An Unsolved Riddle

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Abstract: Dearomatization is a versatile synthetic tool for transformation of a simple planar molecule to a more functionalised diverse non-planar molecular skeleton allowing a fast access to synthetic complexity. Oxidative dearomatisation is a fantastic protocol for developing rapid and controlled generation of complex, readily functionalizable three-dimensional structures from simple planar starting materials is a highly attractive goal, as it allows fast access to diverse molecular architectures. Dearomatization of arenes is a powerful approach that has been proposed as a key component in putative biosynthetic pathways for a range of bioactive natural products, inspiring a range of elegant syntheses. A highly desirable factor in such constructions is the induction of asymmetry into the product, which has generally been achieved by three distinct chemical approaches: diastereoselective dearomatization of a substrate bearing an existing stereocenter. However, generalized, cheap and scalable approaches towards this reaction are scarce and none is catalytic. Cyclohexadieneones and naphthalenones are important structural motifs which serve as effective molecules towards complex natural product synthesis. Notably, the last decade has seen a tremendous urge to develop sustainable versions of this transformation which can be applied to a wider context. Important functionalisation along with conversion of these planar molecules to three dimensional molecules like Aminocyclohexadieneones, azido-naphthaleneones and Peroxo-cyclohexadieneones constitute the central core for a vast set of medicinally important molecules and thus create an extreme focus of attention. Certainly, a generalised oxidative strategy which carefully accomplishes this “trio” of reactions aminative, azidative and Peroxidative dearomatisations can be a reaction of tremendous synthetic importance. This trio of reactions has been accomplished using Phenyl trimethyl ammonium tribromide(PTAB) as an effective reagent

**AP-2****Prof. Dayanidhi Patnaik Memorial Award**

V^{IV}, V^{IV}O, V^VO, and V^VO₂ Systems: Exploring their Interconversion in Solution, Protein Interactions, and Cytotoxicity

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Abstract: There is a contemporary interest in vanadium chemistry, which stems from the broad range of relevance and application of vanadium in biological as well as industrial processes. Therefore, the development of new vanadium complexes with improved pharmacological activity is of current interest. In contrast to the well-known oxidovanadium(IV)/(V) complexes, relatively few non-oxido V^{IV} and V^V complexes, the so-called “bare” complexes, have been isolated and structurally characterized. On the other hand, it is well known that, for an oxido and alkoxido vanadium system, the solid-state chemistry may be different from that in solution. In fact, in solution the complexes may undergo ligand exchange, in some cases also redox reactions and/or formation of dimer and oligomers; thus, the main species present in solution may differ from that of the parent solid. Over the past few years, we have been working in the field of vanadium chemistry incorporating several mono and dibasic ligand systems, and have successfully isolated several oxidovanadium(V),¹⁻⁴ oxidovanadium(IV),⁵ mixed valence oxidovanadium(IV, V),³ and some rare stable nonoxido-vanadium(IV) complexes^{4,6} and accessed their solution chemistry and biological activity. In this presentation I will focus on some of our recent interesting results.

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AP-3

Prof. G.B. Behera Best Thesis Award

Preparation and characterization of carbohydrate based hybrid nanocomposite hydrogels for *in vitro* release of drugs

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Abstract: Recently, nanocomposite hydrogels have gained a special interest in drug delivery applications due to their unique combination of distributed nanostructural phase and cross-linked hydrophilic network. Out of these nanostructural materials, specially noble and inorganic nanomaterials like nano silver, nano gold, nano ZnO, and their analogues have enormous demand. It is because of their high surface-to-volume ratio which may offer active binding sites to the drug molecules. It is worth mentioning that, various research groups have devoted their expertise in the synthesis of non-toxic polymeric hydrogels which has created a special interest for encapsulation of various drugs. There is a challenge to overcome this problem for which we have chosen carbohydrates and polysaccharide material to enhance the degradability. Generally, nanocomposite hydrogels offer enhanced swelling capacity as well as higher gel strength at higher nanostructural content due to active participation in improving cross-linking density. Hydrogel materials are extensively applied in drug delivery applications due to their soft and wet polymeric network which not only able to imbibing huge quantities of water or biological fluid in its porous structure but also mimic the nature of extracellular matrix.

The present thesis reveals designing of low cost ecofriendly carbohydrate based hybrid nanocomposite hydrogels towards *in vitro* release of drugs such as ornidazole (OD), and ciprofloxacin (CFX). In the first research work, we have synthesized nano silver and nano ZnO and their incorporation within the dextran based hybrid nanocomposite hydrogels. The chemical interaction of hybrid nanostructures (PAM/D@Ag and PNIPAM/PEG-D@ZnO) is studied by FTIR whereas the structural behaviour of the nanocomposite hydrogel is evaluated by XRD pattern. The change in morphological attributes of porous PAM/D and PNIPAM/PEG-D hydrogels due to incorporation of Ag NPs and nano ZnO hybrid nanostructures is examined from field emission scanning electron micrographs. HRTEM analysis is performed for all nanocomposite hydrogels to locate the orientation and position of hybrid nanofillers in hydrogel surface. Swelling, thermal, antibacterial, mechanical and rheological behaviours of the synthesized nanocomposite hydrogels are

studied in detail along with their *in vitro* drug release (OD/CFX) with respect to pH and temperature. Moreover, we have designed cellulose based hybrid nanocomposite hydrogels (PAM/C-Au and PPO/PEO-C@Ag). FESEM and HRTEM analysis are performed to monitor the change in surface morphology due to incorporation of Au NPs and Ag NPs. Swelling, water retention, thermoresponsive; thermal, rheological and drug release performances of the prepared hydrogel and nanocomposite hydrogels are studied in detail.

In next piece of work, we have prepared soy protein based hybrid nanocomposite hydrogels (PAM/SP-Ag). All prepared nanocomposite hydrogels are characterized by FTIR whereas; the structural behaviour is investigated by XRD. The morphology and the nano filler orientation in the hydrogel structures are examined by FESEM and HRTEM. Swelling, thermal, rheological and drug diffusivity, cytotoxicity analysis of all synthesized hybrid nanocomposite hydrogels are investigated in detail. Furthermore, in another piece of work, we have designed nanocomposite hydrogels are structurally and morphologically characterized with XRD, FTIR, FESEM and HRTEM to correlate with their flower like structure. Swelling, water retention, thermoresponsive; thermal, rheological and drug release performances of the prepared hydrogel and nanocomposite hydrogels are studied in detail. Further in another study, thermal responsive hydrophobic gels of oleylamine and oleic acid as capping ligands in toluene for target drug delivery.

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AP-4

Prof. R. C. Tripathy Memorial Award (Outside the State) (For the Year 2020)

Ultrathin Plasmonic Tungsten Oxide Quantum Wells with Controllable Free Carrier Densities

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Abstract: Localized surface plasmon resonances (LSPR) of nanostructures can be tuned by controlling their morphology, local dielectric environment, and free carrier concentration. Here we report the colloidal synthesis of an ~3 tungsten–oxygen (W-O) layer thick (~1 nm), two-dimensional

(2D) WO_{3-x} nanoplatelets (NPLs) ($x \approx 0.55-1.03$), which display tunable near-infrared LSPR properties and additionally high free electron density (Ne) that arises predominantly from the large shape factor of 2D NPLs. Importantly, the W to O composition ratios inferred from their LSPR measurements show much higher percentage of oxygen vacancies than those determined by X-ray diffraction analysis, suggesting that the aspect ratio of ultrathin WO_{3-x} NPLs is the key to producing an unprecedentedly large Ne, although synthesis temperature is also an independent factor. We find that NPL formation is kinetically controlled, whereas thermodynamic parameter manipulation leads to Ne values as high as $4.13 \times 10^{22} \text{ cm}^{-3}$, which is close to that of plasmonic noble metals, and thus our oxide-based nanostructures can be considered as quasi-metallic. The unique structural properties of 2D nanomaterials along with the high Ne of WO_{3-x} NPLs provide an attractive alternative to plasmonic noble metal nanostructures for various plasmon-driven energy conversions and design of photochromic nanodevices.

AP-5

Prof. Dayanidhi Patnaik Memorial Award (For the Year 2020)

Facile synthesis and photocatalytic efficacy of UiO-66/CdIn₂S₄ nanocomposites with flowerlike 3D-microspheres towards aqueous phase decontamination of triclosan and H₂ evolution

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Abstract: In the current scenario, the increasing global population and rapid development of industries are major concerns which are leading to energy crisis and environmental pollution. To find cost effective, green and sustainable route for the production of renewable energy sources and mitigate environmental pollution are the major challenge for researcher around the globe. The solar light driven photocatalysis is one of the promising technology to deal with environmental pollution and renewable energy generation. The construction of porous hetero-structure photocatalyst material with improved surface and optoelectrical properties is a practical and effective strategy for mineralization of toxic organic pollutants and water splitting reaction under visible light irradiation. In this work, we have developed a facile hydrothermal route to prepare a series of novel UiO-66/CdIn₂S₄ heterojunction nanocomposite materials containing finely dispersed UiO-66 spherical nanoparticles (20-40 nm) anchored over high aspect ratio CdIn₂S₄ nanosheets. Comprehensive characterization of the UiO-66/CdIn₂S₄ nanocomposites revealed a hierarchical 3D micro-flower structure with enhanced surface reactive sites, better channelization of charge carriers, high resistance to charge recombination and a favorable band alignment between the two semiconductor components. The optimal photocatalyst (30UiO-66/CdIn₂S₄) showed improved photocatalytic efficiency towards triclosan degradation with rate constant (0.0094 min⁻¹) twelve times higher than the pure CdIn₂S₄ (0.0007 min⁻¹). The 30UiO-66/CdIn₂S₄ photocatalyst also exhibited higher H₂

evolution rate (2.95 mmol-g-1h-1) with apparent conversion efficiency of 20.8%. The important results generated in this work will be discussed in the seminar.

AP-6

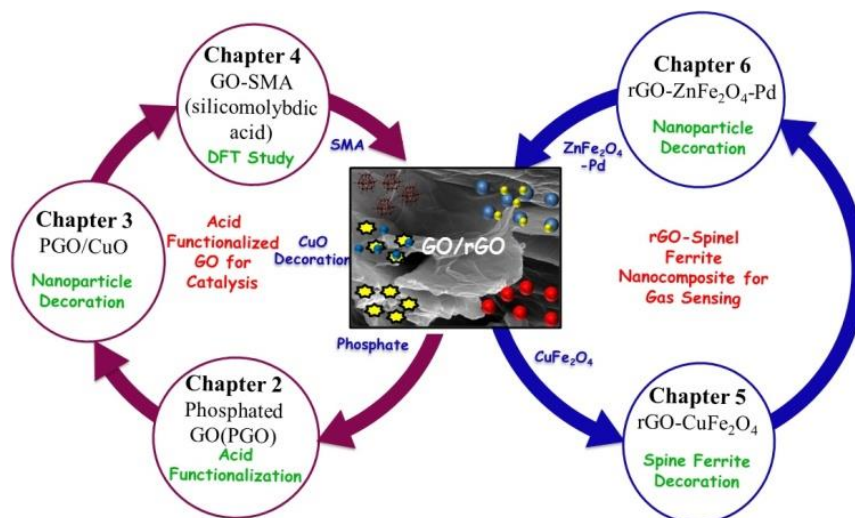
Prof. G. B. Behera Best Thesis Award (For the Year 2020)

Rational Design of Highly Active and Sensitive Graphene Oxide-based Catalyst and Sensor Materials

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Abstract: Graphene oxide (GO), a functionalized graphene with oxygen-containing chemical groups has shown great promise in various applications due to its unique properties such as high surface area, mechanical stability, tunable optical and electrical properties [1, 2]. The presence of surface functional groups has opened new route for the synthesis of GO-based hybrid materials. Keeping this in mind, my PhD thesis is focused broadly on two objectives; (1) synthesis of acid functionalized GO-based hybrid materials for catalytic applications and (2) synthesis of spinel ferrite decorated rGO-based hybrids for gas sensing applications. In the catalysis part, it documents the use of acid functionalized GO (PGO) for the synthesis of biologically important nitrogen-based heterocycle such as pyrimidones (Chapter 2, *Chem. Eng. J.*, 2018, 331, 300). Highlighting the effect of nanoparticle decoration on acid functionalized GO, the second project focuses on the design of highly efficient CuO decorated PGO catalyst for the synthesis of β -amino carbonyl compounds (Chapter 3, *Catal. Today*, 2020, 348, 137). Continuing this narrative, DFT studies has been carried out to find out the synergistic effect between GO and acidic groups in GO-SMA catalyst (Chapter 4, *Communicated*). In the gas sensing part, attempts have been taken to design rGO-CuFe₂O₄ nanocomposite and use as a promising gas sensor for the detection of NH₃ gas (Chapter 5, *Sens. and Actuators B: Chem.*, 2018, 272, 100). Later on, the effect of nanoparticles decoration has been done in order to design rGO-ZnFe₂O₄-Pd nanocomposite as an efficient H₂ gas sensor at room temperature (Chapter 6, *Int. J. Hydrog. Energy*, 2020, 45, 5073). All the materials presented in this thesis proved to be stable, efficient, sensitive and recyclable system for the above applications which are of biological and environmental significance.



References

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AP-7

Prof. R. C. Tripathy Memorial Award (inside the state) (For the Year 2020)

Hybrid of Patronite sheets: An emerging material for Electrochemical Water Splitting

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Abstract: Electrochemical water splitting has proven to be one of the most cost-effective and efficient methods for the generation of hydrogen (H₂) and oxygen (O₂). State-of-the-art techniques adopt catalysts made from precious elements like Pt and Ir to reduce the overpotential required to overcome the kinetic barrier associated with the hydrogen bond in a water molecule. However, improving the scale of production of H₂/O₂ through the aforementioned precious catalysts is not cost-effective and suffer from poor cyclic durability that restrict the commercial use. Therefore, cheaper and better alternatives need to be developed that would not only help us achieve better catalytic efficacy but also improve the durability of the water-splitting device.

This work reports the hybridization of patronite (VS₄) sheets with reduced graphene oxide and functionalized carbon nanotubes (RGO/FCNT/V_S₄) through a hydrothermal method. The synergistic effect divulged by the individual components, i.e., RGO, FCNT, and VS₄, significantly improves the

efficiency of the ternary (RGO/FCNT/VS₄) hybrid toward the oxygen evolution reaction (OER). The ternary composite exhibits an impressive electrocatalytic OER performance in 1 M KOH and requires only 230 mV overpotential to reach the state-of-the-art current density (10 mA cm⁻²). Additionally, the hybrid shows an appreciable Tafel slope with a higher Faradaic efficiency (97.55±2.3%) at an overpotential of 230 mV.

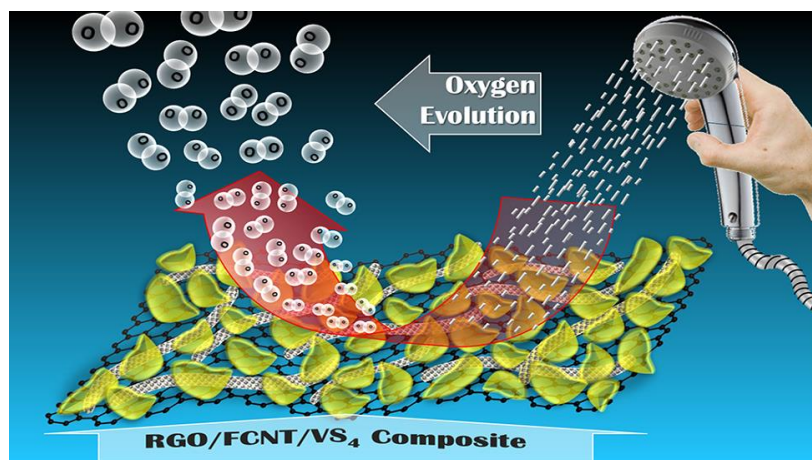


Figure 1: Scheme showing the electrocatalytic activity of the RGO/FCNT/VS₄ composite towards evolution of oxygen.

Oral Presentations

OP-1

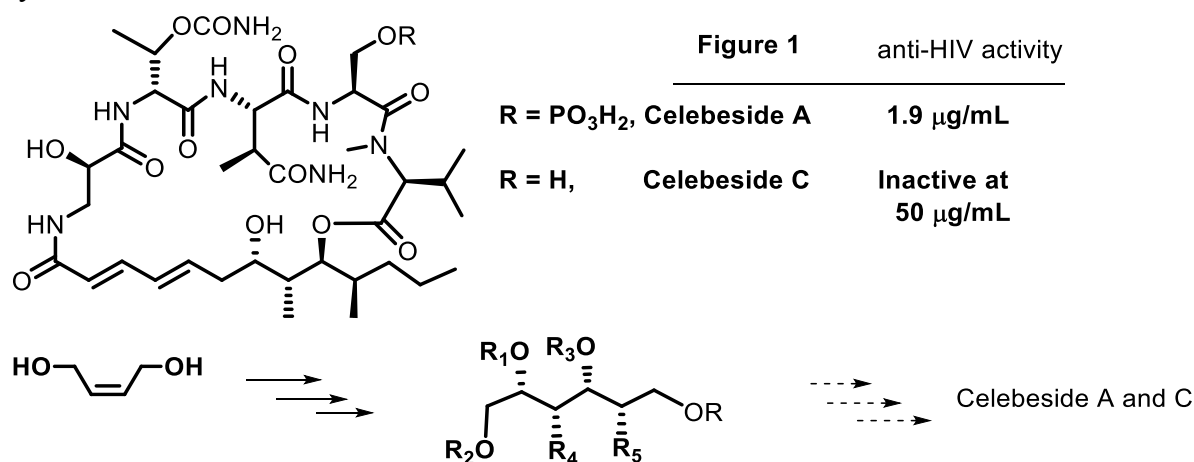
Heterodetic Cyclodepsipeptides: Celebesides A and C

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Abstract: Depsipeptides are heterodetic peptides in which at least one amide bond has been replaced with one ester bond. Depsipeptides from natural sources show relevant biological activities. Naturally occurring cyclic depsipeptides have emerged as an important source of pharmacologically active compounds or promising lead structures for the development of novel synthetically derived drugs. Cyclic depsipeptides are well known for exhibiting a diverse spectrum of biological activities. Depsipeptides are large group of natural products produced by fungi, actinomycetes, cyanobacteria, higher plants and marine organisms. Isolation, structural elucidation and biological activities cyclic depsipeptides Celebesides A-C were reported by Plaza-Jessica-Bewley *et al.* Celebesides A and C were evaluated in single round HIV-1 infectivity assay against viruses and cytotoxicity assay using human colon tumor cell line HCT-116. The celebeside A inhibited HIV-1 entry with an IC₅₀ value of $1.9 \pm 0.4 \mu\text{g/mL}$. Diversity of biological activities, their architecture and the challenge to synthesize the depsipeptides in optically pure form made them as attractive targets for their total syntheses.



OP-2

SrSn_{1-x}Fe_xO_{3- δ} (x=0-0.2) Perovskite Oxides as Promising Functional Materials for Oxygen Sensor

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Abstract: Cubic phase (S.G.: P23) of iron substituted strontium stannate, $\text{SrSn}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$ ($x = 0, 0.05, 0.1, 0.15$ and 0.2) were prepared by solid state reaction method. Linear decrease in lattice parameter with iron (Fe) substitution was observed using powder X-ray diffraction method. Electrical conductivity measured on bulk pellets of the above compositions using AC impedance spectroscopy shows that this functional material is a mixed ion & electron conductor (*MIEC*) and the conductivity increases with the Fe dopant concentration. The activation energy (E_a) deduced from their Arrhenius plots are in the range of $0.3 - 0.5$ eV which implies that the mechanism of electrical conduction is same for all the compositions. X-ray photoelectron spectra show a divalent state for Sr, tetravalent state for Sn and a divalent state for oxygen irrespective of the composition leaving only Fe responsible for the increase in conductivity. Mössbauer spectroscopy studies reveal that Fe-ions in tetravalent, trivalent and divalent states with their relative proportion remain more or less same across the compositions. The increase in conductivity is mainly due to Fe^{3+} and/or Fe^{2+} ions because the isovalent Fe^{4+} substituted for Sn^{4+} do not contribute to changes in electrical conductivity as SrSnO_3 being an insulator with all Sn-ions in +4 valence state. Oxygen partial pressure dependence electrical conductivity studies of $\text{SrSn}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$ ($x = 0, 0.05, 0.1, 0.15$ and 0.2) shows that $\text{SrSn}_{0.9}\text{Fe}_{0.1}\text{O}_{3-\delta}$ and $\text{SrSn}_{0.85}\text{Fe}_{0.15}\text{O}_{3-\delta}$ exhibit significant change in conductivity as function of oxygen partial pressure and have the potential to be tailored/engineered as percentage level oxygen sensors. Of these two compositions, $\text{SrSn}_{0.85}\text{Fe}_{0.15}\text{O}_{3-\delta}$ has less interference from moisture and therefore a more promising material

OP-3

Modulated Triple-Material Nano-Heterostructures: Scope and Challenges

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Abstract: For efficient charge separations, multi-material hetero-nanostructures are being extensively studied as photocatalysts. While materials with one heterojunction are widely established,² the chemistry of formation of multijunction heterostructures is not explored. This needs a more sophisticated approach and modulations. To achieve these, a generic multistep seed mediated growth following controlled ion diffusion and ion exchange is reported which successfully leads to triple-material hetero-nanostructures with bimetallic-binary alloy-binary/ternary semiconductors arrangements. Ag_2S nanocrystals are used as primary seeds for obtaining AuAg-AuAgS bimetallic-binary alloyed metal-semiconductor heterostructures via partial reduction of Ag(I) using Au(III) ions. These are again explored as secondary seeds for obtaining a series of triple-materials heterostructures, AuAg-AuAgS-CdS (or ZnS or AgInS_2), with introduction of different divalent and trivalent ions. Au controls growth of triple-materials heterostructure in a unique way by manipulating metal-ligand binding energy.

OP-4

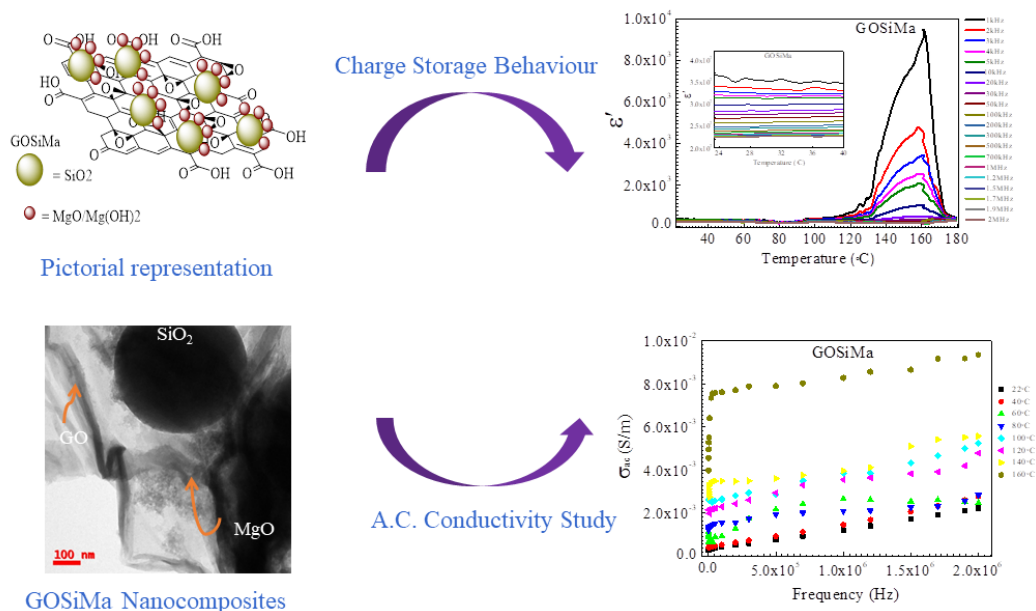
Spherically overlapped SiO₂@MgO NPs on GO sheet and effect on dielectric behaviour

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Abstract: This work aims to design graphene oxide-based silica@magnesium oxide (GO-SiO₂@MgO) / (GOSiMa) hybrid nanocomposite through a green sol-gel technique from naturally abundant precursors like Carbon-based GO and magnesium chloride (MgCl₂) and chemically modified tetraethyl orthosilicate (TEOS). The physical, chemical and morphological study of designed hybrid nanocomposites is investigated by several experiments including TEM, FESEM, EDAX, FTIR, XRD, DLS, and BET. The cyclic voltammetry (CV) behaviour is studied at both N₂ and O₂ atmosphere and found to be observed with a significant result using Ag/AgCl electrode as a reference. An effective surface area of 107.6 m²/g with an average porosity value of 97.86 Å is observed from the BET experiment providing an important factor for the enhanced dielectric behaviour. The dielectric study has shown dielectric constant/permittivity ϵ' from 10² up to 2.5 × 10⁴ with the minimal permittivity loss ϵ'' of $\leq 10^2$ at all range of temperature 22-185 °C with the 10³ - 10⁶ Hz frequency range. The effect of polarization, structural orientation and atomic rearrangements are the prime factors for the enhancement of the dielectric constant. Conductivities (σ_{ac}) of this hybrid nanocomposite are measured as 8 × 10⁻³ S/m in the low-frequency region at 1 kHz and 1 × 10⁻² S/m at a high-frequency region of 2 MHz at a temperature of 160 °C for proving the hybrid nanocomposites as a potential power electronics candidate for application in the charge storage device. The current work emphasized the dielectric and charge storage behaviour [1, 2] of the prepared hybrid nanocomposite in a safe, cost-effective and green method.



OP-5

Impact of Heteroatom Substitution on Photophysics of Dual-State Emissive 2-(2'-hydroxyphenyl)benzazole Dyes

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Abstract: The excited state intramolecular proton transfer (ESIPT) of 2-(2'-hydroxyphenyl)benzimidazole derivative (bis-HPBI), has been studied in different solvents. Unlike 2-(2' hydroxyphenyl)benzimidazole, it shows exclusive ESIPT even in protic solvents. Though bis-HPBI has two HPBI units, the tautomer emission of bis-HPBI is due to only a single proton transfer. The experimental studies and theoretical calculations corroborate the finding. However, its thiazole analogue (bis-HPBT) is insoluble in most of the organic solvent and aqueous medium. Owing to its good solubility in THF and insolubility in H₂O, the nanoparticles of bis-HPBT prepared in THF/H₂O mixture and the optical behaviour of nanoparticles were explored.²

OP-6

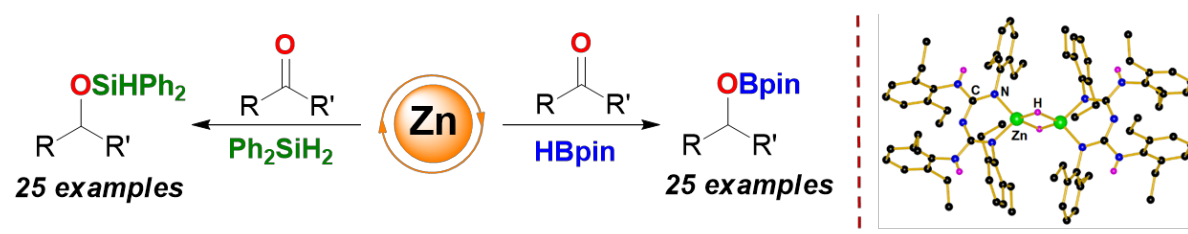
CBG Zinc Hydride: Synthesis, Reactivity, and Catalysis towards Hydrofunctionalization of Ketones

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Abstract: A popular NacNac or β -diketiminato analogue, conjugated bis-guanidinate (CBG) stabilized and well-defined dimeric zinc hydride **1**, [LZnH]₂; [L = {(ArNH)(ArN)-C=N-C=(NAr)(NHAr)}]; Ar = 2,6-Et₂-C₆H₃] has been reported.^[1] Next, A series of structurally characterized Zinc (II) complexes [e.g., Formamide, Amide, and Alkoxides] has been synthesized from highly reactive zinc hydride complex, **1**.^[2,3] Further, we report that the earth-abundant, cheaper, sustainable zinc catalyzed the hydrofunctionalization of ketones to alcohols. This catalyst covers a broad substrate scope, including inter- and intramolecular chemoselectivity.^[4]



- ✓ **Wide substrate scope**
- ✓ **Excellent yield**
- ✓ **Low catalyst loading**
- ✓ **Intermolecular chemoselectivity**
- ✓ **Solvent free, Atom economical**
- ✓ **Sustainable catalysis**

OP-7

Smallest Shannon Radii Transition Metal Ion Ni(II) for Stabilizing α -CsPbI₃ Perovskite Nanocrystals

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Abstract: Lead halide perovskite nanocrystals are recently emerged as one of the most efficient nanomaterial emitters having all visible color tunable emissions. However, the phase sensitivity of red emitting α -CsPbI₃ nanocrystals remained the major concerned. Even though several reports already established with near unity photoluminescence quantum yields, but their phase and optical stability in ambient exposure had always some limitations. Ni(II) ions, having smallest transition metal Shannon radii were explored for B-site doping in red emitting α -CsPbI₃ nanocrystals (**fig. 1a**).

This successfully stabilized the cubic phase and retained the intense emission of nanocrystals for nearly two months (**fig. 1b**). The photoluminescence quantum yields also obtained ~80 % for the ~1% doping (atomic percentage). Being smallest ion, the halide octahedra in the perovskite lattice were expected to provide high restrain ability towards δ -CsPbI₃. Comparing with post synthesis iodide treatments, the importance of doping in high temperature reaction was discussed. With varying the doping concentration, its impact on the stability of the nanocrystals is also reported. Finally, these doped nanocrystals were explored for photovoltaic devices and showed comparable efficiency (9.1%) to different other similar doped nanocrystals.

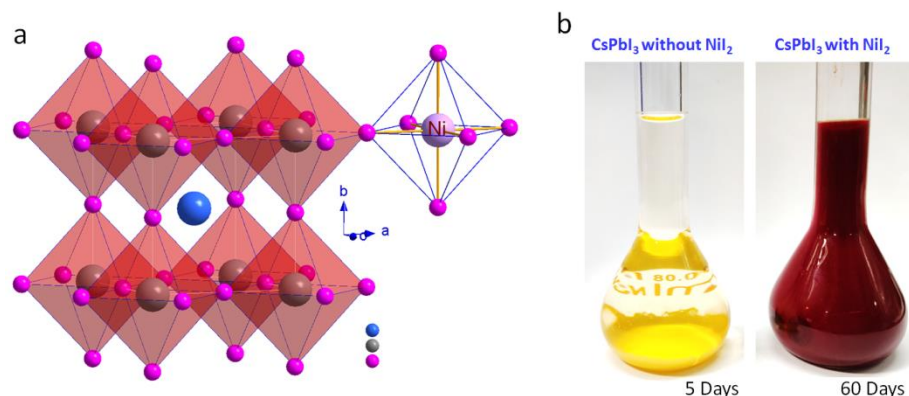


Fig. 1. (a) Atomic model showing Ni(II) in Pb-site of the perovskite α -CsPbI₃ crystal. (b) Digital images of undoped and Ni (II) doped CsPbI₃ dispersed nanocrystals solution after 5 and 60 days respectively.

OP-8

Ultrasonic Investigation of Different Electrolytes In Aqueous Dimethylsulphoxide Medium

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Abstract: The density (d), ultrasonic velocity (U) and viscosity (η) have been measured for electrolytes like potassium chromate, sodium chromate, and sodium thiosulphate in aqueous solution of dimethyl sulphoxide (DMSO) at 293K, 298K, 303K, 308K and 313K. By using the experimental data the other parameters like adiabatic compressibility(β), relative change in adiabatic compressibility($\Delta\beta/\beta_0$), change in adiabatic compressibility($\Delta\beta$), apparent molal volume (Δv), apparent molal compressibility (Δk), intermolecular free length (L_r), specific acoustic impedance(Z), limiting apparent molal compressibility (Δk_0), limiting apparent molal volume (Δv_0) and their

constants(S_k , S_v) have been calculated. The results obtained from above mentioned parameters are helpful to determine the solute-solute and solute-solvent interactions. With increase in concentration ultrasonic velocity increases as the structure is more closely packed. The decrease in adiabatic compressibility indicates the presence of strong bonding between the solute and the solvent. The negative value of apparent molal volume proves more electrostrictive solvation throughout the system. The negative value of apparent molal compressibility indicates strong solute-solvent interactions. The positive value of S_v provides information on strong solute-solute interaction. The higher apparent molal compressibility values of sodium chromate than those of potassium chromate and sodium thiosulphate confirms its more effective structure making behavior

OP-9

Developing Hybrid Aqueous Na-ion Capacitors by Electrodes Synthesized in Facile Electrochemically Exfoliated Method

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Abstract: The electrochemical energy storage devices (EESD) such as batteries and supercapacitors have been relied upon the ability to store the charge in the wide potential region with high Coulombic efficiency and long-term stability. However, transition metal oxides are well known, for their high theoretical specific capacity but suffer from low electronic conduction and capacity fading during cycling. To address these shortfalls metal oxides are usually, embedded within a conductive carbon-based matrix. The use of graphene would afford easy pathway for electron movement and increases the surface area for higher interaction of active electrode materials with electrolyte. Subsequently, graphene-based transition metal oxides composites have attracted active research pursuits in synthesizing the low cost effective electrode materials for EESD. Additionally, the few layers of graphene and metal oxides adorned on graphene as electrode materials can be generated by electrochemical exfoliation methods easily in less time and less hazardous chemicals. In this context, highly exfoliated graphene and MnO_2 @Graphene composites were developed by economic approach with an aim to achieve improved performances and scaling up for mass production. Further, the materials were tested as electrodes in aqueous Na-ion capacitors. The details of this experimental

work and its outcome will be presented. Such scheme could serve as precedent for development of potential electrode materials for EESD.

OP-10

Variation in metal elements from soil to leaf and their possible role in silk synthesis in tropical tasar silkworm *Antheraea mylitta* Drury

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Abstract: Synthesis of silk by sericigenous insects is a complex process that involves a cascade of biochemical pathways involving different enzymatic system. The natural spinning process in silkworm involves the conformation transition of the liquid silk protein present in the silk gland to make fiber. This conformational transition is influenced by many factors, and change in the metallic ion concentration is one of them. *Antheraea mylitta* the tropical tasar silkworm produces Vanya silk of commercial importance, so it is reared over a large area covering eastern and central India. Due to the life cycle strategy of tasar silkworm to different rearing seasons, marked difference have been reported in the quantity of silk produced by silkworm along with regional variation. A study was conducted to find out the relationship of soil and leaf micronutrients with the silk yield of tasar silkworm reared in two ecologically different locations on two host plants over rainy and autumn rearing seasons. The study revealed significant variation in silk traits both in place and season with highest values recorded at Kendujuani in the cocoons formed on *Terminalia tomentosa*. Silk filament length was significantly more (855 m) in autumn crop than rainy (512 m) at Kendujuani, while the trend was similar but with significantly less value ($P < 0.01$) at Chandua. Among the nine micronutrients studied, Mg, Ca, Na and Zn were found to be significantly in higher concentration in host plant leaves during autumn crop ($P < 0,05$) with highest value in Kendujuani ($P < 0.01$) whereas no significant difference recorded for S, B, Fe, Mn and Cu. There was significant variation in nine soil micronutrients in two places over two rearing seasons. Since the larval feeding period during autumn crop is more (45 days) in comparison to rainy crop (28 days), the selective accumulation of different nutrients by silkworm and their role in silk synthesis and associated physiological processes is preminent. Further, the role of Mg^{2+} , Cu^{2+} , Zn^{2+} , Ca^{2+} and K^+ in the protein conformation transition and helical conformation to β -sheet of silk along with associated factors is discussed in this paper.

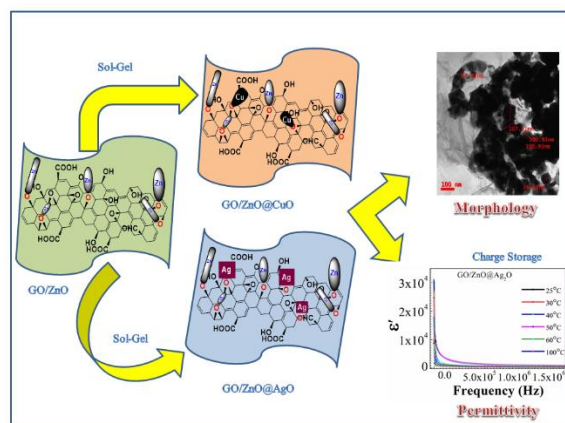
Graphene oxide embedded by morphologically varying cubical and quasi-spherical like ZnO@Metal Oxides nanocomposites and its study on dielectric behaviour

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Abstract: This work aims to highlight the significant dielectric permittivity and electronic properties of GO-based ZnO, CuO and Ag₂O mixed ternary nanostructured composite via a modified sol-gel based hetero-selection synthesis approach. The morphology of the designed hybrid nanocomposites played a remarkable factor in the development of dielectric properties. The synthesized material is studied in detail by using sophisticated instruments like TEM, FESEM, FTIR, XRD, Zeta and BET. The dielectric behaviour is studied at different ranges of frequency 10³ Hz to 2×10⁶ Hz and temperature of 25°C-200°C. The permittivity constant, loss and σ_{ac} conductivities (at 200°C) for GO/ZnO@Ag₂O are found to be $5 \times 10^2 - 3.1 \times 10^4$, ≤ 4 and 1×10^{-3} S/m and 1.2×10^{-2} S/m respectively at all ranges of given frequency and temperature. The presence of highly quantified oxygen moiety, dipolar formation, interfacial polarization and atomic arrangements became responsible for the enhancement of dielectric permittivity and minimal loss of such composites. Similarly, the highest permittivity (60°C) and σ_{ac} conductivities (at 200°C) of GO/ZnO@CuO are observed to be 2.6×10^3 and 2.25×10^{-4} S/m at 1 kHz respectively. This value is found to be dependent on frequency and increases linearly with the increase in frequency. The specific surface area of such composites is found to be better than free GO/ZnO composites, with a moderate average porosity value and also partially participated for the dielectric property growth. The present work provides an interesting morphology and can be applied for charge storage uses.



Conformational Polymorphs and Solvates of 1-(6-aminopyridin2-yl)-3-phenylthiourea

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Abstract: Three conformational polymorphs and two solvates of an asymmetrical N, N'-disubstituted thiourea derivative namely, 1-(6-aminopyridin2-yl)-3-phenylthiourea (PTU) have been reported here. In all the polymorphs and solvates, the PTU molecules self-assemble into dimers in the solid state, via two complementary N-H...S bonds resulting the formation of $R_2^2(8)$ -type of H-bond motif. The two PTU molecules in these dimers interact with each other in a head to tail fashion. Furthermore, the PTU molecule adopts trans, cis- conformation with an intramolecular N-H...N interaction in all the crystals. However, the orientation of the aminophenyl ring with respect to the phenyl ring plays crucial role in the solid state packing of the polymorphs and solvates. Additionally, three polymorphs are distinguishable by C-H... π , N-H... π and π ... π interactions. The polymorph PTU-1 crystallizes in P-1 space group with $Z'=2$, whereas the polymorphs PTU-2 and PTU-3 crystallizes in Pbcn and R-3 space group respectively, with $Z'=1$. On the other hand, the solvate PTU-DMSO crystallize in P2₁/c with 1:1 host-guest ratio, and PTU-Morpholine exists in P-1 space group with 2:1 host guest ratio. Hirshfeld surface analysis was carried out to compare the intermolecular interactions in the three polymorphs and two solvates of the title compound. The 2D fingerprint analysis of each of the polymorphs reveals that besides the H...H interactions, C...H and S...H interactions contribute more to the generation of polymorphs. The contribution of C...H interactions in both PTU-2 (31.6%) and PTU-3 (32.1%) are much higher than that of any molecule in PTU-1 (19.8% and 23% for Molecule A and B respectively). Additionally, a tiny amount of π ... π interaction was observed (C...C interaction, 4.5%) in polymorph PTU-1, which was absent in PTU-2 and PTU-3.

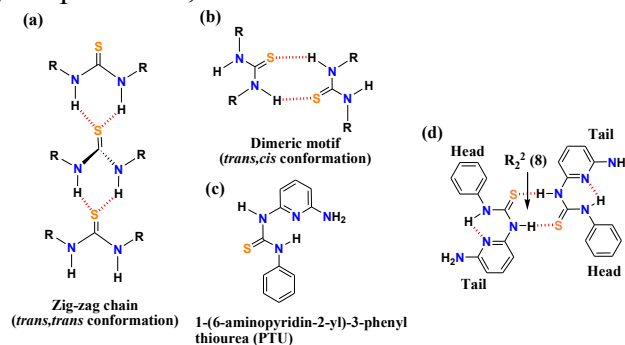


Figure 1: (a) and (b) Hydrogen-bonding motifs typically observed for disubstituted thiourea in the solid state; (c) Structure of 1-(6-aminopyridin2-yl)-3-phenylthiourea (PTU); and (d) Formation of dimers through $R_2^2(8)$ -type of cyclic motif via two complementary N-H...S interactions.

Poster Presentations