POSTER-1

ENHANCEMENT OF PHOTOCHEMICAL HETEROGENEOUS WATER OXIDATION BY MANGANESE BASED SOFT OXOMETALATE IMMOBILIZED ON GRAPHENE OXIDE MATRIX

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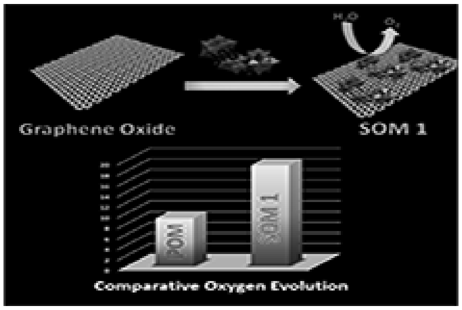
Development of efficient and oxidatively stable molecular catalysts having abundant transition metals at active site is an immediate challenge to synthetic chemists in order to photochemically split water into clean fuels oxygen and hydrogen to serve ever-increasing energy demand. Herein we report a soft-oxometalate (SOM)-based heterogeneous photocatalytic system which effectively performs water oxidation giving oxygen. In the present work we placed a double sandwich type manganese-based molecular polyoxometalate (POM), $Na_{17}[Mn_6P_3W_{24}O_{94}(H_2O)_2].43H_2O$ on an electro active graphene oxide matrix and synthesized a new SOM $Na_{17}[Mn_6P_3W_{24}O_{94}(H_2O)_2].43H_2O$ @ graphene oxide] **1** and performed water oxidation with it. The efficiency of the photocatalytic water oxidation by SOM **1** is almost double than in the case of $Na_{17}[Mn_6P_3W_{24}O_{94}(H_2O)_2].43H_2O$ alone. The rationale lies in the electron accepting nature of the graphene sheets which effectively relay the electrons generated in the water oxidation reaction, thus facilitating the forward reaction and increasing the oxygen yield.



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POSTER-2

PORE WALL FUNCTIONALIZED MIXED LIGAND METAL ORGANIC FRAMEWORKS AND THEIR APPLICATION IN SELECTIVE CARBON DIOXIDE ADSORPTION

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The efficient storage and separation of CO_2 from industrial emissions under atmospheric pressure has attracted significant research interest due to the alarming rise of carbon dioxide concentration in the atmosphere. Carbon dioxide is one of the major greenhouse gases contributing to global warming leading to various environmental disorders. So concerns about global warming, there is an immense interest in removing CO_2 from exhaust streams of fossil fuel combustion to combat the greenhouse gas effect. For flue gas, the high temperature and low CO_2 partial pressure make this separation particularly challenging. Separations involving CO_2 are also important in a variety of other applications such as upgrading of natural gas and hydrogen purification. Adsorption and membranebased separation technologies hold many advantages for these problems, particularly because of their low energy requirements. MOFs exhibits tunable architecture as well as the functional pore wall through judicious design and selection of organic ligands, which shows well CO_2 adsorption selectively over other gases. Hence we are interested to present the syntheses and characterization of a series of mixed ligand metal organic frameworks (MOFs) by using different N,N′-donor ligands and aliphatic and aromatic dicarboxylates as a coligand; which have different polar functionality (−N=N−, – CH=N–N=CH– and –CMe=N–N=CMe–, $-NH_2$ group) in their pore surface and high void volume in their dehydrated forms to accommodate CO_2 selectively in the channels. Enhancement of CO_2 selectivity with incorporation of hydrophobic groups in the pore wall would also be presented. Compounds containing hydrophobic group adsorb less amount of water in low pressure, which is very important since considerable amount of water (7-9%) along with CO_2 and N_2 is present in the flue gas.

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POSTER-3

LIQUID CRYSTAL FOR COLON TARGETED DRUG DELIVERY

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Abstract

The lyotropic liquid crystal of food grade capable of responding pH variations that have a reversible switch in both the structure and physical properties. In the presence of water at 37°C and 150 mM ionic strength, the monolinolein and the linoleic acid have the capability to reversibly change from continuous lm3m cubic phase to a H_2 reverse columnar hexagonal phase. When changing the pH from neutral (pH 7) to acidic (pH 2) conditions. The system is demonstrated on a model hydrophilic drug Phloroglycinal by both release and diffusion studies at different pH, followed by ultraviolet −visible (UV−vis) spectroscopy.

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Acknowledgement

This is a review article prepared by us to study and to make advancement in the novel drug delivery system with the help of liquid crystals and to bring new dimension in the application of crystal in pharmaceuticals.

POSTER-4

ANION DEPENDENT STRUCTURAL DIVERSITY OF CADMIUM(II) COMPLEXES: SYNTHESIS, CRYSTAL STRUCTURES, SUPRAMOLECULAR INTERACTIONS AND LUMINESCENCE PROPERTIES

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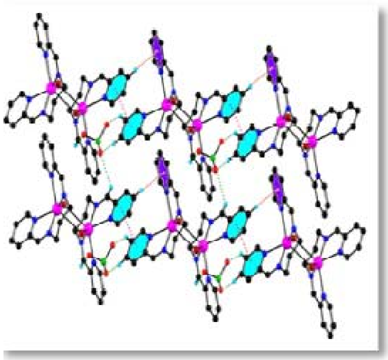
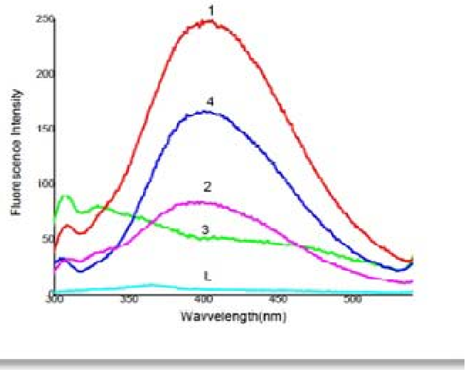
Portugal Four photoluminescent Cd(II) complexes, $[Cd_2(L)_2(\mu\text{-}Cl)_2](ClO_4)_2$ (**1**), $[Cd_2(L)_2(\mu\text{-}Br)_2](ClO_4)_2$ (**2**), $[Cd(L)I](ClO_4)$ (**3**) and $[Cd(L)(NCS)_2]$ (**4**), derived from the tetradentate ligand (**L** = N,N'-bis(2-pyridylmethylene)-1,3-propanediamine), have been synthesized and characterized by various spectroscopic techniques, elemental analysis and X-ray crystallography. Complex **1** and **2** are chloro- and bromo-bridged dinuclear complexes whereas complex **3** and **4** are mononuclear iodo and thiocyanato complexes, respectively. The stabilization of the crystal lattices is maintained by interesting, relatively strong hydrogen bonds and π–π interactions which lead to various supramolecular architectures.



Crystal structure



Luminescence property

POSTER-5

ANALYSIS OF HALOGEN MEDIATED HYDROGEN BONDING IN DINUCLEAR MN(III) COMPLEXES

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The studies of polynuclear coordination complexes of various nuclearities has attracted a great deal of attention over many years due to their potential applications in numerous areas including coordination polymer, polyoxometalates (POMs), catalysts , single-molecule magnets (SMMs), fluorescence and so on [1]. Specially, the discovery of single molecule magnet (SMM) behaviour has motivated synthetic chemists to focus on producing coordination clusters which may provide examples of functional materials with enhanced and specified properties [2].

Two new halogen mediated dinuclear manganese(III) complexes have been synthesized from a single pocket ligand 4-bromo-2-[(3-hydroxy-propylimino)-methyl]-phenol (H_2L) . The ligand and the complexes were characterized by conventional methods, e.g., FT-IR , ^1H NMR, CHN analysis, ESI-MS and UV-Vis spectroscopy. The single crystal X-ray crystallographic study reveals that both the compounds $[Mn_2^{III}(L)_2Cl_2(MeOH)_2]$ (**1**) and $[Mn_2^{III}(L)_2Br_2(MeOH)_2]$ (**2**) are isostructural, crystallized in monoclinic space group $P2_1/c$. The detail crystallographic analysis and Hirshfeld surface analysis reveals that the structures are made with halogen mediated H- bonding which is the basis of the 3D supramolecular interaction in both the complexes. The oxidation state assignment for the Mn-ions are made using charge balance considerations, interatomic distances [Mn-N and Mn-O] , Jahn-Teller distortion and BVS calculations. The BVS calculation data are also a good fit for the +3 oxidation state of the Mn centres.

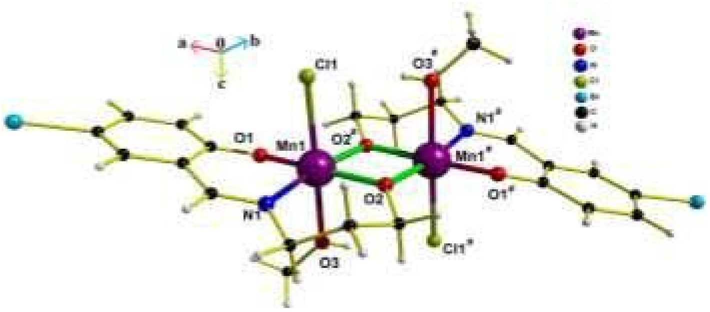

Figure 1. Molecular structure of $[Mn_2(L)_2Cl_2(MeOH)_2]$ (**1**).

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Acknowledgement:

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POSTER-6

VALENCE TAUTOMERISM INDUCED NUCLEOPHILIC IPSO SUBSTITUTION IN A COORDINATED TETRABROMOCATECHOLATE LIGAND AND DIVERSE CATALYTIC ACTIVITY MIMICKING THE FUNCTION OF PHENOXAZINONE SYNTHASE

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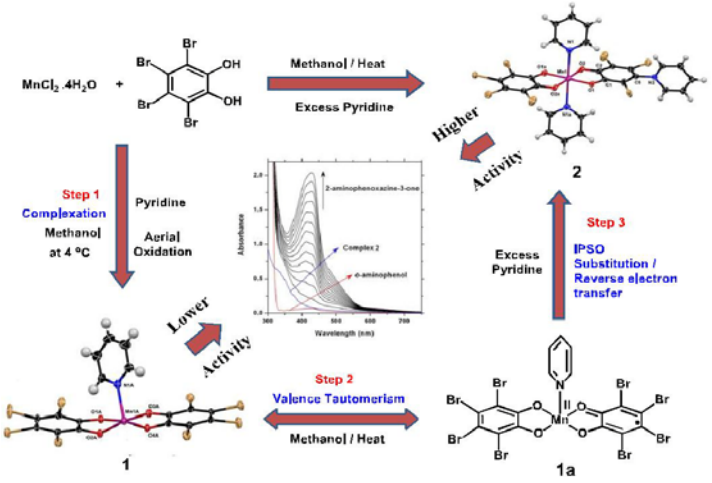
Two new manganese(III) complexes, [pyH][Mn($Br_4Cat)_2$(py)] (**1**) and [Mn(Br_4Cat)(Br_3pyCat)$(py)_2$] (**2**), where py is pyridine, Br_4CatH_2 is tetrabromocatechol and $Br_3pyCatH_2$ is 3,5,6-tribromo-4-pyridiniumcatechol, derived from redox 'noninnocent' bromo-substituted catecholate ligands are Synthesized. Both complexes were characterized by various spectroscopic techniques in addition to the single crystal X-ray crystallography, and the electrochemical behavior of these complexes was investigated by cyclic voltammetry. Variable temperature UV–vis spectral studies for complex **1** reveal an unprecedented observation in which a dramatic increase of the ligand-to-metal charge transfer band at 592 nm associated with concomitant change in color of the solution from olive-green to dark-green is noticed with increase in temperature. This unprecedented spectral feature is consistent with the formation of a new species **2** in which valence tautomerism induced aromatic nucleophilic substitution of a tetrabromocatecholate ligand by pyridine is observed. To the best of our knowledge, the nucleophilic aromatic substitution of tetrabromosemiquinone by pyridine to generate this pyridinium-containing catecholate ligand is the first example of valence tautomerism induced nucleophilic ipso substitution by a nitrogen containing ligand. Although the electrochemical behavior of both complexes is similar, the probable role of a positive charge on the ligand backbone has been discussed in order to justify the significantly higher catalytic activity of complex **2** over complex **1**



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POSTER-7

SYNTHESIS, CHARACTERIZATION AND CATALYTIC PROPERTIES OF SOME MULTINUCLEAR COPPER(II) COMPLEXES

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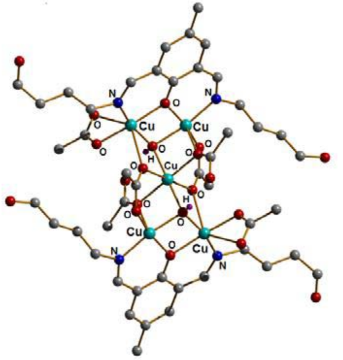
Transition metal complexes of Schiff-base ligands have become center of attraction to the researchers over few decades because of their diverse structures and their applications in various fields *e.g.* magnetism, biology, and catalysis (1-3). Polynuclear copper complexes with N,O donors have been used as catalysts in different organic transformations, *e.g.* epoxidation, sulfoxidation, olefin aziridination, atom transfer radical addition (ATRA) (2). Even though copper(II) Schiff-base complexes are known for a long time, they were barely used as catalysts in olefin epoxidation reactions in homogeneous medium.



Here synthesis, characterization and catalytic properties of four tetranuclear [$Cu_4(O)(\mathbf{L^{\mathit{n}}})_2(CH_3COO)_4$] (**$1.3H_2O.CH_3CN$**, **2**, **$4{\cdot}CH_3CN$** and **5**) and one pentanuclear [$Cu_5(OH)_2(\mathbf{L^3})_2(CH_3COO)_6$] (**$3{\cdot}H_2O$**) with N_2O-donor Schiff-base ligands are being reported here, where **HL^1** = 4-methyl-2,6-bis(2-hydroxyethylimino methyl)phenol for **1**, **HL^2** = 4-methyl-2,6-bis(3-hydroxypropyliminomethyl)phenol for **2**, **HL^3** = 4-methyl-2,6-bis(4-hydroxybutyliminomethyl)phenol for **$3{\cdot}H_2O$**, **HL^4** = 4-methyl-2,6-bis(5-hydroxypentyl iminomethyl)phenol for **$4{\cdot}CH_3CN$** and **HL^5** = 4-methyl-2,6-bis(6-hydroxyhexyliminomethyl)phenol for **5**. These complexes have been characterized by elemental analysis, FT-IR, UV-vis spectroscopy and single crystal X-ray diffraction study. X-ray analysis reveals that complexes **$1.3H_2O.CH_3CN$**, **$4{\cdot}CH_3CN$** and **5** are μ_4-oxido-bridged tetrameric copper(II) complexes. Pentanuclear complex, **$3{\cdot}H_2O$**, has been found to have two μ_3-hyoxido bridging ligands which connect three copper atoms. These complexes have been used as the catalysts for epoxidation of cyclohexene, styrene, α-methyl styrene and *trans*-stilbene in acetonitrile in the presence of *tert*-butyl hydroperoxide as the oxidant.

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POSTER-8

SYNTHESIS, CHARACTERIZATION AND CATALYTIC ACTIVITIES TOWARDS EPOXIDATION OF OLEFINS OF TWO DINUCLEAR COPPER(II) COMPLEXES

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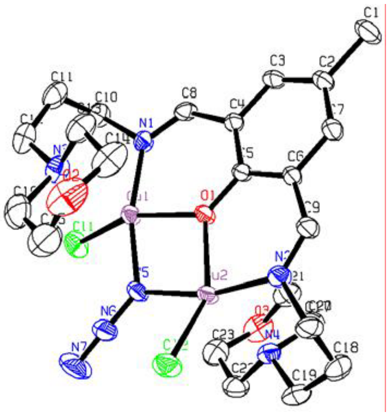
Multinuclear transition metal complexes of Schiff-base ligands have drawn attention of the researchers over few decades because of their diverse structures and their applications in various fields *e.g*. magnetism, biology, and catalysis (1-4) *etc*. Copper(II) complexes have been used as catalysts in different organic transformations, *e.g* . epoxidation, sulfoxidation, olefin aziridination, atom transfer radical addition (ATRA) (2,3). Even though copper(II) Schiff-base complexes have been well known for a long time, they have been less employed as catalysts in olefin epoxidation reactions in homogeneous medium. Epoxidation of olefins is an important reaction in organic chemistry because epoxides are versatile building blocks for the synthesis of many bioactive molecules and organic fine chemicals (5).



Two copper(II) complexes, $[Cu_2(\mathbf{L}^1)Cl_3].2H_2O$ (**1**) and $[Cu_2(\mathbf{L}^2)(N_3)Cl_2]$ (**2**) where $\mathbf{HL}^1$=4-methyl-2,6-bis ((2-morpholinoethylimino)methyl)phenol and $\mathbf{HL}^2$=4-methyl-2,6-bis((3-morpholinopropylimino)methyl) phenol have been synthesized and characterized by elemental analysis, various spectroscopic methods, TGA and single crystal X-ray diffraction analysis. Single crystal X-ray diffraction analysis reveals that in both the complexes, two copper atoms are linked by phenoxo oxygen atom and a bridging ligand, namely chloride and azide, respectively. These complexes have been used as catalyst for the epoxidation of cyclohexene, styrene, α-methylstyrene, *trans*-stilbene and norbornene using *tert*- butyl hydroperoxide as the oxidant in acetonitrile under mild conditions. All of the substrates undergo conversion to produce respective epoxide as the major product.

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POSTER-9

TUNING OF STRUCTURAL TOPOLOGY OF DNA INTERACTING COORDINATION SOLIDS OF BIOACTIVE PHENATHROLINE INVOLVING BENZOATES AND SUBSTITUTED BENZOATES

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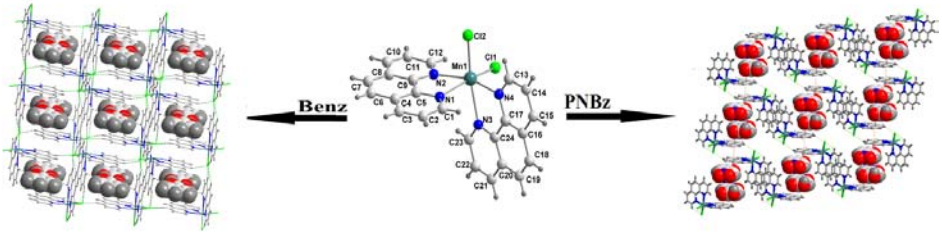
Abstarct

Research on transition metal complexes with hetero aromatic N-donor chelating ligands has been of great interest in the past decade. The carboxylate group in the organic ligands has been widely used for construction of a number of metal–organic frameworks because of their versatility in coordination modes and their ability to form robust and flexible hydrogen-bonding networks.[1] Transition metal complexes of 1,10-phenanthroline (phen) are also widely employed in studies of DNA in view of their applications in several research areas, including bioinorganic and biomedicinal chemistries as well.[2] Herein, a few new supramolecular metal-organic compounds involving phenanthroline, benzoate and substituted benzoates have been synthesized and characterized. In the precursor **1**, two Phen ligands are coordinated orthogonally to the metal centre Mn(II) and fulfilled its octahedral geometry with two more Cl coordination. The benzoic acid (Benz) hydrogen bonded dimer is encapsulated by inversion related two hosts with cavity size 7.658Å × 11.595Å (Phen centroid to centroid) without subtracting π-distances in **2** whereas in **3** the p-nitrobenzoic acid (PNBz) hydrogen bonded dimer is encapsulated by inversion related two hosts with cavity size 8.524Å × 10.047Å (phen centroid to centroid). In **1**, **2** and **3** C−H···Cl, C−H···π , O−H···O and C−H···O interactions play a key role in the construction of 3D supramolecular network. These interactions have been theoretically characterized with the help of topology of electron density involving quantum theory of atoms in molecules (QTAIM). ITC study shows exothermic nature of binding to CT-DNA for **2** and **3** respectively.



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Acknowledgement
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POSTER-10

CATECHOLASE ACTIVITY OF A CO(III)- AND A NI(II)SCHIFF BASE COMPLEXES

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The ubiquitous plant enzyme catechol oxidase catalyzes exclusively the oxidation of catechols to the corresponding *o*-quinones in presence of molecular oxygen. The resulting highly reactive *o*-quinones autopolymerise to form brown polyphenolic catechol melanins, a process thought to protect the damaged tissues of the plants from pathogens or insects. Active site of catechol oxidase contains antiferromagnetically coupled (EPR silent) dicopper(II) centre at the active site.[1] In continuation to our present interest in non-copper catecholase active systems[2,3] the synthesis, X-ray structure and catecholase activity of two newly synthesized complexes $[Co(L)_3]$ (**1**) and $[Ni(L)_2]$ (**2**) [HL =2-((*E*)-(2-pyridine-2-pyridin-2-ylthio)ethylimino)methyl)phenol] (Figs. 1 and 2) will be presented. The compounds catalyze 3,5-ditertiarybutylcatechol at room temperature in methanol in presence of molecular oxygen with first order reaction kinetics, and turn over numbers for each synthetic model are 3.47568×10^3 h^{-1} (**1**) and 2.683×10^3 h^{-1} (**2**).

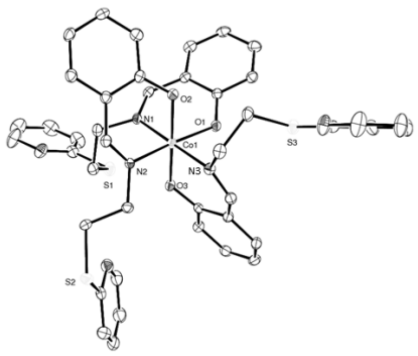

Fig 1. TEP of **1**

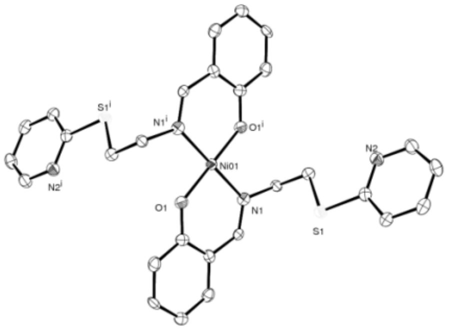

Fig 2. TEP of **2**

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POSTER-11

A CONVENIENT CHIRON APPROACH TO (4*R*,5*R*)-5-HYDROXYALKYLBUTAN-4-OLIDES AND THE CORRESPONDING 7-OXA ANALOGUES FROM D-(+)-MANNITOL VIA AN ADVANCED COMMON PRECURSOR

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5-Hydroxyalkylbutan-4-olides are widely distributed in Nature. They show diverse biological activities. One such molecule is Muricatacin. It was isolated several years ago by McLaughlin and co-workers from the seeds of *Annona Muricata*. Both the enantiomers are found in nature, and both exhibit the same potent cytotoxicity towards several human tumor cell lines. Another molecule, (4*R*,5*R*)-(−)-5-hydroxy-4-decanolide and its diastereoisomer (4*R*,5*S*)-(−)-5-hydroxy-4-decanolide were the first two compounds to be identified as male sex pheromone in the parasitic Hymenoptera. Some unnatural analogues of muricatacin have been also prepared and evaluated for their antitumor activities. One such molecule, 7-oxa-(−)-muricatacin was designed as a possible muricatacin bioisostere. It has been reported as a more potent and selective antitumor compound than muricatacin.

A simple, short, and general chiron approach had been achieved that gave access to not only various enantiopure (4*R*,5*R*)-5-hydroxyalkylbutan-4-olides but also their 7-oxa analogues starting from inexpensive D-(+)-mannitol via a common key intermediate. The stereochemistry inherited from C-3 and C-4 of D-mannitol was translated to the desired stereochemistry at C-4 and C-5 of the target molecules.

Using this flexible methodology, we accomplished successfully the total synthesis of naturally occurring (−) -muricatacin and (4*R*,5*R*)-(−)-5-hydroxy-4-decanolide as well as the synthesis of unnatural 7-oxa-(−)-muricatacin and a hitherto unknown γ-lactone, (4*R*,5*R*)-(−)-7-oxa-5-hydroxy-4-dodecanolide.

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POSTER-12

SUPRAMOLECULAR PACKING FEATURES OF SOME BIOLOGICALLY IMPORTANT PYRIDAZINE DERIVATIVES AND THEIR SALTS

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Pyridazines are important drug intermediates in the synthesis of several drugs such as Cefozopran, Iclusig (ponatibib), Vardenafil etc. These drugs are used for the treatment of pneumonia, sepsis, urinary and abdominal infections [1-2]. Because of the increasing interest in the biological and chemical aspects of this class of compounds, we have crystallized four salts, a solvate and a co-crystal of them and have studied their molecular geometries and supramolecular interaction patterns [3].

Our presentation would highlight the important findings on the above aspects.

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POSTER-13

SELF ASSEMBLIES IN (R)-9-(2-HYDROXY PROPYL) ADENINE AND ITS SALTS

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Studies on antiviral drugs towards HIV-1 reverse transcriptase reveals that drugs containing adenine moiety with N^9-aliphatic side chain with two carbon length has no antiviral activity and its activity starts from aliphatic chain with three carbon (propyl derivative) length. It has been reported that 3-hydroxy propyl adenine has moderate activity towards HIV-1 Reverse transcriptase[1]. The present work discusses about a derivative of adenine namely (R)-9-(2-hydroxy propyl) adenine (HAP) (I) and its nitrate (HPANA) (II) and perchlorate (HPAPA) (III) salts. The HPA (I) crystallizes with one molecule in the asymmetric unit. The asymmetric unit of HPANA (II) salt built by one HPA cation (N^1 protonation) and one nitrate anion. The HPAPA(III) salt consists of one diprotonated HPA cation (N^1 and N^7 protonation) and two perchlorate anion in 1:2 ratio. The supramolecular self assemblies of HPA and its salts construct through several (N-H...O, O-H...N, N-H...N and weak C-H...O) hydrogen bonds[2] and aromatic π-π stacking/anion-π interactions[3]. The cumulative interactions generate supramolecular sheet like architecture.

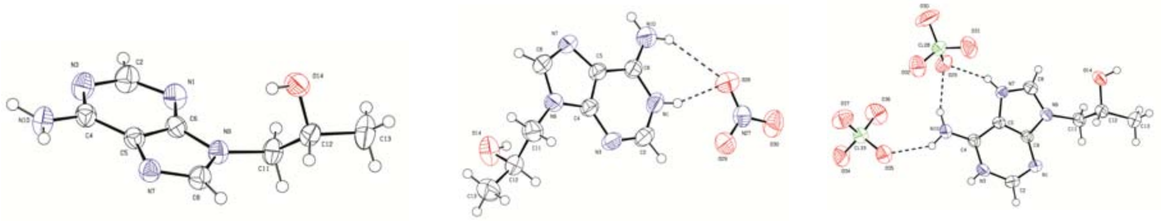

Figure 1. ORTEP view of the compounds (I-III)

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POSTER-14

Molecular Dynamics of Kv1.3 Ion Channel and Structural Basis of Its Inhibition By Scorpion Toxin-OSK1 Derivatives

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Kv1.3 is one of the widely distributed *Shaker* type voltage gated potassium channel which performs the outward flow of K^+ ions in excitable cells. In immunological synapse, Kv1.3 plays a pivotal role in antigen dependent activation and proliferation of lymphocytes along with the $K_{Ca}3.1$. The up-regulation of Kv1.3 leads to several T-cell-mediated autoimmune diseases, hence considered as an attractive pharmacological drug target. Here, we have employed molecular modeling, docking and simulation techniques to examine the dynamical properties of Kv1.3 in both open and closed state conformation embedded in DPPC membrane as well as its modes of inhibition against the popularly known scorpion venom OSK1 and its three mutant analogues. The Kv1.3 in open conformation took comparatively more time to get stabilized than the closed state. Both conformations ascertain their stability and the transition between closed to active states is more consistent with the paddle model of channel gating. The binding modes of channel-toxin complexes are well established by identifying strongly interacting amino acids lining at their polar surfaces. Our findings suggest that, two mutant derivatives OSK1-K16,D20 & OSK1-P12,K16,D20 have increased inhibitory potency against Kv1.3 . We also pointed out some particular residues responsible for binding of OSK1 with Kv1.3 over other *Shaker*-type ion channels. We believe the insights came from Kv1.3-OSK1 interaction will be valuable in pharmacological studies for strategic development of both potent and selective therapeutic drugs against T-cell-mediated autoimmune diseases.

POSTER-15

SYNTHESIS, STRUCTURE AND CATALYTIC ACTIVITIES OF NI(II) COMPLEXES BEARING N_3O TETRADENTATE SCHIFF BASE LIGAND

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Abstract

Two new nickel(II) complexes $[Ni(L)Cl_2]$ (**1**) and $[Ni(L)(NCS)_2]$ (**2**) of a neutral tetradentate mono-condensed Schiff base ligand 3-(2-(2-aminoethylamino)ethylimino)butan-2-one oxime (L) have been prepared and characterized by usual physicochemical techniques e.g. elemental analyses, spectroscopic (IR, Electronic, NMR) methods, conductivity and molecular measurements. The crystal structure of complex (**2**) has been determined by using single crystal x-ray diffraction method and it suggests a distorted octahedral geometry around Ni(II) having NiN_6 coordinating atmosphere (Figure 1). The non-coordinated N–O groups on the ligand L are engaged in H-bonding interactions with thiocyanate S atoms. These H-bonding interactions lead to O--S separations of 3.132 Å and play prominent role in crystal packing. These complementary interactions in terms of H-bond donor and acceptor lead to 1D supramolecular sheet-like arrangement. The catalytic behavior of the complexes for oxidation of styrene has also been observed. The dependence of catalytic behaviour on the oxidation of styrene was studied by varying solvent, reaction temperature, reaction time and ratio of substrate to oxidant.

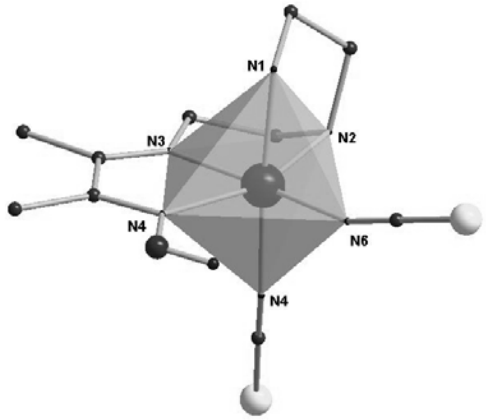

Figure 1: Neutral mononuclear Ni^{II} complex (**2**) with octahedral coordination sphere

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POSTER-16

CITRAZINIC ACID AND MELAMINE DERIVED TWO-COMPONENT HYDROGELATOR: SYNTHESIS, INTRIGUING ROLE OF REACTION PARAMETERS AND IODINE ADSORPTION STUDY

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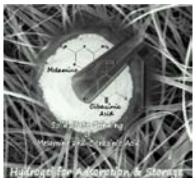
Herein, we have implemented an intimate grinding-mixing protocol (GMP) for the synthesis of a new hydrogelator from citrazinic acid and melamine. Ground mixture upon sonication, just for few second, in a suitable solvent/mixed-solvent system finally results in a gel matrix. Citrazinic acid, is decorated with ureidopyrimidone functionality and melamine is enriched with amino-pyridine functionality. Therefore, the necessary non-covalent interactions (like hydrogen bonding and π-π stacking) become a part-and-parcel, bringing a nanofibrous gel material in existence. A thorough and complete solvent dependent gelation investigation suggests that water must be present as the sole solvent or one of the members of other mixed-solvent system to successfully result in gel formation. The gel shows entangled network morphology. Different micro-analytical studies (FTIR, Powder XRD, FESEM, TEM, Rheology etc.) have been conducted for complete characterizations of the gel sample. Again, it is worth mentioning that here GMP plays a key role to strongly initiate and improvise solid state self-assembly. Different non-covalent interactions procure the suitable hydrogen-bonded motif which presumably propagates upon activation in solution phase after mild sonication favouring spontaneous formation of fibrous architectures. It was also noticed that without grinding, the solid state interactions are jeopardized and only partial gel structure prevails. Finally the available porosity in the gel framework and the enriched π-electron density within, make the gel a suitable host for adsorption of guest molecules. We studied the reversible adsorption-desorption equilibrium of molecular iodine within the dried-gel matrix. The guest entrapment into the host occurs both from the solution and also from gas phase iodine. The complete analysis suggests that our material presents a high storage capacity of this halogen species.



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POSTER-17

2:1 CO-CRYSTAL OF 4-NITROPHENOL AND 2,4-DINITROPHENOL WITH PIPERAZINE: A CRYSTALLOGRAPHIC STUDY

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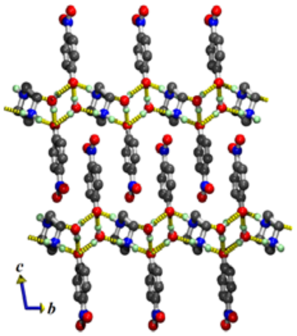
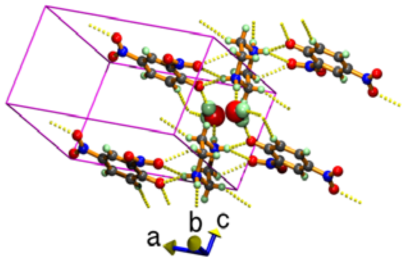
Co-crystals are crystalline solids in which at least two different molecules are assembled through the use of non-covalent interactions.[1] Among various binary and ternary co-crystals reported so far, pharmaceutical co-crystals[2] have drawn most of the attentions due to their obvious importance in medicinal chemistry. Besides this practically important class of co-crystalline materials, study of co-crystals in the general area of crystal engineering[3] is also important as it augments our knowledge regarding the design of multi-component crystalline materials with the help of non-covalent interactions.

Nitrophenols are important aromatic compounds which have many practical uses as indicator, fungicide, dye etc. Here we report the co-crystallizing behavior of 4-nitrophenol and 2,4-dinitrophenol with piperazine. The X-ray crystal structure of 4-nitrophenol with piperazine reveals that the acidic phenolic -OH group of the nitrophenol readily donate the proton to the basic piperazine. Doubly protonated piperazine molecules are involved in double NH···O hydrogen bonding with solvent water molecules as well as deprotonated nitrophenol molecules and helps in a two tear molecular assembly. X-ray crystal structure of 2,4-dinitrophenol with piperazine reveal a nearly similar role played by both the components. Presence of an additional nitro group slightly changes the organizing motif. Two tear layered assembly is prevalent in this crystal also but the π··· interaction between the nitrophenol molecules is widely different. In summary present study reveals that nitrophenol class of molecules can readily be co-crystallized with bases like piperazine where piperazine induced NH·O hydrogen bonding and solvent water molecules play important role.



4-Nitrophenol + piperazine



2-4-di-Nitrophenol + piperazine

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POSTER-18

SUPRAMOLECULAR AGGREGATION IN BTC CONTAINING CO(II) COMPLEXES

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The highly symmetrical 1,3,5-tricarboxylate (btc) ligands posses interesting features that are beneficial for the construction of versatile coordination architectures [1-2]. The multicarboxylate groups on the molecule which, when linked with metal containing units, yield a variety of polymeric and supramolecular aggregates of metal-carboxylates. While metal-btc derivatives themselves can take up diverse structural features, incorporation of auxiliary ligand can bring about substantial structural tuning which would be very relevant for many functional applications [3]. Three supramolecularly aggregated coordination solids *viz.*, $[Co_2(btc)_3.12H_2O]_n$ **1**, $[Co_3(btc)_2(dmp)_8]_n$ **2** and $[Co(bpy)_4(btc)_2(H_2O)_{10}]\cdot(bpy)\cdot4H_2O$ **3** (bpy= 4,4'-bipyridine, dmp= 3,5-dimethylpyrazole), have been synthesized and are structurally characterized. The molecular and crystal structures of these compounds were determined by X-ray diffraction analysis. The zig-zag 1D polymeric chains in **1** are bridged by btc anions wherein the metal centres adopt the octahedral coordination geometry. Compound **1** participates in exhaustive hydrogen bond formation among the chains that lead to a robust 3-D supramolecular network in the solid state. The principal building units of compound $[Co_3(btc)_2(dmp)_8]_n$ are the tetrahedral and octahedral Co(II) centres bridged by the tris-monodentate btc ligands. Each btc anion bridges two neighbouring $Co(dmp)_2$ units forming a tetrahedral geometry around the Co(II) ion that extends along the crystallographic *b*-axis. The btc anions are further connected to $Co(dmp)_4$ units forming an octahedral coordination of the metal ion in an another direction giving rise to a 2D network structure. The 2D polymeric layers are interacting with each other through C–H···π non covalent interactions and C/N–H···O weak hydrogen bonds. In compound **3**, the discrete trinuclear complex molecules are self-assembled into infinite chains through inter-molecular O–H···N hydrogen bridges and π–π stacking interactions between anti-parallelly aligned unidentate bpy molecules. The chains and uncoordinated bpy molecules are further assembled into 2D, which are stacked to give a 3D supramolecular architecture with the uncoordinated water molecules in the cavities. All the compounds have been tested for their thermal as well as chemical stability.

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POSTER-19

GRADED IR-FILTERS FOR SUPRAMOLECULAR SYNTHONS: DISTINGUISHING DIFFERENT GEOMETRIES OF SAME INTERACTION

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The concept of the supramolecular synthon is increasingly finding greater importance in crystal engineering, with applications in many diverse fields. While single crystal X-ray diffraction (SXRD) is one of the most suitable techniques to obtain accurate information on the structures of molecular assemblies in the solid state, it has also been found that obtaining a single crystal is in itself often a challenge. Computational crystal structure prediction (CSP) is an alternative approach in such cases. It is noteworthy that despite the large number of crystal structures known today, CSP is a challenging task that is fraught with difficulties. Synthon assisted CSP is a promising strategy in this overall endeavor. There is accordingly a need to obtain basic synthon information in polycrystalline samples. A simple, robust, rapid and high throughput analysis protocol that can identify synthons accurately is especially important in this current scenario. Infrared spectroscopy (IR) is a well-established technique if a process to effectively remove overlapping bands, and thereby identify bands arising specifically due to the interacting groups of the synthon in consideration, can be developed. Based on this concept an 'IR-marker' method[1] has been developed for simultaneous identification of multiple strong as well as weak H-bonded synthons[2] and their transferability has also been probed.[3] In the most recent study, we have been able to distinguish more challenging topological and geometrical variations, namely **P**, **Q**, and **R** types in the same $NO_2\cdots I$ halogen bonded synthon[4] by means of 'Graded IR filter'. [5] We have employed a five step method that incorporates a gradation in the identification protocol to distinguish between the synthons in samples with unknown structures.

POSTER-20

RECOGNITION OF FLUORIDE ANION AT LOW PPM LEVEL INSIDE LIVING CELL AND FROM FLUOROSIS AFFECTED TOOTH AND SALIVA SAMPLES: FROM MOLECULE TO DAILY USE DEVICE

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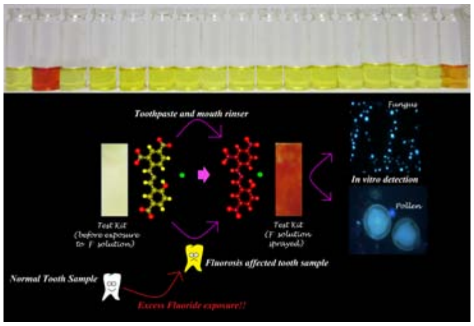
A simple Schiff base chemosensor 2-((2-(2,4-dinitro phenyl)hydrazono)methyl)-4-nitrophenol (L) has been developed as a colorimetric and fluorimetric '*turn on*' sensor for fluoride (F^-). F^- recognition at ppm level from mouth rinser and toothpaste water solution has been successful. From health related concern of rural Indians it is highly necessary to detect F^- from fluorosis affected tooth as well as saliva samples for quick and easy diagnosis of dental fluorosis in rural and remote part of India as twenty states of India are suffering from fluorosis. Dental specimen of different category patients from different parts of rural places of district Burdwan of West Bengal, India were collected and thereafter examined. To the best of our knowledge, in the history of Supramolecular Chemistry this is possibly the first ever evidence of detection of F^- from fluorosis affected tooth and saliva samples by colorimetric way (yellow to intense reddish brown) in presence of a newly developed Schiff base chemosensor (L).

Development of Test kit for F^- detection from DMSO:water (1:1) mixture is also engineered. Intracellular F^- from pollen grains of *Techoma stans* and *Candida albicans* (a diploid fungus), grown in 10^{-6}(M) F^- contaminated water has been successfully detected under fluorescence microscope.



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POSTER-21

Formation Of Ferromagnetic End-To-End Pseudohalide Bridged Homochiral Helical Copper(II) Schiff Base System Via Spontaneous Chiral Resolution

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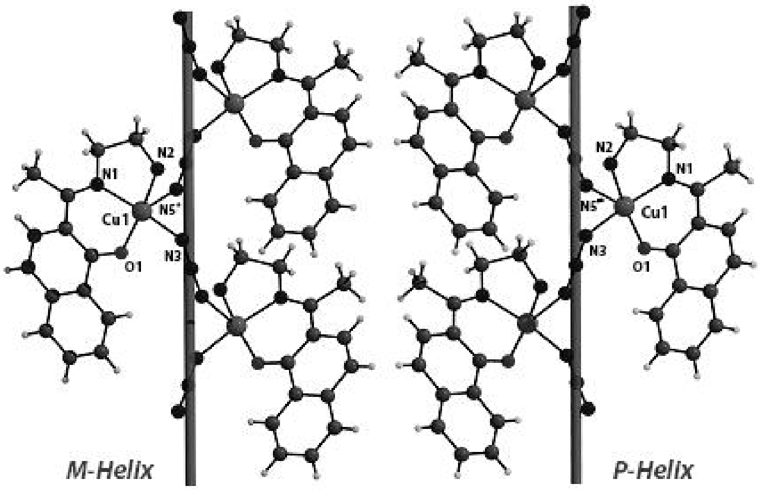
Homochiral helical coordination polymers of copper(II) have been synthesized using achiral precursors via spontaneous chiral resolution. Structures have been confirmed by single crystal X-ray diffraction studies and solid state CD spectroscopy.



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POSTER-22

APPLICATION OF A NOVEL 2D CADMIUM(II)-MOF IN THE FORMATION OF A PHOTO-SWITCH WITH SUBSTANTIAL ON–OFF RATIO

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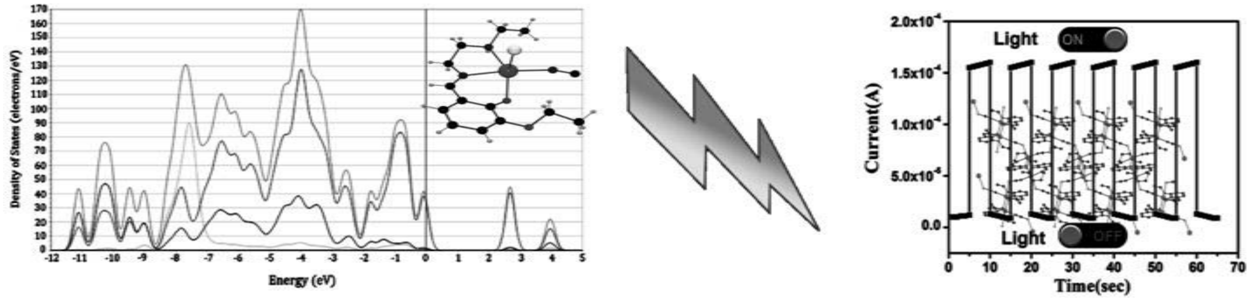
A novel thiocyanate bridged 2D MOF, $[CdL(\mu\text{-}1,3\text{-}SCN)_2]_n$, has been synthesized and characterized by x-ray crystallography. The band of the synthesized material in solid state has been determined by experimental measurement and compared with the theoretical value found from DFT calculation.



Acknowledgement :

We are thankful to Partha Pratim Ray, Department of Physics, Jadavpur University, Kolkata 700032, India, Antonio Frontera. c Departament de Química, Universitat de les IllesBalears, Crta. deValldemossa km 7.5, 07122 Palma de Mallorca (Baleares), Spain.

POSTER-23

SYNTHESIS, BIOLOGICAL EVALUATION AND MOLECULAR DOCKING STUDIES OF BENZOFURAN-THIAZOLE HYBRID MOLECULES AS POTENT ANTICANCER AGENTS

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Developing new selective, potent and less toxic antimicrobial agents to combat against life threatening invasive microbial infections and their ever growing multi-drug resistant is a major concern to chemists. Heterocyclic compounds offer a high degree of structural diversity and possesses wide range of economically useful therapeutic agents. Confining selective bioactive heterocyclic pharmacophores to construct new hybrid molecules have emerged as an interesting area for developing new potential pharmaceutical agents as their chemical characteristics clearly differ from those of existing agents. Benzofurans and thiazole scaffold are very interesting heterocycles, which are available in nature and show a wide range of pharmacological properties such as antimicrobial, anti-inflammatory, anti-HIV, antioxidant, analgesic and anticancer agents. In continuation of our research work on the synthesis and extraction of bioactive compounds, we report here some new hybrid *N*-(4-(benzofuran-2-yl)-3-aryl/hetaryl thiazol-2(3*H*)-ylidene)-aryl/hetarylamines bearing varied substituents have been synthesized to yield potent and hopefully selective drugs **4a-p**. Molecular docking approach is adopted for their aptness in regulating the functions, have been studied from their interaction energies (figure), within a shorter computational time frame without compromising the accuracy. The structure–activity relationship (SAR) of the newly synthesized compounds were evaluated using various cell lines and most of the obtained products were found to possess anticancer properties.

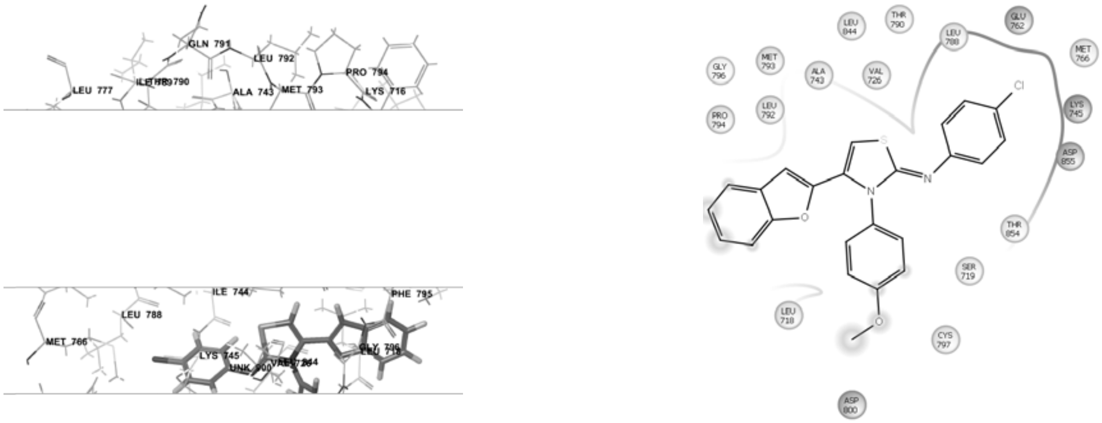

Fig. Possible 3D orientations and 2D interactions of compound **4d** in active site of EGFR receptor protein

POSTER-24

SYNTHESIS AND STRUCTURES OF SOME CUX BASED COORDINATION POLYMERS VIA IN SITU REDUCTION OF COPPER(II)

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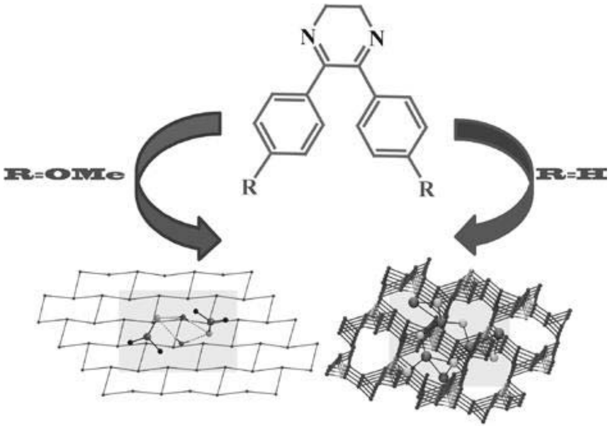
The one-pot synthesis of some CuX based coordination polymers, upon reduction of copper(II) at ambient conditions. The structures have been confirmed by single crystal X-ray diffraction analysis. All complexes are found to be highly inert toward oxidation.



Acknowledgments

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POSTER-25

Preparation Of Coinage Metal-TiO$_2$ Hybrid Nanocatalysts For Improved Photocatalytic Activity Under Sunlight Irradiation

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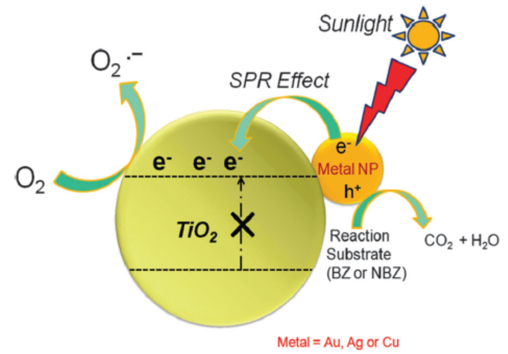
Abstract: This study demonstrated the comparative co-catalysis activity imparted to TiO_2 by as prepared coinage metal (Au, Ag and Cu) quantum dot particles of similar sizes (3-5 nm) as a function of their plasmonic interactions with TiO_2 under visible light irradiation as shown in scheme 1. The physiochemical and interfacial properties (1-5) of this metal-TiO_2 composites are studied by optical band gap, XRD, XPS, TEM, surface area, time resolved spectroscopy, current-voltage characteristics, GC and GC-MS analysis. It revealed that optical band gap is shifted to 2.9 eV from 3.2 eV of bare TiO_2 and the specific surface area 50 m^2g^{-1} of TiO_2 is notably reduced to 20-33 m^2g^{-1} after metal nanoparticles impregnation (M-TiO_2). The average relaxation time≈ 18 μs (bare TiO_2) < 20 μs (Cu-TiO_2) < 24 μs (Au-TiO_2) < 27 μs (Ag-TiO_2) of photoexcited charge species and the highest conductance value 1.65×10^{-7} S of Ag-TiO_2 as revealed by current-voltage studies strongly established that Ag-TiO_2 interface acts as a better electron sink to capture and store photogenerated electrons, thus displaying superior photocatalytic activity than Au/orCu-TiO_2 interface. Thus, Ag-TiO_2 exhibited the highest rate constant $k = 4\times10^{-2}$ min^{-1} relative to $k = 2.7\times10^{-2}$ min^{-1} (Au-TiO_2) and $k = 1.93 \times10^{-2}$ min^{-1} (Cu-TiO_2) for the oxidative degradation of benzaldehyde and nitrobenzadhyde to CO_2 under direct sunlight (40-50 mW/cm^2) exposure.



Scheme 1 Surface plasmon resonance effect of metal nanoparticles (Au, Ag or Cu) for TiO_2 photocatalysis under sunlight irradiation.

Keywords: Metal-TiO_2 interfacial energetics; Coinage metal-TiO_2 nanocomposites; Plasmonic nanoparticles; Plasmonic interaction; Visible light photoactivity

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POSTER-26

MOLECULAR DOCKING SIMULATION, SYNTHESIS AND *IN VITRO* ANTITUMOR ACTIVITY OF TRIAZOLO-OXADIAZOLES : SEARCH FOR ANTICANCER AGENTS

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Heterocyclics have seen unparallel progress owing to their wide natural occurrence, specific chemical reactivity and broad spectrum of pharmacological activities. The emergence of new viral pandemics, resurfacing of microbial diseases, increasing prevalence of systemic diseases coupled with the unvanquished scourge viral infections underline the imperative need for the discovery of new drug scaffolds. The ability to bind easily with the enzymes and receptors in organisms through hydrogen bonding and other weak interactions, azole heterocycles have been attracting increasing interest in pharmaceutical chemistry. Although the extensive clinical use of triazole anti-infective agents has ever revolutionized the treatment of several infectious diseases, some of them are still limited by poor activities towards intractable fungi, high frequency of renal toxicity and several adverse effects as well as emergence of increasing resistant microbes. These situations force scientific community to develop structurally new antimicrobial agents. Quinazolines exhibit extensive potentiality in medicinal chemistry with the latent ability to exert interactions with various active sites in organisms. Medicinal fields have been increasingly attracting a special interest, due to their potential outstanding contributions in the prevention and treatment of diseases such as HIV, microbial infections and also used in the treatment of several other diseases like leprosy and mental disorders. Many oxadiazole based compounds are core structures in various synthetic pharmaceuticals. Inspired by this and in continuation of our ongoing research program aiming at bioactive leads with potential chemotherapeutic activities has given impetus to design and synthesize a novel series of 4-((3-(2-chlorophenyl)-[1,2,4]triazolo[3,4-b][1,3,4]oxadiazol-6-yl)methylthio)-2-phenylquinazoline **6a-j**. *In-silico* molecular docking approach is adopted for biological evaluation of the compounds **6a-j** to study their aptness in regulating the functions, within a shorter computational time frame without compromising the accuracy. This virtual investigation showed a narrow variation in binding patterns and minimum binding energy of most of the newly synthesized compounds and may emerge as potential anticancer lead molecules.

POSTER-27

LATTICE STRUCTURE - MAGNETIC PROPERTY SYNERGISM IN UNCONVENTIONALLY FERROMAGNETIC MANGANITE NANOPARTICLES

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The present study investigates the prediction of temperature dependent magnetic phase transitions by crystal structure refinement. Crystal structure of magnetic materials might alter with the magnetic phase transitions but such alterations are mostly visible when the space group also varies across different temperatures.[1] Within the same space group, so far there was no evidence of lattice changes at transition temperatures although few reports on doped $A_{1-x}A'_xMnO_3$ (A = rare earth metal, A´ = alkaline earth metal) type manganites are available where a break in the slope of thermal variation of the crystal parameters was observed at the ferromagnetic transition temperature (T_c) studied by synchrotron or neutron diffraction studies.[2,3] In this work we have shown that refinement of laboratory X-ray diffraction (XRD) data can predict all the magnetic transition temperatures viz. ferromagnetic (T_c), antiferromagnetic (T_N), and spin-glass (T_{SG}) transitions. We synthesized undoped $PrMnO_{3+\delta}$ (PMO) nanoparticles by a unique non-aqueous sol-gel method by which very small (~12 nm) manganite nanoparticles can be stabilized.[4] Although bulk PMO is antiferromagnetic, our nanosized undoped or lightly-doped PMO was found to be ferromagnetic.[5] Due to a dominant antiferromagnetic character of bulk PMO, generation of ferromagnetic ordering at the nanoscale induces all possible magnetic transitions and this forms the basis of choosing this particular system. With the help of Rietveld refinement of XRD patterns, all possible magnetic phases were detected and most of the refined structural parameters show a characteristic *U*-turn at T_c. Moreover, the antiferromagnetic character was found to be maximum just above T_c, which is not possible to observe through routine magnetic measurements The rare observation of increased antiferromagnetism leading to a ferromagnetic ordering was found due to atomic deformations and reduced Mn-Mn separation. This long-range correlated structure-magnetic synergistic trend was never observed earlier and was generalized with the Pr (A-site) and Mn (B-site) vacancy doped nanoparticles.

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POSTER-28

DIVERSE SELF-ASSEMBLY OF DISCOTIC TRICARBOXYAMIDES: A CRYSTALLOGRAPHIC INSIGHT

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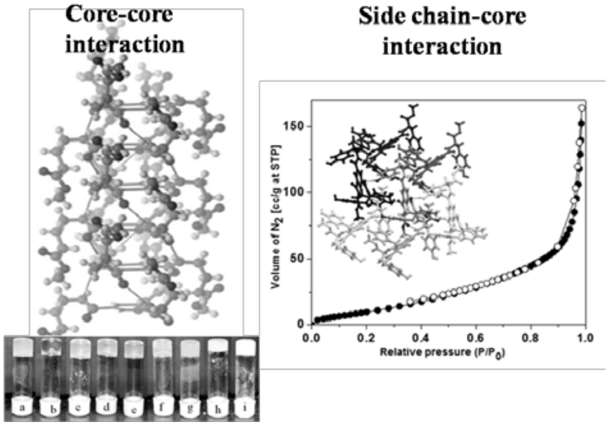
The organization of the cooperative building blocks through H-bonding, metal–ion complexation, electrostatic interactions and hydrophobic interactions is the key step towards the fabrication of new materials and devices. Discotic benzene-1,3,5-tricarboxyamides(BTA) is one of the most important candidate in this area.[1] We have synthesized various C=O-centered and N-centered discotic BTA and studied their assembly pattern at atomic level. The symmetric BTAs aggregate by core-core interactions and three fold amide-amide hydrogen bonding to give columnar structure. These BTAs form gel in large range of organic solvents which can be used to fabricate novel lanthanide nanocrystal decorated fibers.[2] We have studied the effect of side chain –side chain interactions on further assembly and gelation of the columner structures (Figure 1, left).[3] We have also introduced the effect of side chain-core interactions on the self-assembly of BTA which is very rare upto date. Specifically, we will show that the side-chains-core interactions have significant effect on self-assembly of chiral benzene-1,3,5-tricarboxyamide. The non columnar tricarboxyamide exhibits 10 times higher N_2 sorption than the columnar one (Figure 1 right).[4] Moreover, these non-columnar disk-like building have formed dimer and used to immobilize luminescence CdSe quantum dots. The electrochemical response shows that the oxidation potential has decreased and reduction potential has increased by CdSe doping. Photoelectric study exhibits that the conductivity of the CdSe-doped conjugate has enhanced by 200 orders of magnitude.[5]


Core-core interaction

Side chain-core interaction

Figure 1. Columner packing by core-core interactions and cage-like packing by side chain interaction

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POSTER-29

STRUCTURAL DIVERSITY: SUPRAMOLECULAR SHEET AND DOUBLE HELIX OF γ-PEPTIDES

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Nature creates a wide range of single and double helical macromolecules from the combination of regular building blocks such as twenty amino acids and four nucleobases. Molecular motions and folding of designer molecules and supramolecular architectures held together by intermolecular noncovalent interactions are highly important for understanding the structure-function relationship of biological macromolecules.[1] We have designed and synthesized a series of aromatic γ-peptides from *m*-aminobenzoic acid and N, N′-dicyclohexylurea. We have reported that the inter-strand hydrogen bonding and π-π stacking interactions significantly increased the hybridization constant of aromatic γ-peptide foldamers.[2] Structural transformation of biopolymers is a natural fact and is responsible for a wide range of diseases. We have also explored the remarkable solvent assisted structural transformation and aggregation behaviour of the γ-peptides.[3] In polar protic solvent, the helical strand interacts with the solvent molecules and expands to a more open (extended) structure, which further self-assembles to form a supramolecular sheet like structure (Figure 1). But in chloroform, the peptides dimerized as a parallel double helix stabilized by intermolecular hydrogen bonding interactions (Figure 1). Moreover, we have introduced the effect of halogen bonds on the self-assembly of aromatic γ-peptide which is very rare upto date. Specifically, we shall show that the compound exhibited different photoluminescence intensity and lifetimes in crystals obtained from ethyl acetate and methanol.[4] X-ray crystallography revealed that the intermolecular C=O…Br halogen bond directs the heavy atom effect to produce the phosphorescence.

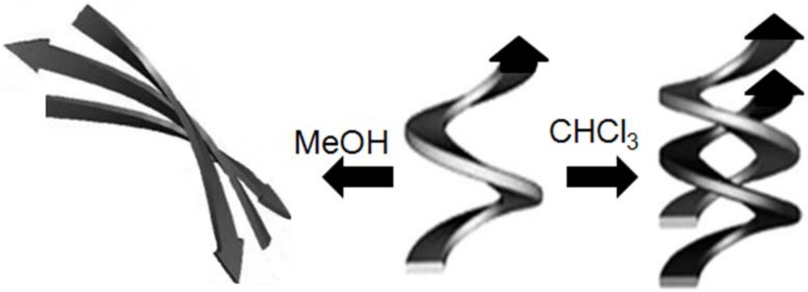

Figure 1. Solvent assisted structural transformation of a short aromatic γ-peptide.

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POSTER-30

STRONG SINGLE BAND BLUE EMISSION FROM COLLOIDAL CE^{3+}/TM^{3+}-DOPED NAYF$_4$ NANOCRYSTALS FOR LIGHT EMITTING APPLICATIONS.

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Lanthanide doped materials are interesting as a phosphors due to narrow luminescence peak and long life time, these narrow peaks lead to high color purity. Which is potentially useful for developing phosphor based LEDs. Our objective is to develop a colloidal phosphor which can display strong blue light for developing blue LED. Blue LEDs are interesting because they are used for various applications, such as blue ray disks, blue lasers for high density DVDs, and laser projectors to name a few. This is achieved by Ce^{3+}/Tm^{3+} doped NaYF$_4$ nanocrystals.

We report for the first time the observation of an unusual strong single band blue emission from water dispersible Ce^{3+}/Tm^{3+}-doped NaYF$_4$ nanocrystals. The Ce^{3+} ions act as sensitizer for the Tm^{3+} ions to produce intense single band near 450 nm. Sensitization by Ce^{3+} ions is quite interesting as it enhances the luminescence quantum efficiency of the lanthanide ions. The water dispersibility is achieved by capping the nanocrystals with citric acid molecules. The high dispersibility of the nanocrystals is explored for the nanocomposites formation which is developed by incorporating the Ce^{3+}/Tm^{3+}-doped NaYF$_4$ nanocrystals into polymers such as poly(vinyl alcohol). The resulting polymer nanocomposites possess high transparency and retain the optical properties of the nanocrystals. Furthermore the nanocomposite material was coated on commercially available 280nm UV LED, which displayed intense blue light upon electrical activation. The strong single band blue emission and the high transparency of the nanocomposites suggest that the developed materials can be of potential interest for the development of phosphor based blue light emitting diodes (LEDs).

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POSTER-31

MICROMOTORS:AUTONOMOUS MOVEMENT INDUCED INCHEMICALLY POWERED ACTIVE SOFT-OXOMETALATES

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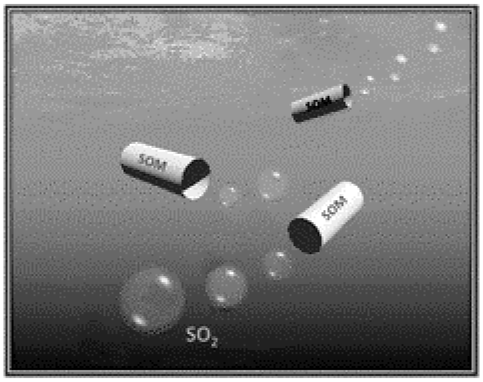
Synthesis of autonomously moving micro or nanoscale objects is an immediate challenge in current nanoscience and nanotechnology. Although micro as well as nanomotors have been designed by various groups, in most cases their synthesis is tedious and their motion is relatively slow. In this work, we report a system based on soft-oxometalates (SOMs) which is very easy to synthesize, moves with a high velocity (~369 body lengths s^{-1}) in response to chemical stimuli and also shows collective behaviour like school of fishes. We also explain in detail the reaction kinetics, and power conversion efficiency of these active soft materials using two different chemical fuels that exploit redox chemistry latent to SOMs.



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POSTER-32

DIRECT SYNTHESISOF CONTROLLED SIZE NANO SPHERES INSIDE NANO CAVITIES OF SELF-ORGANIZED PHOTO POLYMERIZING SOFTOXOMETALATES [PW12O40]N(N=1100–7500)

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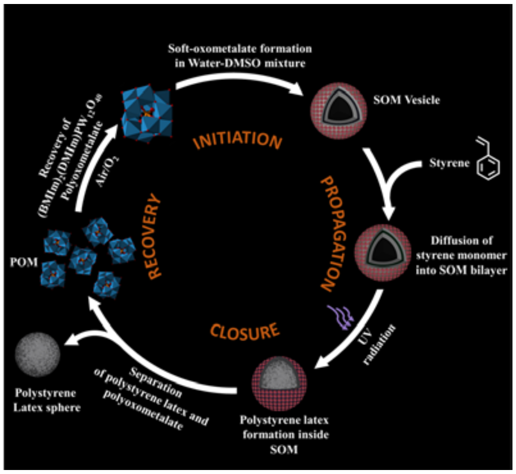
The unusual self-assembly of $\{(BMIm)_2(DMIm)[PW_{12}O_{40}]\}_n$ (n=1100–7500) (BMIm=1-butyl-3-methylimidazolium, DMIm=3,3’-dimethyl-1,1’-diimidazolium) soft oxometalates (SOMs) with controlled size and a hollow nanocavity was exploited for the photochemical synthesis of polymeric nanospheres within the nanocavity of the SOM. The SOM vesicle has been characterized by using several techniques, including dynamic light scattering (DLS), static light scattering (SLS), attenuated total reflection (ATR) IR spectroscopy, Raman spectroscopy, microscopy, and zetapotential analysis. The self-assembly and stabilization of this soft-oxometalate vesicle has been shown by means of counter- ion condensation. The immediate implication of such stabilization— the variation of the dielectric constant with the hydrodynamic radius of the vesicle—has been used to synthesize vesicles of controlled size. Such vesicles of varying size have been used as templates for polymerization reactions that produce polymeric spheres of controlled size. Direct evidence shows that the SOM behaves as a model heterogeneous catalytic system. Such surfactant- and initiator- free photochemical synthetic routes for obtaining uniform latex spheres could be used in the making of optical bandgap materials, inverse opals, and paints.



Schematic representation of the complete photocatalytic cycle of $(BMIm)_2(DMIm)PW_{12}O_{40}$.

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POSTER-33

EFFECT OF HETEROATOM(S/SE) JUGGLING IN D-A-D FUSED SYSTEMS : SYNTHESIS AND ELECTROCHEMICAL POLYMERIZATION.

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Synthesis of fused donor-acceptor-donor (D-A-D) type of small molecules **1-3** using thiophene/selenophene as donor and benzothiadiazole (BDT)/benzoselenadiazole (BDSe) as acceptors were synthesized. Their structural, photophysical and electrochemical properties were studied. Electrochemical polymerization was done and the polymers were characterized both electrochemically and by spectroelectrochemistry. **1-3** shows high fluorescence quantum yield, positive solvatochromism and high stokes shift. Head to head dimerization was observed through S….N interaction with intermolecular distance of 3.274 Å for **2** (the sum of van der waal radii between S and N 3.35 Å), whereas in **3** the dimerization takes place through Se….N interaction with the distance of 2.944 Å (the sum of van der waal radii between Se and N 3.45 Å).

POSTER-34

SULPHUR AND SELENIUM CONTAINING NEW BUILDING BLOCKS FOR CONJUGATED SYSTEMS AND THEIR TRANSISTOR PROPERTIES

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The development of new conjugated organic materials for dyes, sensors, imaging, organic light emitting diodes, field-effect transistors, and organic solar cell has largely relied upon assembling p-conjugated molecules and polymers. Though the development in this field has grown rapidly in the last fourty years, the conjugated electroactive building blocks with promising properties are limited.

The synthesis of new conjugated building blocks, Diselenolodiselenole (C_4Se_4) derivatives and Thienopentathiepine (C_4S_6) derivatives, is described for the first time. Here, we introduce two new synthetic approaches to synthesize these building blocks from their diyne precursors with elemental sulphur and selenium. Crystal structures of thiophene and selenophene capped Diselenolodiselenole showed planar conjugated backbone exhibited resolute intermolecular interactions through heteroatoms form a 2D brick-like structure in bulk. This 2D crystal packing with several nonbonding interactions facilitate the intermolecular charge transport. In FET device performance thiophene and phenyl capped (C_4Se_4) shows reasonably good p-type mobility 0.02 and 0.001 $cm^2 V^{-1} s^{-1}$. Improved planarity from phenyl capped to thiophene capped (C_4Se_4) moieties (around 43 °) is responsible for better device performance. Chalcogenophene (Thiophene, Selenophene and Bithiophene) capped thienopentathiepines undergos electrochemical polymerization to produce three new conjugated polymers **P1** **P2** and **P3**. Optoelectronic properties and spectroelectrochemistry of these polymers were studied.

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POSTER-35

FACILE SYNTHESIS OF FLUORESCENT PROTEINS CHROMOPHORE FROM AMINO ACIDS

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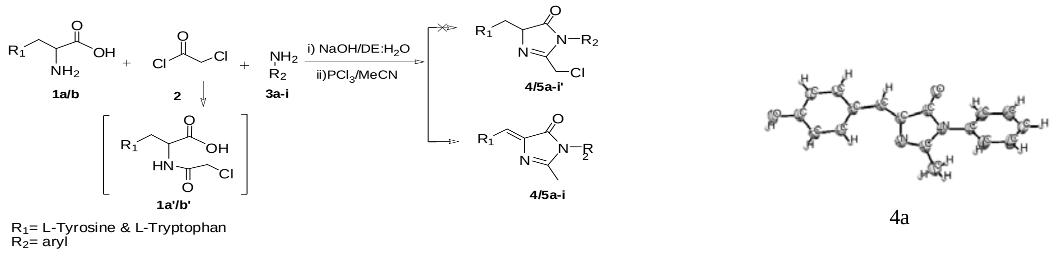
Nitrogen containing heterocycles are of special interest in synthetic organic chemistry,[1] since they occur in a wide variety of natural products. Among them, imidazolinone is a fundamental non-aromatic naturally-occurring heterocycle that has been intensively used in the synthesis of functional materials and pharmaceuticals.[2] The imidazolinone substructures are found to act as the chromophores of the fluorescent proteins (FPs), for example, green fluorescent protein (GFP), cyan fluorescent protein (CFP), blue fluorescent protein (BFP) and for red kaede fluorescent protein (RFP).[3] Imidazolones also show various biological and pharmaceutical activities. The omnipresent of 4-arylidene-5-imidazolinones and their intrinsic photochemical phenomena have made it intriguing synthetic targets and useful chemical models for investigating the mechanism of the fluorescence proteins.[4]

Herein we report a new phosphorous-catalyzed tandem approach for the synthesis of 4-arylidene-5-imidazolinones (4/5a-i), which are Green FPs and Cyan FPs chromophore respectively. The reaction involve assembly of *N*-chloroacetyl-amino acids (1a'/b') and anilines (3), wherein (1a'/b') are generated *in situ* by the direct use of the corresponding aromatic amino acids (1) and acyl chlorides (2) in one pot (Scheme 1). In these reactions, at least four different active sites are involved; two C-N bonds, one C=N bond, one C=C bond and new rings are constructed with all reactants efficiently utilized in the chemical transformation.



Scheme 1. Synthesis of 4-arylidene-5-imidazolinones in one-pot system

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POSTER-36

SYNTHESIS OF HEXAGONAL PHASE EU^{3+}-DOPED GDF$_3$ NANOCRYSTALS AT HIGHER TEMPERATURES TO ENHANCED THE LUMINESCENCE EFFICIENCY

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Abstract: The formation of orthorhombic phase GdF$_3$ nanocrystals (thermodynamically controlled product) requires higher activation energy than that required for the formation of hexagonal phase GdF$_3$ nanocrystals (kinetically controlled product). As a result, at higher reaction temperature, formation of the orthorhombic phase GdF$_3$ is generally preferred. However, the thermodynamic product is always more stable than the kinetic one at lower temperature. Here, we report a simple and facile microwave assisted method to synthesize stable hexagonal phase polyvinylpyrrolidone (PVP) functionalized Eu^{3+}-doped GdF$_3$ nanocrystals at higher temperatures (upto 220ºC). This is achieved by tuning the viscosity of the solvents as well as using KF as fluoride source. Both morphology and size of the GdF$_3$ nanocrystals are also varied by tuning the reaction conditions. PVP functionalization of the nanocrystals makes them water dispersible. The Eu^{3+}-doped hexagonal GdF$_3$ nanocrystals show more intense red emission compared to orthorhombic GdF$_3$ nanocrystals.In addition Eu^{3+} ions possess longer luminescence lifetimes in hexagonal GdF$_3$ nanocrystals. The high luminescence efficiency of the Eu^{3+}-doped GdF$_3$ nanocrystals together with high dispersibility in water can have potential use in bioimaging and MRI imaging applications.

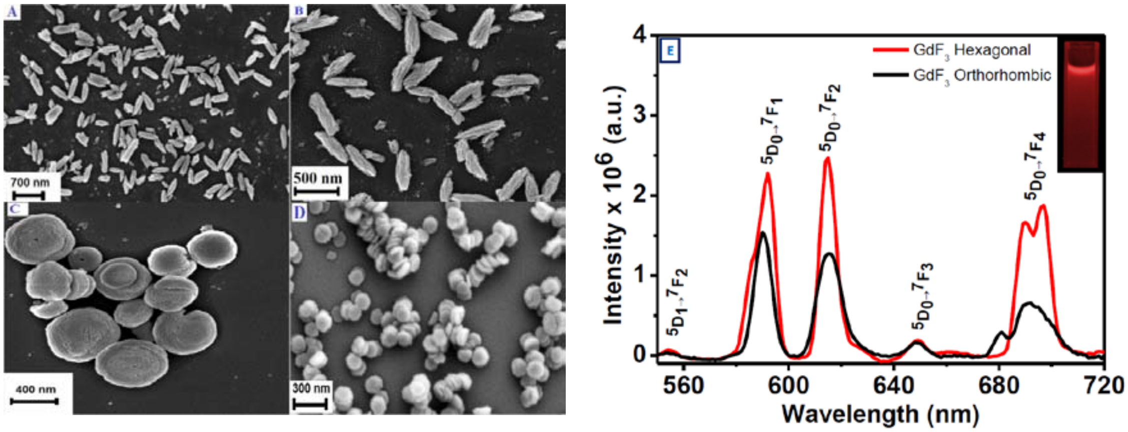

Figure. 1SEM images of Eu^{3+} doped GdF$_3$ nanocrystals (A to D) at different reaction conditions along with the photoluminescence (PL) spectra of Eu^{3+} ions in hexagonal and orthorhombic GdF$_3$ nanocrystals (E).Inset shows the digital image of the red emission of hexagonal GdF$_3$nanocrystals in water.

POSTER-37

STRUCTURE OF METHANE CHEMISORPTION ON PT(111) SURFACE -A DFT STUDY

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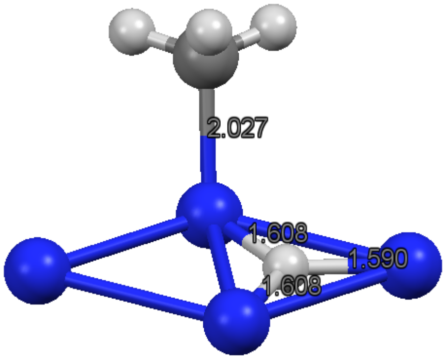
Abstract

Chemisorption mechanism of methane on Pt (111) surface studied using density functional theory methods. During one C—H bond dissociation, surface CH_3 intermediate has been formed. When two C—H bonds dissociation takes place, surface CH_2 will be formed. Similarly, during three C—H bond dissociation surface CH species has been identified. We calculated the minimum energy barriers and adsorption energies for theses three different types of approaches on the Pt(111)surface.



Transition State

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POSTER-38

CO-CRYSTALLIZATION APPROACH TO CONVERT THERMALLY INNOCENT SOLIDS INTO THERMOSALIENT CO-CRYSTALS BY USING THERMORESPONSIVE TEMPLATE

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Thermomechanical effects of the single crystals like bending, hopping, jumping, moving, splitting and exploding have potential applications for designing mechanical sensors, probes for smart medical devices, artificial muscles, bioelectronics including components of microfluidic devices. Thermosalient crystals can be remarkably useful due to their inherent high sensitivity to external stimuli, coupled with actuating behaviour. To the best of our knowledge this is the first report of the thermosalient co-crystals. The co-crystal approach provides an opportunity to tune the properties by altering crystal structure in a predetermined fashion, hence can allow the design of more effective crystals of the active compound, for example with high durability, stability and better sensitivity property. In the present work, we have chosen three compounds, SAL-4ABA (1), SAL-4ABA-BPY (1A) and SAL-4ABA-BPE (1B) among which 1A and 1B are co-crystals that show impressive jumping behaviour. The crystals of 1 also show colour change from yellow to orange upon heating above 240-250oC, followed by the characteristic thermosalient effect at 265.5-266.5oC, when heated at 0.5oC/min in DSC profile.

Here the thermosalient phenomenon is reversible .The crystals of 1A also show the characteristic colour change from yellow to orange at 205oC followed by the appearance of sawtooth profile at 220-239oC and thermosalient behaviour at 240oC. The crystals of 1B also display its characteristic colour change from orange to orange-red and to red, followed by multiple jumps around at 200oC. The crystals melted at 238oC and on cooling, the recrystallization endotherm is found at 150oC. In this work, we demonstrate how one can successfully convert a non-TS compound into a TS compound using a TS co-former as a template. This paves the way for not only tuning the properties of the TS-active component, but also design the multi-functional co-crystals where both the co-formers offer different function, hence may act as smart functional co-crystals.

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POSTER-39

SUPRAMOLECULAR CHEMISTRY ON ACCOUNT OF THE FACT THAT THE OH GROUP CAN OFFER BOTH HYDROGEN-BOND DONOR AND ACCEPTOR SITES

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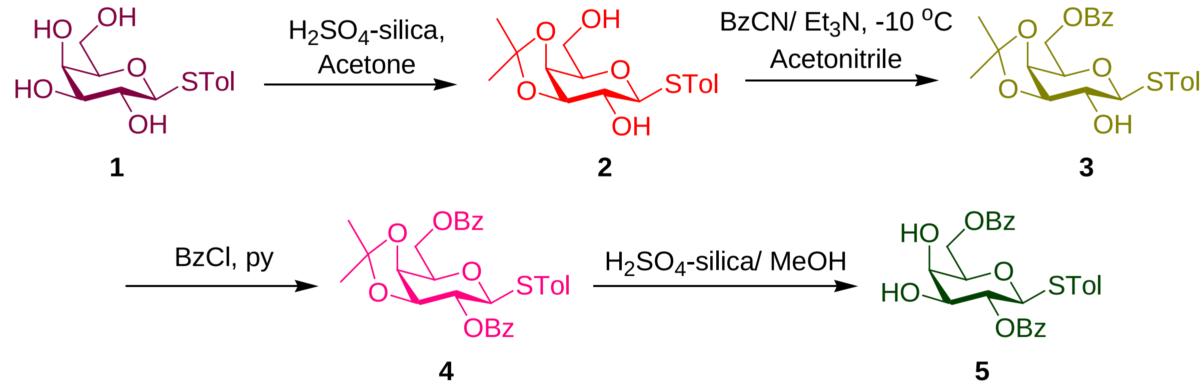
Abstract

Sugars are interesting as synthons in supramolecular chemistry on account of the fact that the OH group can offer both hydrogen-bond donor and acceptor sites. In our present study, we have synthesised five galactose derivatives through protecting group manipulations (**Scheme 1**). Having obtained this series of compounds, together with their crystal structures, the effects of different protecting group manipulations on the product of the reaction, as well as on the packing arrangements of these molecules in the solid state, can be examined. Notably, we report the crystallographic evidence of the change in regular chair conformation to a skew boat conformation in a partially protected sugar derivative. Crystallographic correlation with four more analogous derivatives indicate a particular O–H···O hydrogen bonding network is responsible for the change in conformation. Besides that in our study, we have tried to correlate single crystals of galactosides**1**, **2** and **3** (intermolecular hydrogen bonded system) with their gelation ability. Among these three only compound **1** shows effective gelation in various solvent,while **2** and **3** do not act as gelator.



Scheme 1. Synthesis of the thio-galactoside compounds **1**-**5**

POSTER-40

COMPLETE EXCHANGE OF METAL IONS CONSTITUTING THE FRAMEWORKS OF METAL-ORGANIC FRAMEWORKS

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With growing interests on metal-organic frameworks (MOFs), post-synthetic modification receives considerable attention to get more control over the materials, as a pre-synthesized highly porous and desirable framework can be chosen for further modification to fine tune the pore environment without disrupting the framework topology. However, substitution or replacement of framework-constituting components from a pre-assembled framework without changing the framework topology or structure has not been explored. Herein, I present the complete exchange of framework-constituting metal ions from robust microporous frameworks keeping the original framework topology intact. To exchange the framework-constituting metal ions it is desirable to have an open access of the metal ions through solvent accessible channels or pores of the framework.

Recently, we and other groups demonstrated that metathesis, that is, the replacement or exchange of integral parts of the frameworks, can be applied to MOFs as post-synthetic modification without altering the basic structure or topology of the frameworks. Herein, I report the synthesis of a Mn(II) framework and the metal-ion exchange of the Mn(II) framework to produce Fe(III), Co(II), Ni(II), and Cu(II) frameworks, which were difficult—if not impossible—to achieve through direct synthesis. We observed a facile metal-ion exchange without altering the framework structure or structural integrity of the MOF. Although this process involves the simultaneous breaking and formation of several dative bonds between the ligands and the leaving/incoming metal ions, the ion-exchange processes occurs in a single-crystal-to-single-crystal transformation manner. These materials showed similar high porosities.

POSTER-41

GREEN SYNTHESIS, CHARACTERIZATION AND EVALUATION OF ANTIBACTERIAL AND CYTOTOXIC POTENTIAL OF *AVERRHOA CARAMBOLA* MEDIATED SILVER NANOPARTICLES

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Abstract

Silver nanoparticles (AgNPs) were biosynthesized from aqueous extract of *Averrhoa carambola*, characterized and their potential as antimicrobial and anti-proliferative agents were evaluated in this present study. AgNPs were produced through environmentally friendly procedures by reduction of silver nitrate with *A. carambola* extract. The green synthesized AgNPs were characterized by UV-visible spectroscopy, Transmission electron microscopy (TEM), Atomic force microscopy (AFM) and fourier transform infrared (FT-IR) analysis. The UV–Visible spectrum resulted a sharp peak (at 430 nm) represents the strong plasmon resonance of silver. TEM and AFM analysis showed that the formed particles were of spherical morphology with appreciable nanosize. The FTIR data revealed the presence of plant organic constituents and metabolites bound to AgNPs, which contributes for their stability. Bacterial biofilm inhibition activity of AgNPs were assessed by *Pseudomonas aeruginosa* and *K Pneumonia* where biofilms were not observed at upto 72 hours at the lowest dosage of 6.25µg/ml and 12.5 µg/ml, respectively. Antibacterial results based on disk diffusion method demonstrated that *Salmonella* were more sensitive to AgNPs than *E. coli*. Cytotoxicity was determined by MTT assay where AgNPs exerted concentration-dependent cytotoxicity against EAC cells. In MTT assay, cell viability was significantly reduced to 25.35% at a dose of 12 µg/ml though AgNPs showed no significant toxicity against brine shrimp naupli at dosages upto 800 µg/ml. Owing to their excellent antibacterial and antiproliferative activities along with biofilm inhibition properties, these silver nanoparticles can be considered as promising agents for future biomedical applications.

POSTER-42

STRUCTURAL CHARACTERIZATION OF ZN-LI FERRITES

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Abstract

Structural properties of Zn-Li ferrites with the composition $Zn_xLi_{0.45-x/2}Fe_{2.55-x/2}O_4$ (where, x=0.0, 0.1, 0.2, 0.3, 0.4 and 0.5) synthesized by conventional ceramic method have been investigated as a function of Zn content and sintering temperature T_S (where T_S=1000, 1050, 1100, 1150, 1200 and 1250°C). The X-ray diffraction (XRD) analysis confirmed the formation of cubic spinel structure with trace of impurity phase probably hematite in sample x=0, as depicted in Figure between the peaks (111) and (220), (222) and (400). Analyzing the XRD patterns, we notice that the position of the peaks comply with those of the reported values (1,2). The observed peaks (111), (220), (311), (222), (400), (422), (511) and (440) which is either odd or even confirmed the cubic spinel structure of the sample and also in agreement with other workers (3,4).. It is also found that the lattice constant increases with increasing Zn content, obeying Vegard's law. The theoretical density (ρ_{th}), the bulk density (ρ_B), and porosity (P) as a function of Zn content and sintering temperature were also investigated. It is observed that density increases up to 1100^0C and beyond 1100^0C, ρ_B decreases, while porosity shows opposite trend. Scanning electron microscope (SEM) reveals the microstructure of all the samples. The microstructure studies of the present ferrite system also shows that average grain size increases with the function of Zn^{2+} content up to x=0.4. A sudden decrease in average grain is observed beyond x = 0.4, which may be due to the fact that ions like Li^+, Zn^{2+}, Cd^{2+} and Ti^{4+} do not favour grain growth when present in excess quantities (5).

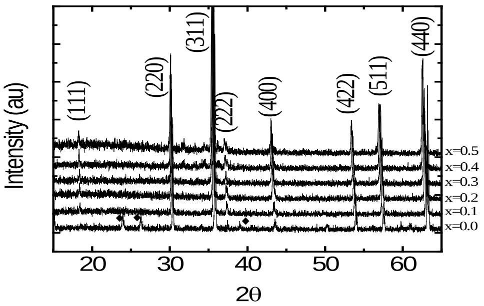

Fig. The XRD patterns for various $Zn_xLi_{0.45-x/2}Fe_{2.55-x/2}O_4$ sintered at 1250^0 in air.

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POSTER-43

HYDROGEN PEROXIDE BIOSENSOR BASED ON THE IMMOBILIZATION OF HORSERADISH PEROXIDASE ONTO GOLD -NANOPARTICLE ADSORBED POLY(BRILIANTCRESYL BLUE) FLIM.

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An amperometric hydrogen peroxide (H_2O_2) biosensor was developed based on the immobilization of horseradish peroxidase (HRP) onto gold nanoparticle (GNP) adsorbed conducting poly(brilliant cresyl blue) (PBCB) film. The electrochemical method was highly selective and sensitive. The modified electrodes showed reversibility towards the reduction of H_2O_2 in 0.1 M phosphate buffer solution (PBS) at pH 7.0. The modification process was characterized by electrochemical methods (cyclic voltammetry and differential pulse voltammetry), scanning electron microscope (SEM) and electrochemical impedance spectroscopy (EIS). The effects of experimental parameters such as the concentration of the mediator (hydroquinone, HQ), pH of the solution, and the working potential were investigated for optimum analytical performance. In the presence of the mediator, the immobilized HRP showed an excellent electrocatalytic activity towards the reduction of H_2O_2. It was found that the peak currents increased with the increasing concentration of H_2O_2. The linear dynamic range from 5 to 150 μM with the regression coefficient of 0.99 was obtained. The detection limit was calculated to be 0.5 μM based on S/N (signal-to-noise ratio) of 3. The reproducibility and stability of the newly developed biosensor were examined and it showed satisfactory results. The performance of biosensor was evaluated with respect to possible interferences and the application to real sample analysis. Seven possible interfering substances (glucose, sucrose, oxalic acid, uric acid, nitrate, chloride, and ferric ion) did not show any observable interference. The concentration ratio of H_2O_2 to interfering species was 1:10. The recovery rate in the range of 98.0% to 101.0% was found which are quite satisfactory. The biosensor exhibited good stability, reproducibility, selectivity, which was successful for practical applications.

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POSTER-44

APPLICATION OF CRYSTALLOGRAPHY IN THE EARTH MATERIALS AND ITS TEACHING METHODOLOGY

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The Planet Earth is a family member of our present Solar System and its orbits around the Sun. The Interior Earth is composed of three broad based layers of solid in the outer surface called as Crust to the inner center is liquid substances called as Core and the middle is Mantle in semi-solid nature. Geologists or Geoscientists deal with the earth materials, since the oldest stage to recent time by hand study, microscopy to x-ray diffraction method and other auto-counting background technique, to identify the different crystalline to non-crystalline form of rock types and minerals. Rock is composed of a single mineral to aggregate of many minerals. The first hand mineral identification is based on the morphological information from the external form of simple crystal form to complex, and structurally, how a crystal structure is built?

The teaching of crystallography is an important tool in the beginning of the geology student for their mineralogical study. Further the geotechnical, foundation engineers and engineering geologists deal theirs geo-resources materials. The chemists, geochemists, physicists deal with their respective goal of investigation for the specific minerals of the finest nature. The purpose of the paper will discuss about the crystallography teaching at the present level in the Department of Geology, University of Dhaka.

POSTER-45

CRYSTAL STRUCTURE OF THE CENTRAL AXIS DF COMPLEX OF *ENTEROCOCCUS HIRAE* V-ATPASE

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In various cellular membrane system, vacuolar ATPases (V-ATPases) function as proton pumps, which are involved in many processes such as bone resorption and cancer metastasis, and these membrane proteins represent attractive drug targets for osteoporosis, osteopetrosis, and cancer (1). *Enterococcus hirae* V-ATPase, which acts as a primary ion pumps similar to eukaryotic V-ATPases, uniquely transports Na^+ or Li^+ instead of H^+ ions (3). This enzyme is composed of nine subunits with the amino acid sequences that are homologous to those of the corresponding subunits of eukaryotic V-ATPases (3). The V_1 domain of this ATPase is composed of a hexameric arrangement of alternating A and B subunits responsible for ATP binding and hydrolysis (2). The V_o domain, in which the rotational energy is converted to drive Na^+ translocation, is composed of oligomers of the 16-kDa c subunits and an a subunit (5). The V_1 and V_o domains are connected by a central stalk, which is composed of D, F, and d subunits and two peripheral stalks, which are composed of E and G subunits of V_1 (6). ATP hydrolysis introduce the rotation of the central stalk (DFd complex) and an attached membrane c ring, which causes ion pumping at the interface between the c ring and a subunit (4).

The crystals of the central axis DF complex of *Enterococcus hirae* V-ATPase were obtained at 293 K, using the sitting drop vapor diffusion method. Developed crystals were analyzed by X-ray diffraction. The collected data sets were indexed and integrated using MOSFLM and scaled with scala from CCP4 packages. The crystal belongs to the space group *C*2, with the unit cell parameters of a=105.79 Å, b=68.43 Å, c=51.15 Å, β=114.99º. The crystal structure of the central axis DF complex was determined using the MAD method.

The crystal structure of the DF complex of *Enterococcus hirae* V-ATPase was determined at 2.0 Å resolution, which was high enough to identify the side chain and atom positions. The final model consisted of residues 7 to 194 of D, residues 1 to 101 of F, 152 water molecules, and a nitrate ion. The structure of the D subunit comprised a long left handed coiled coil with a unique short β-hairpin region that is effective in stimulating the ATPase activity of the V_1-ATPase by two fold. The F subunit is bound to the middle portion of the D subunit and the β-hairpin region of D subunit contributes to close contact with F subunit. The C-terminal helix of the F subunit, which was believed to function as a regulatory region by extending into the catalytic A_3B_3 complex, contributes to tight binding to the D subunit by forming a three helix bundle. Both D and F subunits are necessary to bind the d subunit that links to the c ring. From these findings, the entire rotor complex (DFdc-ring) of V-ATPase was modeled.

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POSTER-46

STRUCTURAL, MAGNETIC AND ELECTRICAL PROPERTIES OF LA AND DY SUBSTITUTED $BiFeO_3$

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Abstract:

Multiferroic $Bi_{1-x}Re_xFeO_3$ (Re = La, Dy; x = 0.3 for La and 0.2 for Dy) ceramics are synthesized by the conventional ceramic method. The X-ray diffraction indicates structural phase transition from rhombohedral to tetragonal and orthorhombic due to La and Dy substitution (1, 2) respectively. The grain size decreases due to La and Dy substitution. The permeability decreases and the relative quality factor increases with La and Dy substitution. The substitution also enhances the ferromagnetic properties. The weak ferromagnetism is ascribed to the suppressed spiral spin structure (3) and magnetically active characteristic of La^{3+}, Dy^{3+} ions together with ferromagnetic coupling of La^{3+} and Dy^{3+} ions with Fe^{3+} ions. Dielectric constant (ε'), loss tangent ($\tan\delta$) and AC conductivity (σ_{AC}) are measured as a function of frequency at room temperature. The La and Dy substitution enhances the dielectric properties of $BiFeO_3$. The dielectric dispersion at lower frequencies ($<10^4$ Hz) is due to the Maxwell-Wagner type interfacial polarization (4, 5). The variation of σ_{AC} is explained in terms of polaron hopping mechanism.

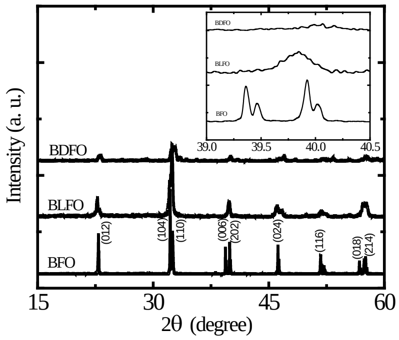

Fig. 1. XRD patterns of $Bi_{1-x}Re_xFeO_3$ ceramics.

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POSTER-47

PURIFICATION, CHARACTERIZATION, CYTOTOXICITY AND CA^{2+} INDUCED STRUCTURAL CHANGE OF A LECTIN FROM *MORINGA OLEIFERA* SEEDS

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Abstract

Lectins are carbohydrate-binding proteins that agglutinate cells and found in large amounts in the food. They are widely distributed, and have been isolated from both plant and animal sources. Lectins are found in fresh and processed foods and the major known potentially toxic lectin containing food groups are grains, legumes, dairy and nightshade. *Moringa oleifera* is a popular vegetable in Bangladesh and has an impressive range of medicinal uses with high nutritional value and medicinal benefits especially in the northern part of south Asia. Different parts of Moringa contain a profile of important minerals and are a good source of protein, vitamins, beta-carotene, amino acids and various phenolics. A lectin was purified from the crude extract of *Moringa oleifera* Lam. seeds by conventional methods with a molecular weight of 17.0±1.0 kDa. This lectin showed strong agglutination activity against rat and human erythrocytes. The lectin activity was inhibited by glucose and lactose. This lectin was stable at the temperature range of 60^{o}C to 80^{o}C and pH range from 4 to 10. This lectin markedly lost its activity in the presence of denaturants urea and DTT. The lectin was a divalent ion-dependent glycoprotein that showed toxicity against brine shrimp nauplii. Furthermore, measurement of fluorescence spectra in the presence and absence of $CaCl_2$ indicated that Ca^{2+} stabilized the protein structure.

POSTER-48

GREEN SYNTHESIS OF SILVER NANOPARTICLES USING STRAWBERRY (*FRAGARIA ANANASSA)* FRUIT JUICE EXTRACT AND STUDY OF ITS ANTIBACTERIAL AND ANTIPROLIFERATIVE ACTIVITIES *IN VITRO*

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Abstract
Green nonoparticles especially biogenic silver nanoparticles show antibactiral, antifungal and antitumor activities due to their small size and surface structures. In the present study, we have synthesized silver nanoparticles from strawberry fruit juice extract and made an effort to investigate the antibacterial and antiproliferative activities of the synthesized AgNPs. AgNPs were synthesized by mixing $AgNO_3$ solution with *strawberry fruit juice* extract and incubated for 4h at room temperature and analyzed by UV-visible spectra (250-800 nm). Intense peak at 430 nm provide evidence of AgNPs synthesis. Synthesis of nanoparticles was confirmed by Transmission Electron Microscope (TEM) and the content of silver was determined by Energy-dispersive X-ray Spectroscopy (EDX). The 3D structure of the AgNPs was studied by Atomic force microscope (AFM). Functional groups were determined by Fourier-transform infrared spectroscopy (FTIR). Synthesized silver nano particles showed moderate antibiofilm activity against *P. aeuroginosa.* The AgNPs inhibited growth of *Salmonella enterica* and *E. coli* significantly as determined by turbidity and disc diffusion method. Cytotoxicity of the silver nanoperticles was studied against Ehrlich ascites carcinoma cells (EAC) by MTT assay. The silver nanoparticles inhibited the EAC cells growth remarkably. Toxicity of the silver nanoperticles was studied against brine shrimp nauplii and it was observed that the nanoparticles is several times lesser toxic than that of the silver nitrate solution.

POSTER-49

MOLECULAR RECOGNITION IN DERIVATIVES OF 2-AMINO-4-THIAZOLIUM CARBOXYLATE / CHLORIDE/NITRATE

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Thiazole moiety is found in variety of natural products and pharmaceutical agents as potent antimicrobial agents, anticonvulsant, antibacterial and antihistamine[1]. 2-Amino-4-thiazole acetic acid is a building block used in the synthesis of different active pharmaceutical products namely Cefotiam[2] (new cephalosporin with a broad spectrum of activity against both Gram positive and Gram-negative microorganisms). The current work deals with some multi-component systems (I-V) of derivatives of 2-amino-4-thiazolium ions with aromatic carboxylates, chloride and nitrate systems. The three dimensional structure of the compounds and their structure functional property could be understand by the preferred molecular recognition, hydrogen bonded patterns and supramolecular architecture which are formed through non-covalent interactions such as hydrogen bonding[3], aromatic π-π stacking interactions, C-H...π and anion...π interactions[4]. The preferred protonated site, primary and secondary interactions of the thiazole moiety with various acid will be discussed in detail.

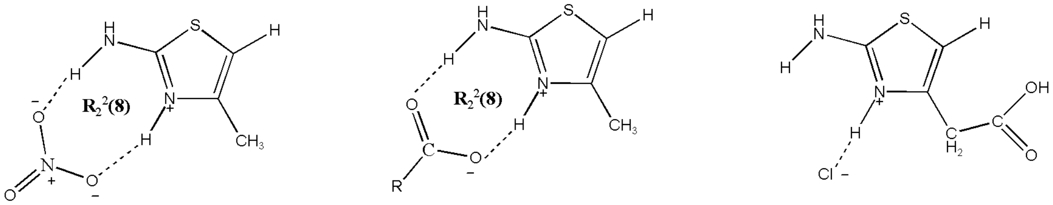

Figure 1. Molecular assemblies in derivatives of thiozolium ion with various acids.

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Poster-50

ANTIBACTERIAL AND ANTIPROLIFERATIVE ACTIVITY OF SILVER NANOPARTICLES SYNTHESIZED BY GRAPES (*Vitis vinifera*) EXTRACT

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Abstract

Nano-biotechnology is an emerging field of biomedical and pharmaceutical areas due to the boost properties of materials in the form of nano-sized particles. There are many noble metals found naturally which are palladium, silver, platinum and gold. Among these noble metals, silver has widely application in jewellery, dental alloy and health additive in traditional Bangladeshi, Chinese and Indian Ayurvedic medicine. The present study was to synthesize green silver nanoparticles (AgNPs) by fruits extract of green colour *Vitis vinifera* and to investigate its antibacterial and anticancer properties. Synthesized AgNPs was analyzed by UV-visible spectra at 250-700 nm. Atomic force microscopy (AFM) images were obtained to analyze the surface morphology of the synthesized AgNPs. AgNPs shape was spherical and nano size particle was measured by field emission electron microscopy (FETEM). The presence of silver in synthesized AgNPs was confirmed by energy dispersive X-ray (EDX) spectrophotometer. Functional groups of AgNPs were identified by fourier transform infrared (FTIR) spectroscopy. Five pathogenic bacteria were used for antibacterial activity of AgNPs. Among them *streptococcus aureus* was the most sensitive bacteria towards assisted *Vitis vinifera* AgNPs. That was also confirmed by the zone of inhibition study. AgNPs were tested against *Pseudomonas aeuroginosa* and *Klebsiella pneumonia* for antibiofilm activity. No biofilm was observed for *K. pneumonia* and *P. aeuroginosa* at synthesized AgNPs up to 96 and 120 h, respectively. Although AgNPs showed a mild toxicity against Brine shrimp nauplii, it showed a remarkable level of antiproliferative activity against Ehrlich ascites carcinoma (EAC) cells as determined by MTT assay.