<table>
<thead>
<tr>
<th>S.No.</th>
<th>Presenter</th>
<th>Title &amp; Abstract</th>
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</thead>
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| 1.    | Mr. Plawan K. Jha | **Title**: An effective chemical reduction of graphene oxide  
**Abstract**: Reduction of graphene oxide (GO) is an extremely important process as it holds the promise to produce a material, reduced graphene oxide (rGO), with physicochemical properties in close resemblance to pristine graphene. Though a number of ways reduction of GO to rGO can be achieved, chemical reduction is desirable from the view point of large-scale production. In conventional chemical reduction, reducing agents, such as sodium borohydride and hydrazine, could not be recycled for further use and thus posing a major challenge to develop efficiently cost-effective methods to produce high-quality rGO. Here, we present one-pot chemical reduction of GO in aqueous medium where rGO is isolated as the precipitate and reducing agent is simply recycled upon treating the filtrate with hydrochloric acid. Ultrahigh performances of as-synthesized rGO in all-solid-state (including flexible) supercapacitor applications along with the recyclability aspect clearly demonstrates that this synthetic approach can be an economically viable industrial process.  
| 2.    | Mr. Avishek Karmakar | **Title**: Hydrogen-Bonded Organic Frameworks (HOFs): A New Class of Porous Crystalline Proton Conducting Materials  
**Abstract**: Two porous hydrogen-bonded organic frameworks (HOFs) based on arene sulfonates and guanidinium ions will be talked about. As a result of the presence of ionic backbones appended with protonic sources, the compounds exhibit ultrahigh proton conduction values ($s$) $0.75 \times 10^{-2}$ S cm$^{-1}$ and $1.8 \times 10^{-2}$ S cm$^{-1}$ under humidified conditions. Also, they have very low activation energy values and the highest proton conductivity at ambient conditions (low humidity and at moderate temperature) among porous crystalline materials, such as metal–organic frameworks (MOFs) and covalent organic frameworks (COFs). These values are not only comparable to the conventionally used proton exchange membranes, such as Nafion used in fuel cell technologies, but is also the highest value reported in |
organic-based porous architectures. Notably, this report inaugurates the usage of crystalline hydrogen bonded porous organic frameworks as solid-state proton conducting materials.


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Mr. Prabhat Prakash

**Title:** Molecular modeling of CO2 absorption in Amino Acid Ionic Liquid

**Abstract:** Amino Acid Ionic Liquids contain multiple amine sites and are promising materials for CO2 absorption at room temperature. In my talk, I will present results on application of Molecular Dynamics simulations to explore the molecular mechanism and timescales of CO2 absorption in tetra-Butylphosphonium lysinate Ionic Liquid1. The structural properties show that CO2 molecules interact with both terminal amine sites of the lysinate anion, where the carboxylate group of the anion facilitates CO2 absorption. The dynamics show that absorption of CO2 leads to increased ionic liquid mobility. Results from our calculations provide insights for improvement in carbon capture by IL in the presence of water which can serve as predictive tool to synthesize novel ionic liquids for enhanced CO2 absorption.

**Reference:** Prakash, P.; Venkatnathan, A. RSC Adv., 2016, 6, 55438.

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Mr. Nandha Kumar

**Title:** Selectivity and Reactivity of Pd-Rich PdGa Surfaces toward Selective Hydrogenation of Acetylene: Interplay of Surface Roughness and Ensemble Effect

**Abstract:** Recent experiments have shown that PdGa nanocrystallites act as highly selective and reactive catalyst for selective hydrogenation of acetylene to ethylene. Motivated by these experimental results we have studied the mechanism and energetics of the above reaction on low indexed (100) and (110) PdGa surfaces using first-principles density functional theory based calculations. We find that the energetically favorable (100) surface created by cleaving the crystal in the less dense region shows reasonably good selectivity and high reactivity. The reactivity on this surface is comparable to that observed on Pd(111) surfaces. Since this surface termination is stable over a wide range of Ga chemical potential and hence is likely to occupy a substantial fraction of the surface area of PdGa nanocrystallites, we suggest this termination is responsible for the selectivity and reactivity exhibited by PdGa. In contrast to other surfaces where hydrogen adsorption and dissociation is followed by acetylene adsorption and hydrogenation, on this surface we identify a novel reaction mechanism in
which hydrogen dissociation occurs in the presence of acetylene. A careful analysis of the factors determining the selectivity shows that selectivity results due to an interplay between surface roughness and chemical nature of the reactive ensemble.


### Ms. Aditi Nandi

**Title:** Cisplatin-induced self-assembly of graphene oxide sheets into spherical nanoparticles for damaging subcellular DNA

**Abstract:** This report describes the hitherto unobserved cisplatin induced self-assembly of 2D-graphene oxide sheets into 3D-spherical nano-scale particles. These nanoparticles can encompass dual DNA damaging drugs simultaneously. A combination of confocal microscopy, gel electrophoresis and flow cytometry studies clearly demonstrated that these novel nanoparticles can internalize into cancer cells by endocytosis, localize into lysosomes, followed by DNA damage leading to apoptosis. Cell viability assays indicated that these nanoparticles were more cytotoxic towards cancer cells compared to healthy cells.


### Mr. Santosh P. Panchal

**Title:** Core-Modification of a Porphyrin into an Antiaromatic Isophlorin

**Abstract:** During the synthesis of porphyrin in 1960, Woodward proposed that condensing pyrrole with an aldehyde under acidic conditions yields the porphyrinogen macrocycle as an intermediate with four pyrrole rings. Its four electron oxidation leads to 20π isophlorin, which undergoes subsequent two-electron oxidation to the 18π porphyrin. Due to its unstable nature, 20π isophlorin has been a synthetic challenge for stabilizing its antiaromatic character. Antiaromaticity in general has not gained significant attention because of the perceived instability of 4nπ systems. However, a stable isophlorin and its derivatives provide a synthetic route into the world of antiaromatic systems. Partial core-modification of a porphyrin can be employed to synthesize a stable 20π antiaromatic isophlorin. Unlike the tetra-, tri-, and dipyrrole derivatives of a porphyrin, a monopyrrole porphyrin exhibits antiaromatic characteristics. It undergoes a two-electron reversible ring oxidation to yield the 18π aromatic dication. 1H NMR analyses provided distinct evidence of the altered electronic characteristics through typical paratropic and diatropic ring current effects for the 4nπ and the (4n + 2) π-electron systems, respectively.

| 7 | Ms. Mehak Malhotra | **Title:** Biodegradable Block Copolymer Nano-carriers in Cancer Treatment  
**Abstract:** There is a dire need for fully biodegradable aliphatic polyester nano-scaffolds as drug delivery vehicles in order to achieve complete enzymatic digestion of the polymer nano-carriers at the intracellular compartments. To accomplish this goal, new classes of biodegradable amphiphilic block and random copolymers based on hydrophilic carboxylic functionalized polycaprolactone (CPCL) and hydrophobic polycaprolactone (PCL) units were designed via ring opening polymerization methodology. The role of polymer topology on the enzymatic digestion of anticancer drug loaded nano-scaffolds at the intracellular compartments was investigated in breast and cervical cancer cells. The "burst" and "controlled" release of drugs from the polymer nano-carriers was directly controlled by chain length in the block copolymers and chemical composition in the random copolymers. In vitro cytotoxicity studies in breast cancer and cervical cancer cells revealed that the nascent polymer was highly biocompatible and non-toxic to cells up to 60 μg/mL whereas their DOX loaded nanoparticles accomplished > 90 % cell death in breast (MCF 7) and cervical (HeLa) cancer cell lines. The newly designed fully biodegradable PCL based block and random nano-carriers are excellent nano-scaffolds for enzyme-mediated intracellular delivery of DOX and the proof-of-concept was established in cancer cell lines.  

| 8 | Mr. Santosh Kumar Singh | **Title:** Direct Experimental Evidence for an $n\to\pi^*$ Interaction  
**Abstract:** $n\to\pi^*$ interaction is an extremely weak but very important non-covalent interaction. Just like any other non-covalent interaction, $n\to\pi^*$ interaction is widely present in biomolecules and materials. However, its existence has been debated extensively due to its counterintuitive nature. Here, we have reported strong experimental evidence of the $n\to\pi^*$ interaction for the first time by probing carbonyl stretching frequency in phenyl formate using IR spectroscopy in isolated gas phase. The current result also demonstrates that the conformational preference in the cis conformer of phenyl formate compared to the trans conformer arises due to the presence of the $n\to\pi^*$ interaction in the former one. The direct proof of this controversial but important non-covalent interaction will stimulate further experimental and theoretical investigation on this intriguing research topic.  
**Reference:** Singh, S. K.; Mishra, K. K.; Sharma, N.; Das, A. |
| 9  | Mr. Abhishek Swarnkar  | **Title:** Luminescence and Solar Cell from Colloidal Cesium Lead Halide Perovskite Nanocrystals  

**Abstract:** In this presentation, I will discuss about a new class of defect-tolerant nanocrystal (NC), namely colloidal CsPbX$_3$ (where X = Br and I) NCs, that exhibit high photoluminescence (PL) quantum yield (50 to 90%), and high power conversion efficiency (10.8%) from sensitized solar cells. Single-NC PL studies suggest reduced blinking in CsPbBr$_3$ NCs, along with similarity of spectral width between the single-NC PL and ensemble-PL. On the other hand, CsPbI$_3$ NCs with cubic phase were prepared, that exhibit a bandgap suitable for solar cell. Solar cell prepared from these colloidal perovskite NCs exhibit an open-circuit voltage of 1.2 V, with power conversion efficiency of 10.8%, and are more stable compared to organic-inorganic hybrid perovskite based solar cells. These devices also function as light emitting diodes (LEDs) with low turn-on voltage and tunable emission. These PL and solar cell properties of CsPbX$_3$ perovskite NCs are superior compared to traditional CdSe based colloidal quantum dots, suggesting CsPbX$_3$ NCs are better candidate for optoelectronic applications.  

**References:**  

| 10 | Ms. Arundhadi Roy  | **Title:** pH-Gated Chloride Transport by Triazine-based Tripodal Semicage  

**Abstract:** Chloride transport across biological membranes is essential for controlling the excitability of diverse neurons, acidification of internal and extracellular compartments, cell volume regulation, cell cycle, apoptosis, etc. Therefore, design and synthesis of synthetic molecular receptors functioning as chloride ion carriers is a rapidly expanding domain of supramolecular chemistry. In the present work, we have described Triazine-based pre-organized tripodal receptors for efficient transmembrane Cl$^-$ carriers. These receptors were designed based on triazine core and 3,7-diazabicyclo[3.3.1]nonane arms to facilitate preorganized cavity formation. Each bicyclic arm was further functionalized to control protonation and lipophilicity which are crucial for their efficient anion binding and effective transport through liposomal membranes. The benzyl substituted receptor was the most effective ion transporter followed by the |
pentafluorobenzyl substituted derivative. The nonsubstituted receptor was least active due to its high polarity. Two active transporters were found to function as mobile carriers for Cl\(^-\) via an antiport exchange mechanism. pH dependent activities were assessed by vesicle leakage assay with the chloride ion selective electrode (ISE) at different pH solutions. Molecular dynamic simulations with the most active receptor show a strong Cl\(^-\) binding within the cavity by direct and water-mediated H-bonds with its N-H groups.