Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information for:

Highlights from Kaleidoscope 2016: A Discussion Meeting in Chemistry, Goa, India, July 2016

The Kaleidoscope-2016 meeting comprised of a total of 9 platform sessions in all areas of chemistry interspersed over 3 days (July 15-17 2016). Sessions were thematic and chaired by a discussion leader who provided a 15 minute overview on the session topic highlighting key challenges and making connections to the presentations in the session. The oral presentations were interspersed with questions and discussions. In addition, each day concluded with a roundtable discussion of all participants, where discussion leaders re-visited key questions and points raised during the presentations and moderated the subsequent discussion. Discussions included blackboard explanations to concepts as well technical clarifications to the questions. Transcripts of the round table discussion for selective sessions are provided below.

Transcripts for Round-table Discussions

Day 1 – Session I: Dynamics in Complex Systems (Chair: Shachi Gosavi)

Talk 1 Tracer Diffusion in a Sea of Polymers with binding zones: mobile vs frozen traps (Rajarshi Chakrabarti)

Talk Summary: Rajarshi Chakrabarti discussed tracer diffusion dynamics through polymer media. He discussed multiple regimes of tracer diffusion dynamics which dependent on the polymer concentration.

Discussions:

Q) Biman Jana: *Can you elaborate on sub-diffusive and normal-diffusive regimes for the tracer?*

A) Rajarshi Chakrabarti: The tracer undergoes normal Brownian diffusion when the number and the binding affinity of the polymer traps are moderate. As the volume fraction and the binding affinity increases the dynamics of the tracer become sub-diffusive. However, it is worth mentioning that the effect of the binding strength is much higher on the dynamics of the tracer in comparison to the number of the polymer traps in the semi-dilute regime considered in our simulations.

Q) Naresh Patwari: *If you eliminate dwell times from the problem do you get to the normal diffusive limit?*

A) Rajarshi Chakrabarti: In the absence of any binding by the polymers the tracer will undergo normal Brownian motion. This is also confirmed by the control simulation, where the dynamics of the tracer is studied in the presence of polymers with no binding zones.

Q) Akash Guliyani/Roop Mallik: *Can you differentiate between diffusion controlled by binding events or those controlled simply by polymer crowding?*

A) Rajarshi Chakrabarti: In the absence of any binding affinity of the polymer the tracer gets bound very rarely even when the system is highly populated. It is the binding strength which primarily control the binding events. This is confirmed from the control simulations.

Q) Akash Guliyani: *Can you extract dwell times? Can you make the transport super-diffusive?*

A) Rajarshi Chakrabarti: Yes, the dwell time can be extracted from the simulations. We have in fact calculated the binding time or the dwell time of the tracer from the trajectories the same. For this we have relied on our own codes. We consider the tracer to be trapped when it is within a minimum distance (1.1σ) from at least two attractive monomers of the any polymers.

In the current system the dynamics of the tracer cannot be super-diffusive. It is possible in the presence of active elements in the system as correctly pointed out by Roop Mallik.

Q) Ravi Venkatramani: *In the plots of mean square deviation vs time, how do you define the zero time point for your trajectory?*

A) Rajarshi Chakrabarti:In the figures of Mean square deviations (MSD) against time, the times plotted are the elapsed time or the lagged time and this cannot be zero. We have recorded data for 5000 time steps, and MSD is calculated for elapsed time varying from 1 to 5000. However, when we plot the MSD in log-log scale, we get zero time point due to the log.

Talk 2 Decoding the language of molecular communication: Water mediated interactions, electrostatics and dynamics (Suman Chakraborty)

Talk Summary: Suman Chakraborty discussed long range water mediated interactions, electrostatics and dynamics in lipid vesicle models.

Discussions:

A) Suman Chakrabarty: The orientation of water dipole is defined with respect to the alignment to the radial vector of the (quasi-)spherical vesicle/reverse micelle. For each water molecule we calculate the angle (θ) between the dipole vector of the water molecule and the radial vector from the center of mass (COM) of the reverse micelle to the COM of the water molecule. For an isotropic (random) distribution of the orientation of water molecules, the probability distribution of the cosine of this angle (cos(θ)) would be uniform, whereas for a reverse micelle with charged interior interface the dipole vector will preferentially align along the radial vector (the sign will vary depending on the positive/negative charge on the interface). This definition remains valid unless the COM of water exactly overlaps with the COM of the reverse micelle (null radial vector), which is extremely rare and ignored if encountered.

Of course, near the center of the vesicle the ensemble average <cos(θ)> approaches zero indicating an isotropic environment due to length-dependent screening of the electrostatic interactions exerted by the charged interface as well as cancellation of the field exerted by other water molecules. Our objective is to understand the length-scale at which the isotropic angular distribution (bulk-like) is recovered as a function of the size of the reverse micelle.

Q) Shachi Gosavi: *How do you differentiate between the effects arising from membrane fluctuation dynamics vs those induced by the electrostatics?*

A) Suman Chakrabarty: The primary objective of this work is to compare the length-scale of perturbation of various structural order parameters of water due to presence of a charged interface. The distances at which the corresponding bulk properties are recovered strongly depend on the properties of interest. While the membrane shape fluctuations can quantitatively alter the length-scale, the relative trend between different order parameters remains the same.

Of course, the shape fluctuations render the radial profile of the structural properties (described in previous comment) less physically meaningful far away from the COM of the reverse micelle. For this reason we have tested a different definition of interfacial and core water to demonstrate that indeed the electrostatic interactions perturb the structural order parameters in the following order of length-scale: number density < tetrahedral order (local) < dipolar orientational order (global).

Q) Prashant Singh: *The hydrogen bonding strength of water at interfaces has been measured to be the same as that in bulk? How do we reconcile/connect these experimental results with observations from your study?*

A) Suman Chakrabarty: Our work highlights the fact that different properties of water are perturbed to different length-scale, i.e. the length-scale of perturbation is highly "context dependent". While the electrostatic interaction due to the charged interface has very long-range effect on the dipolar orientation of the water molecules, it does not affect the local tetrahedral order significantly. The water molecules locally rearrange to maintain the bulk-like hydrogen-bonding pattern. This observation is consistent with the experimental indication that the water-water hydrogen bond strength at interface is similar to bulk water. Water molecules can collectively and cooperatively rearrange in a global sense (dielectric response) while keeping the local hydrogen-bonding network almost intact. In fact, this is the origin of the high dielectric constant of water.

Talk 3: Charge Transfer Transitions in the Absorption Spectra of Proteins (Ravi Venkatramani)

Talk Summary: Ravi Venkatramani presented electronic structure calculations charged amino acids sampled from Molecular dynamics simulations of proteins. The computational data showed that the absorption profile of proteins 300 – 500 nm and beyond could be assigned to charge transfer (CT) transitions arising from charged amino acids.

Discussions:

Q) Akash Guliyani: *How does the absorption spectra from amino acid CT transitions depend on counterion concentration? Has it been systematically tested?*

A) Ravi Venkatramani: The amino acid CT absorption is expected to be sensitive to counterion concentration. Counterions will neutralize/screen the amino acid side-chain charges leading to a reduction in the extent of charge transfer with light absorption. We show through calculations that polar environment around charged amino acids (including water and oppositely charged amino acid head-groups) shift their absorption profile to the blue. Experimental results from our collaborators comparing spectra from high concentration pure lysine solutions with that from high concentration lysine salt solutions indicate that the absorbance at 270 nm (attributed to CT transitions) is attenuated in the case of the latter. However, no systematic examination of the dependence with counterion concentrations have been carried out yet.

Q) Anindya Dutta: *Would confining lysines (or other charged amino acids) in a reverse micelle without water be a better model to test the absorption profile arising from CT transitions*?

A) Ravi Venkatramani: Our collaborators have interrogated the absorption spectra of individual amino acids in high concentration solutions and showed prominent absorption features near 270 nm with tails extending beyond 400 nm. These experiments are similar in spirit to what you propose and highlight the absorption features of multimeric lysine chromophore assemblies. However, the problem in both cases is that the spectral features cannot be mapped back to an underlying molecular structure (as the assembly is by nature polydisperse). On the other hand our protein model allows us to precisely map the positions and interactions between the charged amino acids and link it to their absorption profile. Further, it appears that the three dimensional fold of the proteins enables ordered interactions between the charged amino acids which greatly extend the spectral range of the absorption upto 800 nm.

Q) Naresh Patwari: Do your excitations show couplings similar to those observed in J-aggregates?

A) Ravi Venkatramani: At present I`m not able to comment on the nature of the excitonic couplings. Our analysis is still in the early stages of assigning the spectral band to various chromophores arising from the interaction of charge amino acid side-chains. Only after we narrow down specific spectral windows and associated chromophores can we assess the couplings between excitations.

Q) Janardhan Kundu: *Is the CT coupling through space or through bond? Excitonic couplings are through space?*

A) Ravi Venkatramani: While we have not explicitly calculated CT couplings, based on the sensitivity of the transitions to the conformation of the charged amino acids we anticipate both through bond (the aliphatic part of the side-chain) and through space (direct overlaps between amino-acid head-group and backbone) components to contribute to the CT transitions.

Q) Janardhan Kundu: *Can you distinguish between the spectra of different charged amino acids?*

A) Ravi Venkatramani: The spectra are indeed sensitive to the identity of the amino acids. As shown in our calculations, there is a marked difference between the lysine and glutamate absorption with the latter exhibiting more prominent transitions which extend further down to the visible end of the spectra. Factors which influence the spectra are the chemical nature of the headgroups (π cloud, lone pairs) and the length of the side-chain.

Q) Naresh Patwari: *Can you comment on the effect of hyperconjugation effect to compare Arginine (R) vs Lysine (K) Spectra?*

A) Abhishek De: commented on the hyperconjugation effect.

A) Ravi Venkatramani: Hyperconjugation effects may confer conformational stability to the amino headgroup in both R and K systems. However as the spectral range under consideration are dominated by backbone to headgroup n-π^* or π-π^* transitions, these effects should not be the leading source of differences between the R and K spectral profile. As noted in my earlier responses, factors such as the different headgroups (bulkier amino containing group for R vs that for K) and shorter aliphatic chain length would be leading contributors to differences in the spectra of R and K amino acids.

Q) Rajarishi Chakrabarti: *How would the introduction of a polarizable water model in your simulations, change the results?*

A) Ravi Venkatramani: Our classical MD simulations of the protein in non-polarizable solvent show that water can mediate the interactions between lysine headgroups. While a polarizable water model should refine such interactions making water a more potent glue, the present model already shows extremely close (first interaction shell radius ~4.5 Å) interactions between the N headgroups. Thus, while we do expect some refinements, the major features and results discussed should not change. That being said, we could carry out QM/MM optimizations on the selected snapshots extracted from MD to see the effect of more realistic water model than in the present simulations.

Day I Session III: Biomaterials: Delivering and Transporting Cargo (Chair: Ankona Datta)

Talk 1: Antibacterial Strategies in Engineering Multifunctional Biomaterials (Kaushik Chatterjee)

Talk Summary: Kaushik Chatterjee presented various materials-based strategies that are being developed in his group to prevent bacterial infections associated with the medical implants and devices. He presented and contrasted several strategies that include the use of nanopatterns to mechanically disrupt the bacteria, the controlled release of drugs from materials as a chemical strategy and the use of surface functionalized nanoparticles embedded in polymer matrices as a synergistic physico-chemical approach.

Discussions:

Q) Akash Guliyani: How does the topology of the nanopillars in your engineered surfaces correlate with the size of the bacteria that they penetrate?

A) Kaushik Chatterjee: The pillars are prepared by reactive ion etching. We observe an etching rate of ~100nm/min. Pillars of 1 micron height were optimal for high bactericidal activity without significant cytocompatibility. The tip of the pillar is of the order of tens of nm and varies with etching time. In contrast, the bacterial cells are typically 1-3 microns in size.

Q) Neetu Singh: Won`t human cells covering the surface of the nanostructure render it ineffective in killing the bacteria? Will human cells be harmed by the nanostructures?

A) Kaushik Chatterjee: A co-culture or a sequential culture experiment is essential to investigate this issue, which have not been performed as yet. However, it is envisaged that the utility will be in the case of implants where the bacteria are attached to the implant surface before the device is implanted in the body at the time of surgery. Thus, the nanopillars should help to kill the attached bacteria even before the human cells have contacted the surface.

Q) Kanishka Biswas/Jyotishman Dasgupta: Why are the TiO_2 nanostructures black in color?

A) Kaushik Chatterjee: The cause of the black appearance is not clear but it is unlikely due to changes in chemistry since XPS suggests the surface is primarily titanium oxide. It is likely that the tall nanopillars trap the light resulting in poor reflectivity and thus black appearance. Since this surface is analogous to black silicon, the following has been proposed for black silicon with nanostructures that are 10 microns in height. The low reflectivity of black silicon is attributed to formation of an effective medium within the nanopillars where there is believed to be a continuous change in the refractive index. It is proposed that if the wavelength of light in silicon is similar to the height of this graded layer there is a large decrease in reflectivity giving a black appearance to the surface of the black silicon. Perhaps a similar phenomenon occurs here and needs further studies.

Talk 2: Role of Surface Structure of Cubosomes and its Applications in Drug Delivery (Neetu Singh)

Talk Summary: Knowledge of interaction of different types of nanoparticles with cells can be used to design an efficient drug delivery vehicle. Recent studies have shown that, apart from size, shape, surface charges and surface lipophilicity, the arrangement of surface hydrophilic and hydrophobic groups also plays an important role in deciding intracellular fate of the nanoparticles. Cubosomes are self-assembled liquid crystalline particles and can be loaded with hydrophobic, hydrophilic as well as amphiphilic drugs, an advantage over conventional drug delivery vehicle. Apart from these advantages, since, the cubosomes surface has patterned

hydrophilic and hydrophobic regions, it makes them a good model for studying the cellular uptake mechanism. In this presentation, synthesis and characterization of cubosomes, coating cubosomes with cationic poly-ε-lysine (PεL), their applications in theranostics and effect on cell uptake mechanism upon masking the patterned surface with PεL was discussed. Detailed uptake studies using different inhibitors, revealed the existence of alternative uptake mechanisms for the negatively charged, uncoated cubosomes, which was also discussed.

Discussions:

Q) Ankona Datta: *What are cubosomes? Can you please elaborate on the structural details?*

A) Neetu Singh: Cubosomes are lipid based, biocompatible nanoparticles, formed by self-assembly of amphiphilic lipids when added to water in a specific ratio. Their internal structure is an inverse bicontinuous cubic phase, with hydrophobic and hydrophilic channels, providing them with the ability to carry hydrophilic, hydrophobic and well as amphiphilic drugs.

Q) Shachi: *How do you tune relevant parameters to obtain the structures for targeting?*

A) Neetu Singh: The cubosomes have an inherent negative surface potential. This was used to coat them with poly-ε-lysine (PεL), a positively charged polymer with amine functionality. These amine groups can further be used for conjugation of targeting moieties, like antibodies. The PεL coating also masks the hydrophilic, hydrophobic patterned surface of the cubosomes, thereby also providing a control over intracellular fate of the cubosomes.

Q) Anindya Dutta: *What is the fate of the cubosome after the drug is delivered? What is the mechanism of action and release?*

A) Neetu Singh: Cubosomes are composed of biodegradable lipid, monoolein. After internalization, the cells can metabolize the monoolein to generate energy, or can store it in form a triglyceride in the lipid droplets.

Cubosomes act by hijacking the different uptake mechanisms of cells for intracellular delivery of the loaded drugs, which lack the ability to cross the cell membrane. Depending on the type of drug loaded, the release of drugs can occur by diffusion (hydrophilic drugs) or by degradation of cubosomes (hydrophobic drugs).

Day 2 Session IV: Tools for Probing Biology (Chair: Kana Sureshan)

Talk 2: Imaging Signal Mediators in Biology (Ankona Datta)

Talk Summary: Ankona Datta highlighted challenges in tracking the spatio-temporal dynamics of signal-mediating phospholipids in live biological systems in the context of elucidating phospholipid mediated cell-signalling pathways. She presented her group's work on developing ratiometric cell-permeable sensors for imaging a major class of signal mediating phospholipids, the phosphoinositides.

Discussions:

Q) Naresh Patwari: *Can other negatively charged phospholipids/metabolites perturb your detection of PIP2? What is the underlying mechanism for the sensitivity of the peptide to PIP2?*

A) Ankona Datta: Our *in vitro* studies have been performed in the presence of other negatively charged phospholipids and also in the presence of soluble phosphor-anions. We have found that the detection of PIP2 is not affected in the presence of either.

The underlying mechanism for the selectivity of the peptide towards PIP2 is not completely understood. It is known that the positively charged residues on the C terminal side of peptide can interact with the negatively charged phospholipid head group. Also the N terminal side of the peptide has hydrophobic residues that can interact with the membrane. We are using molecular dynamics simulations in collaboration with Dr. Ravindra Venkatramani (TIFR) to understand the genesis of this selectivity. This is a very important question to address since only if we understand the molecular basis of this selectivity, we can go ahead and design selective sensors for specific phosphoinositides.

Q) Akash Guliyani: *How does one measure the binding affinity of the sensor to PIP2?*

A) Ankona Datta: The binding affinity of the sensor to PIP2 is measured from the fluorescence response of the sensor. We plot the ratio of fluorescence intensities against the phospholipid concentration and fit the data to an appropriate binding model.

Q) Kana Sureshan: *Have you tested the sensor with PIP(3,4)?*

A) Ankona Datta: No, but we plan to.

Q) Shachi: What is the structure of the protein binding to PIP2 and its binding domain?

A) Ankona Datta: The crystal structure of Gelsolin, the PIP2 binding protein on which we have based our peptide receptor design is known. However there is no crystal structure of the phospholipid bound protein.

Q) Roop Mallik: Does the peptide penetrate the membrane? Does the peptide bind to the inner or outer leaflet?

A) Ankona Datta: The peptide penetrates the membrane. We have attached a polarity-sensitive dye to the peptide. Only when the peptide binds to phosphoinositides in the membrane it emits in the blue region of the spectrum. The unbound peptide emits in the green. We can see green fluorescence from the cytosol within 5 min of incubation of the peptide with live cells, in our confocal images. We can also see intensity in the blue region from the plasma membrane and the perinuclear region indicating the presence of phosphoinositides.

Our *in vitro* data clearly indicates that the peptide binds selectively to phosphoinositides. Since phosphoinositides are present in the inner leaflet of the plasma membrane we infer that the peptide binds to the cytoplasmic side of the membrane.

Talk 3: Redox regulation of antibiotic resistance (Harinath Chakarapani)

Talk Summary: Maintenance of redox homeostasis in cellular survival is critical. Cells respond differently to induction of redox stress, where either reducing or oxidizing equivalents are increased. Different cells were expected to respond differently to such stress and may thus pave the way to new drugs. Using natural products as the starting point, a series of simpler analogues that would satisfy the functional aspects of the design i.e. perturbation of redox homeostasis were identified. A simpler compound was found to have potent inhibitory activity against MRSA. The possible mechanism of action of these compounds is enhancement of reactive oxygen species (ROS) that leads to DNA damage. The possible ways forward with such an approach and some interesting leads were presented.

Discussions:

Q) Naresh Patwari:*These days organic chemists can synthesize fairly complex scaffolds including those with chiral centres. Would these be useful in the context of your applications?*

A) Harinath Chakarapani: Chiral centres are useful when specific targets are in play. For example, one enantiomer may interact differently with an enzyme/receptor when compared with another. However, as our design is to induce non-specific stress, chiral centres are not desirable. We generally work with simple scaffolds that do not have chiral centres.

Q) Jyotishman Dasgupta:*Can you design molecules whose mechanism of action is based on iron-chelation chemistry or target ciderophores?*

A) Harinath Chakarapani: Yes, it is possible and there are examples of siderophore delivery agents. Although it is unclear if iron-chelation is the only mechanism operational.

Q) Prasenjit Mal:*What is the mechanism of antibacterial resistance? Is it the same for all drugs?*

A) Harinath Chakarapani: Drug resistance is broadly classified into four mechanisms – one, the drug target is modified; two, an efflux pump is operational; three, a new enzyme that inactivates the drug is operational; and four, the bacteria become less permeable to the drug.

Q) Prasenjit Mal:*How does one find a suitable antibacterial drug from a large pool of molecules?*

A) Harinath Chakarapani: This is the task that all industrial/academic labs are trying to answer. Using large-scale screening of diverse scaffolds, one can try and identify hit compounds. These compounds can then be optimized as leads.

Q) Janardhan Kundu:*Would the ROS not be harmful to the host organism?*

A) Harinath Chakarapani: Yes, ROS is harmful to the host organism. However, there are several examples of compounds that act through ROS generation and are well tolerated. The key may be that mammalian cells may be better at coping with enhanced ROS when compared with certain bacteria. The approach may also find use in cases where multi-drug resistance occurs. Here, the options for therapy become very limited.

Day-2 Session VI: Excited States (Chair: Sayan Bagchi)

Q) Harinath Chakrapani/Jyotishman Dasgupta: *Why is it difficult to do excited state calculations?*

A) Ravi Venkatramani: The lack of structural information of molecules in the excited state is a big bottleneck in computing excited state properties. Typically ground state calculations are initiated near a well-defined reference molecular geometry (e.g from structure determination experimental techniques). On the other hand, excited state calculations are typically seeded at a ground state nuclear geometry and extensive geometry optimizations (accounting for other close lying electronic surfaces) need to be carried out to arrive at the excited state minima from which properties can be calculated. Other problems include the lack of good basis functions and the lack of a general variational principle for excited sate calculations.

A) Vaibhav Prabhudesai: For anion excited states additional complication of the not so well defined configuration also makes the scenario much more difficult to handle. The anion excited states are usually resonances and many times they are addressed using the scattering

calculations with approaches like R-matrix method clubbed with standard quantum chemistry tricks. Complex scaling of potentials have been successful in this to some extent but much more is desired to be done. The only reported excited anion potential energy surface that has been reported so far is for water and many more efforts are needed to be put in.

Talk 1: Molecular Dynamics of Excited Negative Ions (Vaibhav Prabhudesai)

Talk Summary: Vaibhav Prabhudesai from TIFR, Mumbai spoke about his group's efforts to understand chemical reactivity by describing one specific example of electron attachment studies on Ozone. He indulged in describing the velocity slice imaging experimental set up and the way electron spectroscopy is performed on molecular systems.

Discussions:

Q) Akash Guliyani: *How is molecular dynamics inferred from Vaibhav`s experiments on ozone?*

A) Vaibhav Prabhudesai: The experiment involves detecting the fragment negative ion from the low energy electron collision to neutral molecules and measuring their momenta using velocity slice imaging technique (a variant of velocity map imaging technique). As the electrons are attached to the molecule forming an anion which subsequently dissociates giving the fragment anion, knowing the kinetic energy and the angular distribution of the fragment anion w.r.t. the incoming electron beam, one can infer the molecular dynamics the excited anion state undergoes. The kinetic energy of the fragment anion can be used along with the threshold energies known for that fragmentation channel to determine the excess energy in the system that has not shown up in the form of kinetic energy of the fragments. (Although we measure the kinetic energy of only the anion product one can infer the kinetic energies of the corresponding neutral fragments using the energy and momentum conservation principles along with the known structure of the neutral ground state.) The angular distribution of the anion fragment with respect to the incoming electron also helps in understanding the symmetries of the excited anion state involved under axial recoil approximation. Under this approximation which assumes that the molecule does not undergo any rotation before dissociation and the fragmentation of the parent molecule retains the orientation of the dissociating bond w.r.t. the incoming electron beam, we can picture the preferred orientation of the molecule for electron attachment based on the anisotropy observed in the angular distribution. On the other hand, if the molecule undergoes substantial internal motion before dissociation that shows up as lower kinetic energies of the fragment than the expected values. The angular distribution can also be predicted under axial recoil approximation based on the symmetry of the initial neutral state and the final anion state and any deviation from this expected anisotropy will also be used in inferring the molecular dynamics of the anion state leading to dissociation.

In the specific case of Ozone, we observe the velocity slice images of momentum distribution of O^- ion resulting from electron attachment. There are two possibilities of formation of O^- ions namely O^- coming from the end of the tri-atom or the middle O atom becoming the O^- and ejected with the terminal atoms either ejected as O_2 or individual O atoms. All these channels have different threshold and the angular distribution patterns along with the energy of O- help us unravel the underlying dynamics of the anion excited state leading to dissociation. For example, at 4eV electron energy a strong backward anisotropy observed in the O^- angular distribution which shows stronger signal of O^- in the backward direction w.r.t. the electron energy, indicates that for middle O^- atom to give this kind of angular distribution the e must approach preferentially along the principle axis of the molecule and that too from the bent side of it. In that case the terminal oxygen atoms will undergo ejection with them coming together via bending mode vibration of the anion and leaving as O_2 molecule with vibrational excitation. The energetics from the image supports such inference as the O^- ion shows lower kinetic energy than expected from the axial recoil scenario along with the angular distribution not predictable under that approximation. The three body fragmentation channel cannot contribute as its threshold is 4.8 eV which is above 4 eV electron energy. The corresponding O_2^- image shows strong forward distribution is an additional support to this inference.

Talk 3: Tracking Excited State Structural Changes in Conjugated Polymers (Jyotishman Dasgupta)

Talk Summary: Jyotishman Dasgupta described his group's efforts to understand exciton dynamics in conjugated polymers using time-resolved Raman spectroscopy. He introduced the idea by bringing in ideas of controlling excited state reactivity by preorganization and demonstrating that previous work from the lab had shown charge transfer kinetics can be used to map out ground state complexation in polymer-fullerene solution mixtures. He went on to describe the reaction coordinates that lead to exciton relaxation in a donor-π-acceptor backbone. He ended by stating that collaborative work on organic photochemistry with Dr. Kana Sureshan (IISER TVM) started from last year's Kaleidoscope were yielding impressive results.

Discussions:

Q) Shachi Gosavi: *What is the nature of the polymer-electrode interface?*

A) Jyotishman Dasgupta: The polymer attaches itself through physisorption although there can be chemical moieties through which the polymer can be chemisorbed as well. In the case that was presented, the polymer chosen was P3HT (poly-3-hexyl-thiophene) which typically is spin

casted on the electrode surface. However donor-pi-acceptor based low bandgap polymers can have well-defined specific interactions with the electrode surface.

Q) Roop Mallik: *Why was fullerene chosen as the electron acceptor? Can CNTs substitute instead?*

A) Jyotishman Dasgupta: Fullerenes are chosen as acceptors because the fullerene aggregates have good electron mobilities and correctly positioned LUMO energy as compared to other small molecule acceptors. The other reason for the usage is the geometric nature of the structure which allows for stable heterojunction formation by mixing polymer and fullerenes. However the issue has always been the diffusion of the small fullerene balls inside the device which tends to change the performance of the devices. Previous work has shown that these fullernes can be photochemically cross-linked to make the BHJ layer more robust. CNTs have been used previously and they do work but not with as much success as the fullerenes. However the community is on the look-out for an alternate molecular acceptor which can match the fullerene mobilities at a much cheaper price.

Q) Naresh Patwari: *Can you compare linewidths of IR and Raman measurements? Why should they be different?*

A) Jyotishman Dasgupta: The homogenous linewidth of IR and Raman lines are different due to the instrinsic nature of the transitions. Raman linewidths arise from two factors: angular fluctuations of the molecules in liquid state convoluted with the intrinsic vibrational linewidths which have a finite vibrational lifetime. The computation of the Raman linewidths, therefore, is carried out through a Fourier Transform (FT) of the product of two correlation functions: (a) Raman polarizability and (b) fluctuation of the normal mode coordinate. For IR linewidths, the dipole moment fluctuations are considered which are directly calculated by computing the FT of the dipole-dipole correlation function.

Q) Prasenjit Mal: *What was the excitation wavelength and power used for photoreactions involving the C-S bond?*

A) Jyotishman Dasgupta: We used 400 nm LEDs for carrying out the reaction to break the C-S bond. The power was less than <1 mW.

Day-3 Session VII: C-H Activation and C-C coupling (Chair: Sabuj Kundu)

Talk 1: Palladium and Copper in Cross-Coupling and C-H Bond Activation: From Micro to Nanoscale Catalysis (Nidhi Jain)

Talk Summary: Nidhi Jain discussed Palladium and Copper in cross-coupling reactions and their applications towards C-H Bond activation. The focus of the talk was to demonstrate strategies on developing new reactions with both molecular catalysts as well as nanoparticles with ionic liquid capping.

Discussions:

Q) Kanishka Biswas: *How was the size of Pd nanoparticles determined in the presence of ionic liquids?*

A) Nidhi Jain: The size of nanoparticles was determined by DLS analysis. The NPs were washed with ether to remove most of the IL, collected by centrifugation, and then re-dispersed in acetonitrile to record DLS.

Q) Rajarshi Chakraborty: *Nanoparticles size depends on the counterion of Pd ($PdCl_2$ nanoparticle sizes are 5x larger than obtained with other salts), why?*

A) Nidhi Jain: This is due to the lower solubility of $PdCl_2$ in IL, which results in a more heterogeneous distribution, resulting in larger sized Pd NPs.

Q) Neetu Singh: *Question about product stability*

A) Nidhi Jain: The NPs are stable in IL and do not agglomerate.

Q) Naresh Patwari: *What is the mechanism of interaction between the reactants and the Pd nanoparticles? Do reactants displace the ionic liquid capping?*

A) Nidhi Jain: The reaction works at the interface of homogeneous/heterogeneous catalysis. The active Pd(0) particles exposed at the surface interact with the substrate molecules, and initiate catalysis.

Q) Prasenjit Mal: *What is the mechanism for the amination reaction?*

A) Nidhi Jain: CuI forms a six membered chelate with the enolate form of ethylacetoacetate-tagged ionic liquid. This is the active catalyst which undergoes oxidative addition with aryl

halide followed by transamination, and then reductive elimination to yield the aminated product, regenerating back the Cu(I) species.

Talk 2: Highly selective C-C bond formation: From asymmetric catalysis to C-H bond activation (Ravi P. Singh)

Talk Summary: Selectivity in organic transformations, whether chemo-, regio- or stereo is the most challenging to achieve. Often, active molecules of drugs are either single enantiomer of chiral compounds or a single diastereomer. Thus, the design and development of new methods for the synthesis of small molecule drugs and bioactives must address the selectivity efficiently. In this presentation, various examples were discussed where the stereo selectivity of a very broadly applicable reaction such as the vinylogous aldol, Mannich and Micheal reaction were discussed. The talk specifically dealt with selective addition of vinylogous nucleophiles to various acceptors that can be particularly useful in accessing γ-butenolides and γ-lactone frameworks in the total synthesis of natural products and biologically active molecules. These heterocycles behave as a vinylogous nucleophile and after reaction with carbonyl and carbonyl derived compounds (aldehydes, ketones, aldimines, ketimines, enals, enones, and heteroatom-stabilized carbenium ions) offer a multitude of highly functionalized structures. Also, it grants a synthetic track, where a number of functional group and selected stereochemistry can be established. Here, a highly diastereo- and enantioselective organo catalytic asymmetric vinylogous Mukaiyama-Michael addition of various silyoxyfurans to enones, and vinylogous aldol reaction of 2-silyloxyindoles to ketones, which proceeds through the bifunctional catalysis, was presented. Also, vinylogous Mannich reaction of a highly regio- and diastereo- selective TMSOTf promoted synthesis of chiral quaternary 3-aminooxindole butenolides from 2-silyloxy furans and chiral ketimines will be discussed. Highly regio- and diastereo- selective Lewis acid catalyzed vinylogous Mannich reaction of 2-silyloxyindoles with chiral aldimines and vinylogous nucleophilic substitution reaction with diarylmethanols will be highlighted.

Additionally, as an example of site-selective C-H activation, a ligand enabled Cu catalysed intramolecular C-2 site selective Csp^2-H/ Csp^2-H activation method for *N*-substituted prrrole-azole system was discussed. Copper salts, comparatively economical than other transition metal salts and less toxic has also been used for intramolecular C–H coupling reaction between indole-2 and imidazole-2 moieties to deliver annulated polycyclic heteroarenes.

Discussions:

Q) Sabuj Kundu: *What is the mechanism of the cross dehydrogenated coupling?*

A) Ravi P. Singh: In cross-dehydrogenative coupling two unmodified C-H bonds (for C-C bonds) or C-H and N-H bonds (for C-N bond) lead to the formation of C-C or C-N bond. In totality it

occurs with loss of one equivalent of H_2 . The formation of C-C or C-N bond with the loss of H_2 is thermodynamically unfavorable and hence it requires use of oxidant.

Q) Prasenjit Mal: *What is the mechanism for the 1,2 addition product involving cyclohexanone and 2-hydroxyfuran?*

A) Ravi P. Singh: In 1,2- addition product of cyclohexanone activation of carbonyl group by Lewis acid or by hydrogen bonding is required. It leads to generation of positive charge on carbonyl carbon. Further, it is followed by vinylogous attack by 2-furoxy anion.

Q) Nidhi Jain: *What is the order of stability for the amines?*

A) Ravi P. Singh: Amines after dissolution in water form corresponding protonated amines. Also the number of possibilities of hydrogen bonding increases. More the number of hydrogen bonding more is the hydration. The more hydration energy of the molecule, more is the stability of the amine. In terms of hydration energy, tertiary amines are least stable followed by the secondary amine followed by the primary amine.

Q) Jyotishman Dasgupta: *A question for all session speakers: What is the most challenging aspect of C-C coupling and C-H activation reactions?*

A) Ravi P. Singh: The most challenging problem is activation of selective sp3 C-H bonds for formation of C-C bond or other functionalization.

Talk 3: Bi-functional Ru^{2+} complex catalyzed chemoselective transfer hydrogenation and tandem C-C bond formation using alcohols (Sabuj Kundu)

Talk Summary: Synthesis of phenanthroline based 2-(6-methoxypyridin-2-yl)-1,10-phenanthroline (phenpy-OMe), and 2-(2-pyridyl-2-ol)-1,10-phenanthroline (phenpy-OH) ligands and their corresponding ruthenium(II) complexes was discussed by Sabuj Kundu. Bifunctional Ru(II)-(phenpy-OH) complex exhibited excellent catalytic activity in transfer hydrogenation (TH) of ketones and nitriles using 2-propanol as a hydrogen source. Further, exploiting the metal-ligand cooperativity sterically demanding ketones were readily reduced and chemoselective TH of ketones were achieved. Same catalyst was found to be highly efficient to promote the one-pot β-alkylation of secondary alcohols with primary alcohols and double alkylation with different primary alcohols.

Discussions:

Q) Vaibhav Prabhudesai: *Why do your plots seem to show that the rates of the reaction increase linearly upto 100% product formation?*

A) Sabuj Kundu: Reaction rate does not increased linearly upto 100%. Initially, rate was slow due to generation of the active catalyst. After that it speed up significantly. However it

decreased after around 70% conversion of the starting materials. We confirmed this by measuring TOF at different time interval. As the graph is cut off due to limited space it may looks like that.

Q) Ravi K.P. Singh: *How does one determine the role of isopropyl alcohol (solvent) to generate ruthenium-hydride complex?*

A) Sabuj Kundu: Isopropyl alcohol has no substantial role in generating ruthenium hydride species. Hydride is coming from Na isopropoxide via β-hydrogen elimination reaction. When we carried out stoichiometric reaction using Ru-Cl with Na isopropoxide in DCM it smoothly produced the ruthenium hydride species. However, when other base such as NaOH or KOH is used then more isopropyl alcohol helps to produced corresponding isopropoxide which subsequently control the Ru-H formation.

Q) Ravi Venkatramani: *What are the N-Ru bond lengths in the Ru^{2+} catalytic complexes?*

A) Sabuj Kundu: In this complex three Ru–N bonds are (1.953–2.121 Å) based on the crystal structure.

Day-3 Session VIII: Computational Biophysics (Chair: Rajarshi Chakrabarti)

Talk 1: Understanding Protein Dynamics Using Structure Based Models (Shachi Gosavi)

Talk Summary: Shachi Gosavi discussed structure-based models (coarse-grained or atomistic models that encode the structure of the biomolecule and which have been successfully used to understand both the folding and the dynamics of several proteins and RNA) and their evolutionary underpinnings. She then introduced dual-structure based models (dSBMs) which encode two structures: potentially the end points of a conformational transition. Such dSBMs in conjunction with molecular dynamics (MD) simulations can be used to understand conformational transitions. She then spoke about mechanisms of ligand recognition: induced fit and conformational selection and introduced two proteins which are structurally similar but where each protein has a different mechanism of ligand recognition. Finally, she showed that dSBMs predicted the correct mechanism of ligand recognition for each protein and could be used to identify structural elements in the proteins that facilitate the specific mechanism of ligand recognition.

Discussions:

Q) Ravi Venkatramani: *You highlighted the slowest large scale fluctuations in your studies. However, since the conformational changes in proteins correspond to multiple responses,*

including survival in the cell, the functional modes may not be the lowest frequency modes. Can you comment on this aspect?

A) Shachi Gosavi: Not all functional fluctuations will be the lowest frequency modes of a protein. For instance, local amino acid fluctuations are likely to be present in the active site of an enzyme and will aid catalysis. In enzymes which also have much larger conformational fluctuations (such as several kinases) these local catalytic pocket changes are not going to be the lowest frequency modes. Most normal mode analyses make the opposite argument which is: given that the lowest frequency modes require the least amount of energy to excite, it is likely that they have evolved for function. The use of dSBMs do not require that this argument be made because by encoding both structures and varying their energetics you can drive the conformational change that you wish to study.

Q) Jyotishman Dasgupta: *You commented that spectroscopic probes have little effect on protein structure? What is the justification for this viewpoint?*

A) Shachi Gosavi: In general protein structures are assumed to be fairly robust to a variety of changes in condition and so it is likely that they will be robust to the attachment of various spectroscopic probes as well. That being said, the last I checked (which was a while ago) there wasn't consensus about whether or not large dyes affect local protein structure or not. There have been some simulation studies which have claimed that certain FRET dyes had attractive interactions with the protein surface and did affect structure (this is likely to be protein and dye specific). However, FRET experiments generally assume that the dye can rotate freely. More recently, SBM simulations have shown that attaching a GFP molecule to a protein can change its stability. So overall, it seems that one needs to be careful while interpreting the more sensitive experiments!

Day-3 Session XI Novel Methodologies in Synthesis (Chair: Nidhi Jain)

Talk 1: A Novel and General Methodology for Carbasugar Synthesis (Kana Sureshan)

Talk Summary: Sureshan introduced various structurally complex carbasugar natural products and their wide spectra of biological activities. Nature has made a combinatorial library of more than 200 known carbasugar natural products from cyclohexene core by varying the number and position of oxygen functionality, stereochemistry, oxidation state, position of double bond, O-substitution etc. A common strategy to synthesize these molecules would be to have access to the core cyclohexene with multiple hydroxyl groups. Sureshan explained his novel results on the vinylogous opening of orthoesters and ketals of cheaply available inositols producing a hydroxylated cyclohexenal. He has demonstrated the use of this novel methodology for the synthesis of about 25 natural carbasugars.

Discussions:

Q) Jyotishman Dasgupta: *What is the biochemical pathway for carba-sugar synthesis? Is it different from carbohydrate synthesis?*

A) Kana Sureshan: Their biosyntheses are related but not same. Carbohydrate synthesis in plants mainly happens through photosynthesis and the glucose thus produced are converted to other monosaccharides and oligo/poly saccharides enzymatically (using epimerases, dehydrogenases, glycosyl transferases, etc). Animals get most of their carbohydrates from plants. In animals, monosaccharides are also biosynthesized from non-carbohydrate intermediate such as pyruvate, lactate, glycerol etc. Most of the carbasugars are synthesized from carbohydrates or their derivatives through C-C bond forming enzymatic reactions.

Q) Naresh Patwari: *If carbasugars have similar binding affinities to receptors as regular sugar, can they be used to replace regular sugar in food items?*

A) Kana Sureshan: Carbohydrates do many functions. While a few carbohydrates (in the form of monosaccharides) are the source of energy, many others (monosachharides and oligosaccharides) are heavily involved in cell signaling, determining structure of protein, lipids etc. In the case of signaling sugars, they bind to proteins (receptors or metabolizing enzymes) and initiate the cascade of signaling. Once the signaling event is done, the signaling molecule gets metabolized by various enzymes. Aberration in the signaling or activities of these metabolizing enzymes leads to diseases. Carbasugars being structural mimics of these signaling sugars, they competitively bind to the receptors or metabolizing enzymes, thus reducing their activity. Such non-metabolizable competitive inhibitors are potential drug leads and tool to understand the signaling in detail. Also some carbasugars themselves are signaling molecule.

To answer your question whether carbasugars can replace dietary sugars, the answer is a probable ‘no’ for the following reasons. (i) While the sugars are produced in abundance in nature, natural carbasugars are very rare and are produced in minute quantities for plant signaling. (ii) As mentioned earlier, carbasugar can’t be metabolized (which is important for energy release and storage) in the same way as carbohydrates and hence they can’t be a replacement for energy needs. (iii) While we know that monosachharide like glucose gets absorbed to the blood stream from the GI tract, we know little about the absorption of carbasugars. (iv) As carbasugars can interfere with sugar processing enzymes (glycosidases, glycosyl transferases etc), which are essential for many biological processes and vital functions, consumption of carbasugars in large amount can be lethal.

Q) Prasenjit Mal: *How is the electrostatics impacted by the C-> O replacement?*

A) Kana Sureshan: Of course there might be difference in electrostatics of carbasugars and normal sugars. More important is the reactivity. While carbocyclic ring is robust, natural carbohydrates and their derivatives are (hemi)acetal by virtue of their ring oxygen. This key functionality makes them reactive and is important for metabolism. Hence, carbasugars can not be metabolized by sugar processing enzymes.

Q) Harinath Chakrapani: *How is the flexibility impacted by the C→ O replacement?*

A) Kana Sureshan: Both pyranose ring and cyclohexyl ring are expected to have more or less similar conformational flexibility. However, most of the natural carbasugars have a double bond in the ring, which limits the conformational flexibility.

Q) Ankona Datta: *Is finding a glycosylase inhibitor the main goal for developing carbasugar synthetic strategies?*

A) Kana Sureshan: Not really. Finding novel glycosidase inhibitor is just one of the objectives of carbasugar synthesis. As carbohydrates are involved in many cellular signaling, study of carbasugars has wide ranging potentials in development of ligands that interfere with signaling mechanism. Such ligands are essential for understanding the mechanism of cellular signaling in detail and also they could have potential therapeutic applications.

Q) Nidhi Jain: *Have you done a comparative binding analysis between carbasugars and regular sugars?*

A) Kana Sureshan: We have shown a method to access various carbasugars. We have not done any binding studies yet, but we plan to investigate their biological activities and Structure Activity relationship studies with these molecules. Competitive binding studies will be one of such experiments.

Talk 2: Enabling Non-conventional Pathway for Organic Synthesis (Prasenjit Mal)

Talk Summary: With growing public concern on renewable energy and global warming, it is essential to minimize the usage of chemicals in routine synthesis. During the presentation, Prasenjit Mal has demonstrated chemical reaction methodologies under ball milling condition e.g., (a) IBX (2-iodoxybenzoic acid) induced oxidations reactions (b) Electrophilic aryl-halogenation using *N*-halosuccinimides (c) Oxidative amidation (d) Subcomponent synthesis of

supramolecular architectures, etc. It was anticipated that ball milling methodology could possibly be used as a supply of mechanical energy. The reactions reported under this topic were done at solvent free condition and at room temperature. This work was presented as a part of development in the area of mechanochemistry. In addition, it was also discussed about the efforts to develop more viable and efficient synthetic protocols using ultrasound and visible light photoredox catalyst.

Discussions:

Q) Anindya Dutta: *How did you characterize the products yielded in the sub-component reaction approach?*

A) Prasenjit Mal: The reactions were done in open atmosphere and monitored using ^{1}H NMR spectroscopy. During monitoring, milling apparatus was stopped and followed by small portion of the sample was collected from the reaction jar and then dissolved in D_2O to record proton NMR. After this action, the reaction was started again and this operation time was excluded for reporting the reaction timing. After completion of the reaction, products were isolated and washed with small portion of acetone to remove excess pyridine-2-aldehyde, if any. The complexes were characterized using the spectroscopic techniques i.e., NMR (wherever applicable), ESI-MS or X-Ray. The purity of the mechanochemically synthesized $\mathbf{M_4L_6}$ cages was verified upon comparing the powder XRD pattern of the genuine sample of the cages synthesized in solution phase chemistry.

Q) Amit Paul: *Ultrasound frequencies are too low to break a bond, so how does it work in your case?*

A) Prasenjit Mal: Through demonstration of ultrasonically induced scission of the C_{sp3}-C_{sp3} bond in appropriately substituted cyclobutenols (**CB**s), mechanical excitation has been shown to be a probable source of energy to control reactivity of small molecules if they are suitably functionalized to support intermolecular interactions up to an appropriate level, such that, they can collectively compete with covalent interactions and substantially reduce dissociation energies selectively of certain bonds. Such intermolecular interactions can lead to polymeric self-assembly of molecules enabling absorption of mechanical energy through low energy vibrational modes.

Q) Biman Jana: *Are the products from a reaction in solution phase equivalent to those obtained from ball milling?*

A) Prasenjit Mal: In the presented work, the subcomponent synthesis of metallosupramolecular species under ball milling conditions was reported. The results are the same as observed in solution studies. However, it never could be expected, that the specific self-assembly takes place under those drastic conditions. In solution usually relative low concentrations of components are chosen in order to guarantee self-assembly based on thermodynamic control. In the present case the components are used in maximum concentration putting the system under high stress. It is surprising that the self-assembly still works and leads under even milder temperatures and within short reaction times to the products. In addition, even subcomponent exchange could be performed under ball milling conditions.

Talk 3: Galvanic Replacement Reaction (GRR) Strategy Utilizing Cheap Nanoparticle as Sacrificial Templates for Hollow/Alloyed Metallic Nanostructures for Low Cost Nanocatalysis and UV-Vis Plasmonic Nanosensing (Janardhan Kundu)

Talk Summary: Polyhedral Cu_2O microparticle based self-templating strategy has been well-demonstrated for the synthesis of Cu_2O-M heterostructures (M = Au, Pd, Pt) and Au nano/mesocages. However, reports on Cu_2O-Ag heterostructures and the ensuing Ag mesocages are scanty. No reports describe the phenomenon of facet selectivity during the galvanic replacement reaction (GRR) based deposition of Ag on Cu_2O template particles. Here, we have identified the underlying rationale behind the observed difficulty in nucleating Ag nanoparticle on an octahedral Cu_2O template particle. Utilization of an appropriately chosen surfactant/complexant for the silver precursor help us demonstrate the successful fabrication of Cu_2O-Ag heterostructures (octahedral, cubic) with controlled loading density of Ag NPs on the Cu_2O surfaces. This is achieved using Cu_2O template particle that undergoes GRR with silver nitrate in the presence of nitric acid, and 5-sulfosalicylic acid as the surfactant (key role players). We provide evidences that support facet selectivity during the deposition of Ag NPs on Cu_2O cuboctahedral particles. Hollow octahedral Ag and Au-Ag bimetallic mesocages are fabricated that have rough surfaces, uniform morphology, and excellent shape retention. The fabricated heterostructures and mesocages act as excellent SERS substrate. This is the first report on the rational synthesis of octahedral Cu_2O-Ag heterostructures, octahedral Ag hollow mesocages utilizing the Cu_2O self-templating strategy along with the demonstration of facet selectivity of Ag deposition on Cu_2O template particles through GRR. The current approach offers a facile, and versatile protocol for the synthesis of Cu_2O-metal heterostructures and hollow noble metal mesocages that find applications in photocatalysis and SERS based sensing.

Discussions:

Q) Naresh Patwari: *Have you characterized the end products of your dye degradation reaction to ensure that all the carbon has converted to CO_2 and nitrogen to N_2*

A) Janardan Kundu: Degradation products from the present study has not been characterized. However, there are numerous reports on utilizing Cu_2O for photo-catalytic degradation of the same dye utilized here. Such reports have carefully characterized the products of the degradation of the dye and have isolated intermediates of the drgraded products to be aliphatic 3-5 C chain ketones, adlehydes and carboxylic acid that are minimally toxic. The complete mineralization of the dye into CO2 and N2 has been demonstrated for TiO_2 based commercial photocatalysts.

Q) Jyotishman Dasgupta: *How does the shape of the Copper-oxide template the incorporation of silver?*

A) Janardan Kundu: The Ag^+ ions are brought into the close proximity of the Cu2O template surface by the utilized 5-sulfosalicylic acid surfactant. This surfactant, being bidentate, can also bind directly to the surface of Cu2O surface. The acid present in the system reacts with the surface of the Cu2O thereby releasing Cu+ ions that then undergoes galvanic replacement reaction with the near Ag+ ions on the surface of the template. These concerted reactions happen on the surface of the template that leads to the preservation of the template morphology during the replacement reaction. In fact, there are in solution in-situ TEM imaging/video analysis of such galvanic reactions as it happens in real time that depicts the reaction pathway leading to the formation of shape preserved heterostructures.

Q) Akash Guliyani: *What do you envision to do with the hollow nanostructures?*

A) Janardan Kundu: These hollow mono/bi metallic nanostructures are not only useful for SERS but can be utilized in various applications. To name a few: nano-catalysis, suzuki cross coupling reaction catalyst, fuel cell catalyst for Oxygen Reduction Reaction (ORR), bio-imaging (scattering based modalities)

Q) Amit Paul: *Can you elaborate on the ESEM measurement?*

A) Janardan Kundu: ESEM measurements are done for samples that are non conducting in nature where the SEM chamber is maintained with a finite water vapor pressure that serves to conducts the electrons and makes SEM imaging viable