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## ***TIFR Annual Chemistry Conference-2019 (TACC-2019)***

***October 16-18, 2019***

***Tata Institute of Fundamental Research  
Colaba, Mumbai***

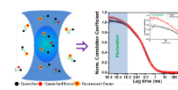
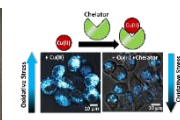
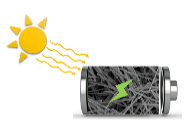
### **Poster Presentations**

**Session 1**    2:00 pm – 3:45 pm (October 16<sup>th</sup>)

**Session 2**    5:30 pm – 7:15 pm (October 16<sup>th</sup>)

**Session 3**    2:00 pm – 3:45 pm (October 17<sup>th</sup>)

***Venue: Homi Bhabha Auditorium Foyer***



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# Full Index of Posters

## List of Poster Presentations (All Sessions)

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49	Sambit Kumar Das	<i>Rapid and accurate composite ab initio models for high-throughput computation of molecular thermochemistry across chemical space</i>
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53	Mithilesh Kumar Nayak	<i>A Novel Access to Bis-Pyrrolinium Dications and their Transition Metal-Like Properties in Reversible Multi-Redox Coupled Bond Activation Reactions.</i>

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55	Simli Dey	<i>Membrane affinity of individual IAPP oligomers measured by single-molecule photo-bleaching</i>
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57	Pritam Eknath Kadam	<i>Hydrogen Bonding Interaction of Carbenes</i>
58	Amaraja Taur	<i>Towards Understanding the Hot electron Chemistry of Plasmonic Nanoparticles</i>
59	Debanjana Das	<i>Copper-Binding Induced Structural Transitions in Small Peptides derived from Azurin.</i>
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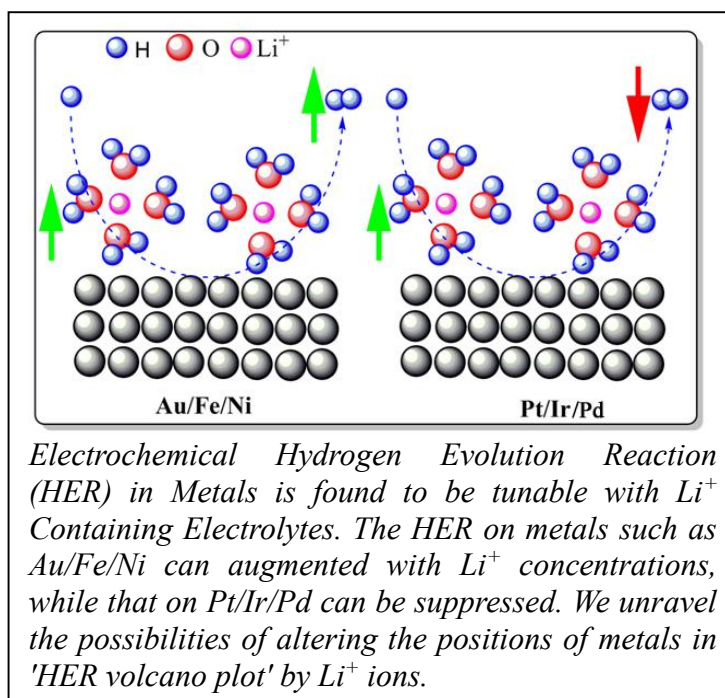
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# Full list of Graphical Abstracts

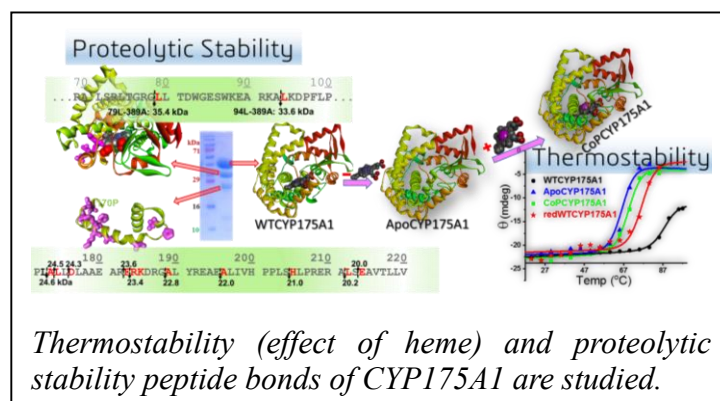
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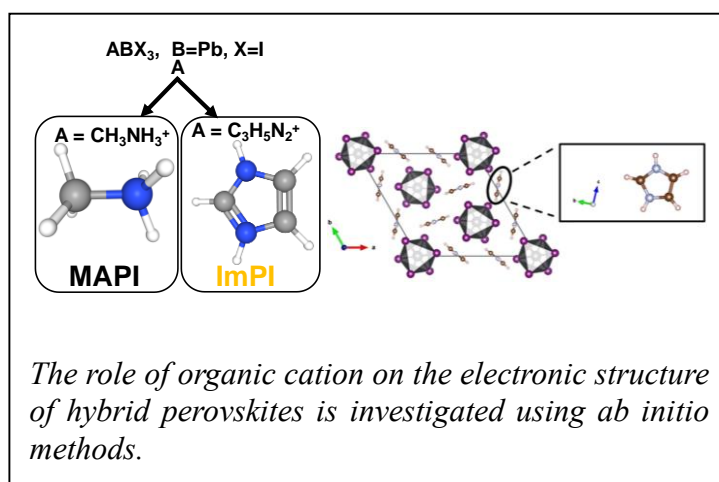
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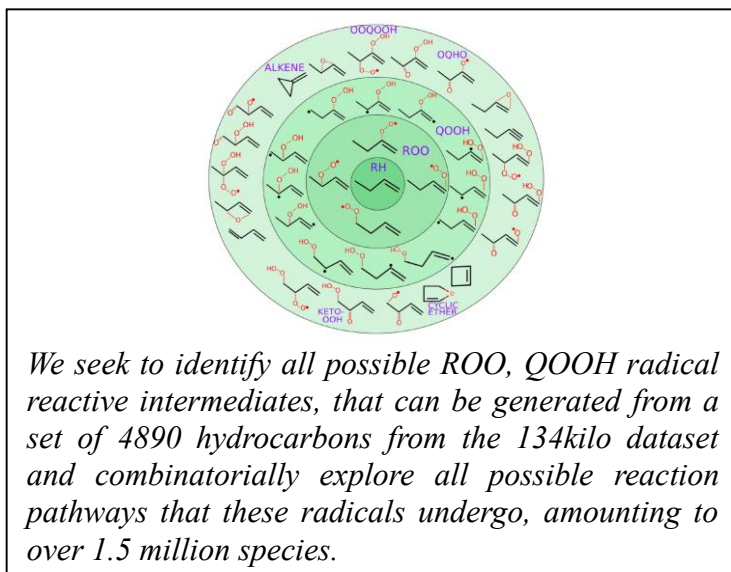
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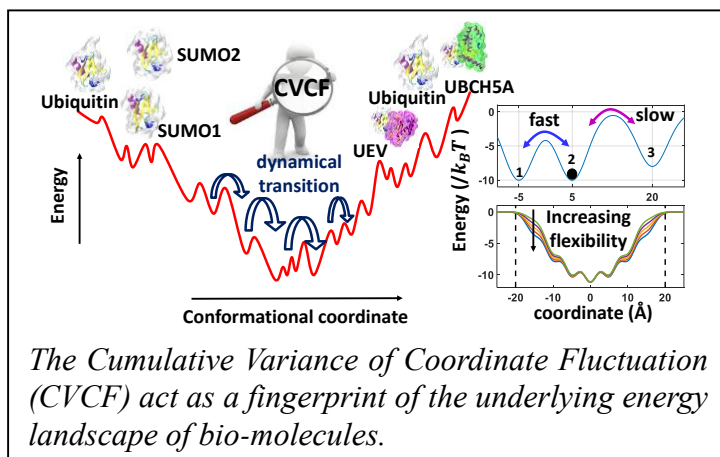
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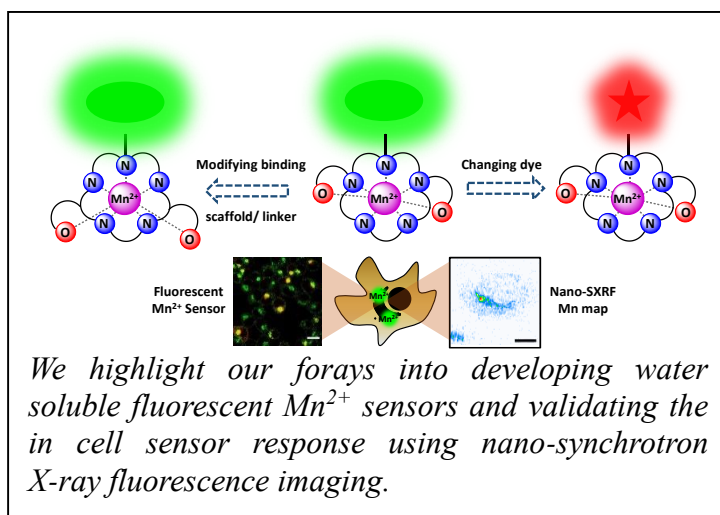
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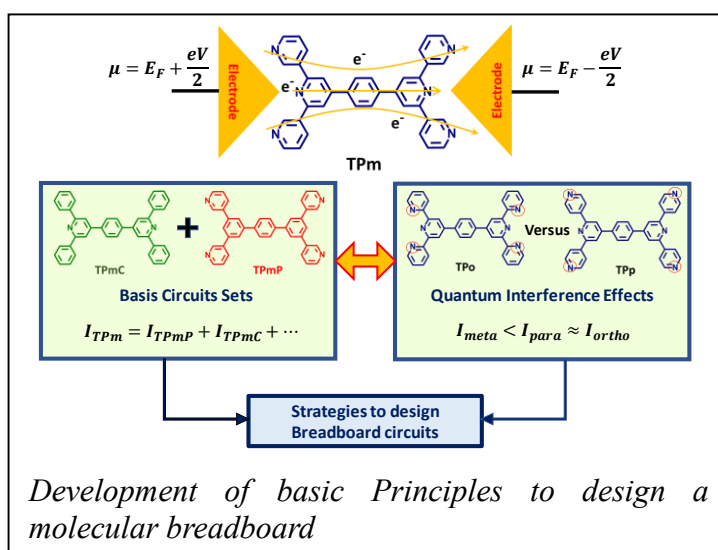
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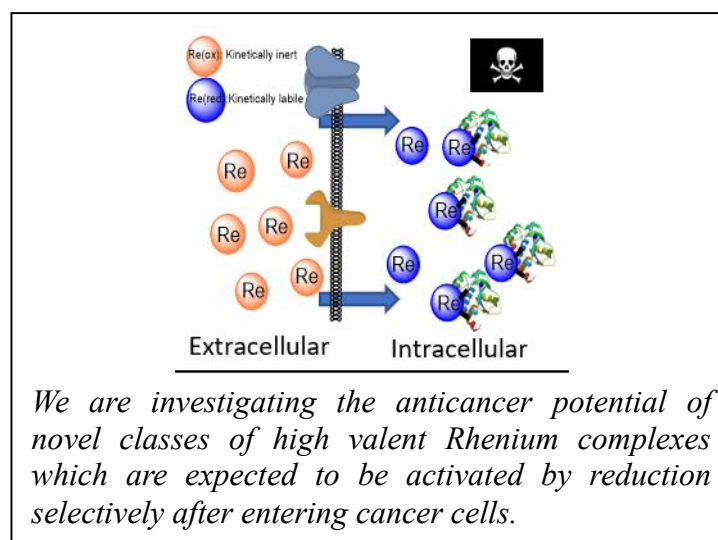
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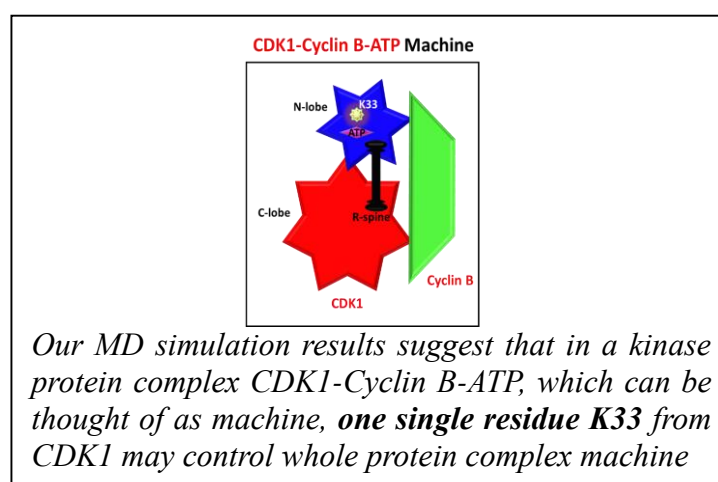
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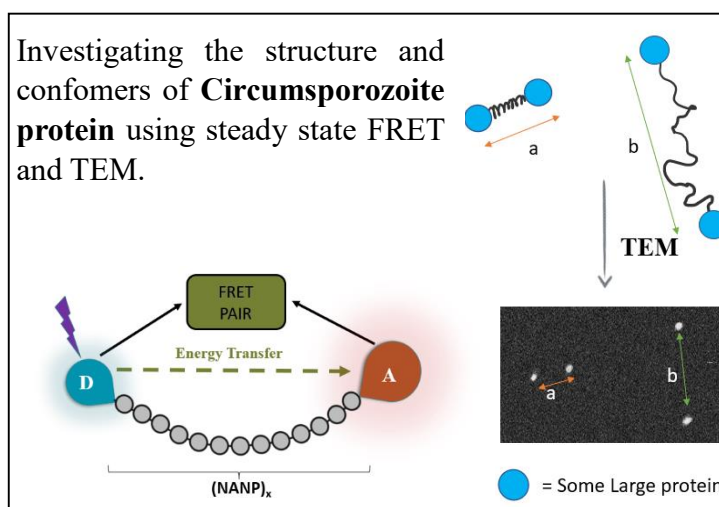
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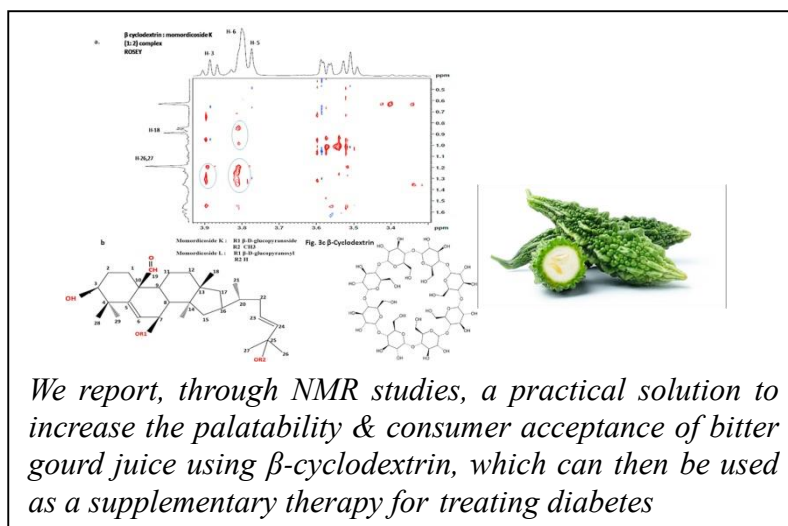
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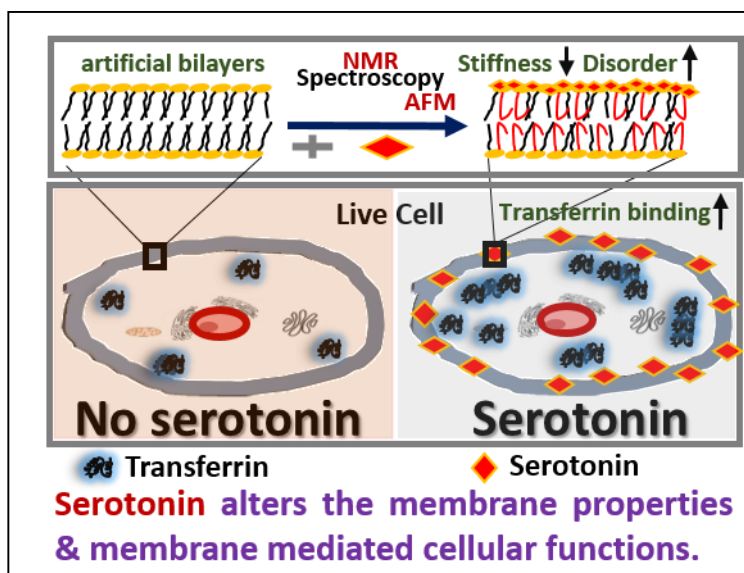
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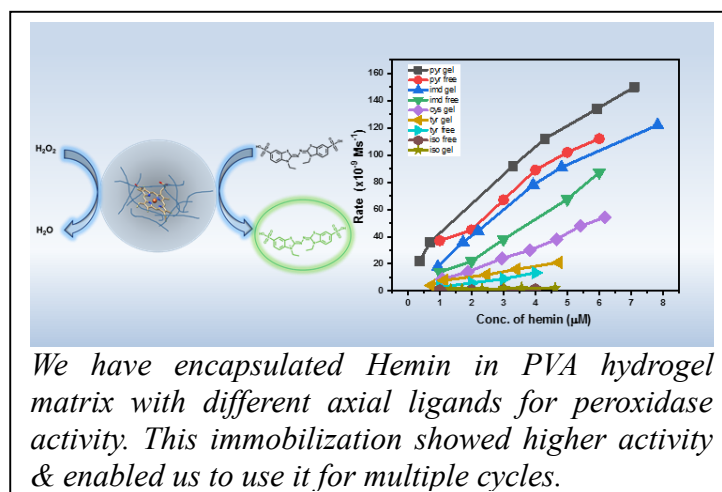
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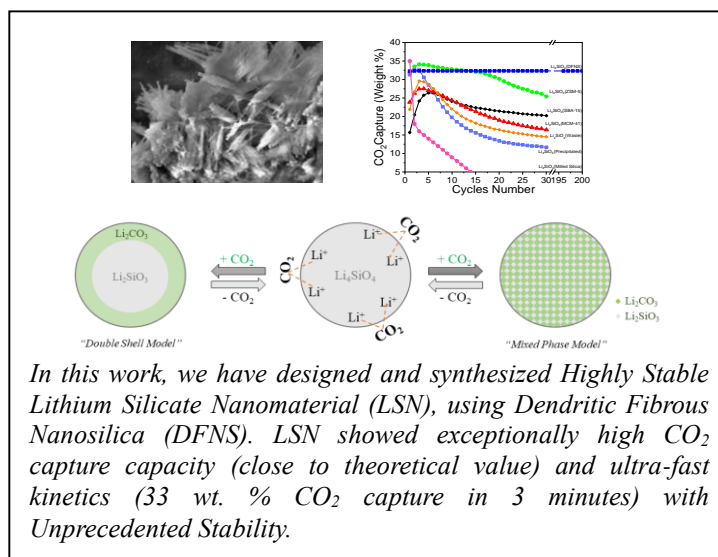
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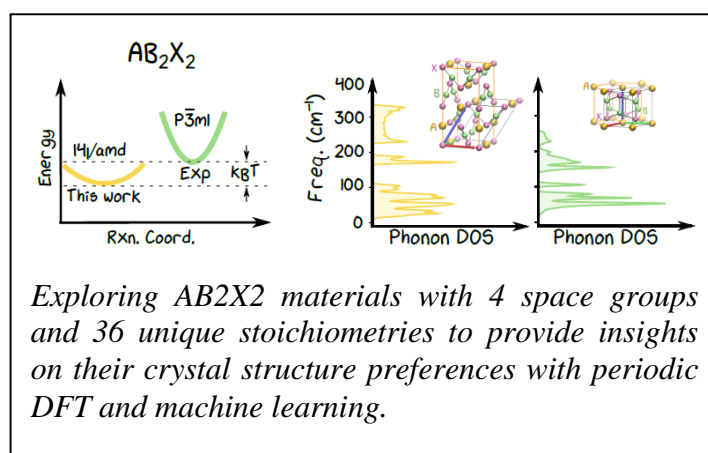
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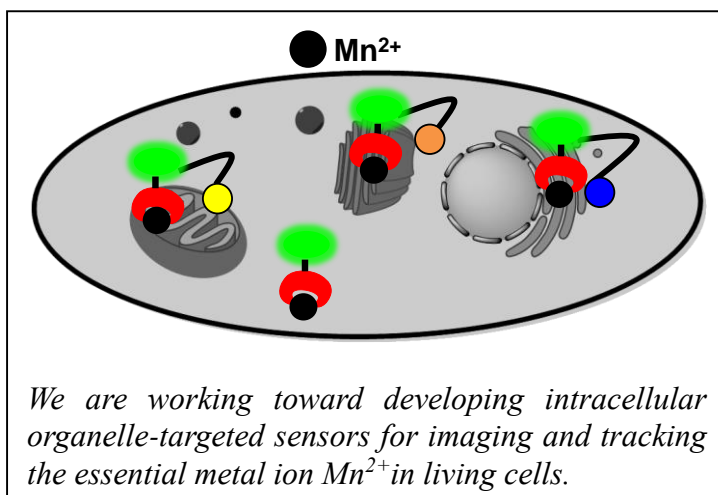
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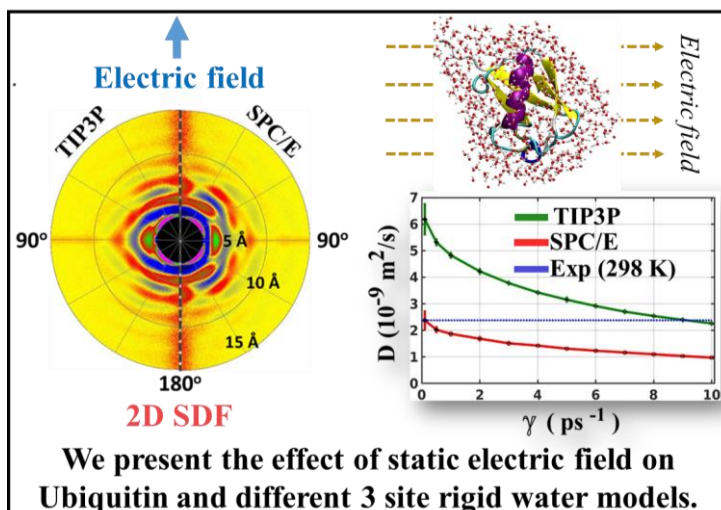
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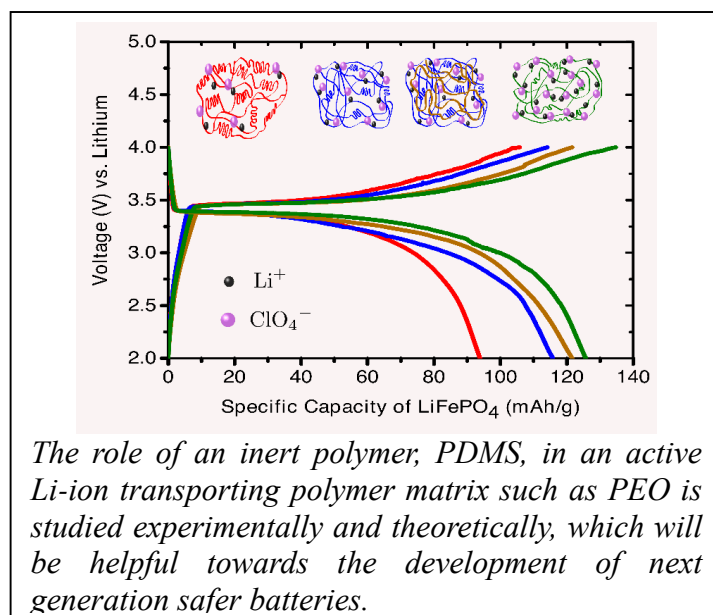
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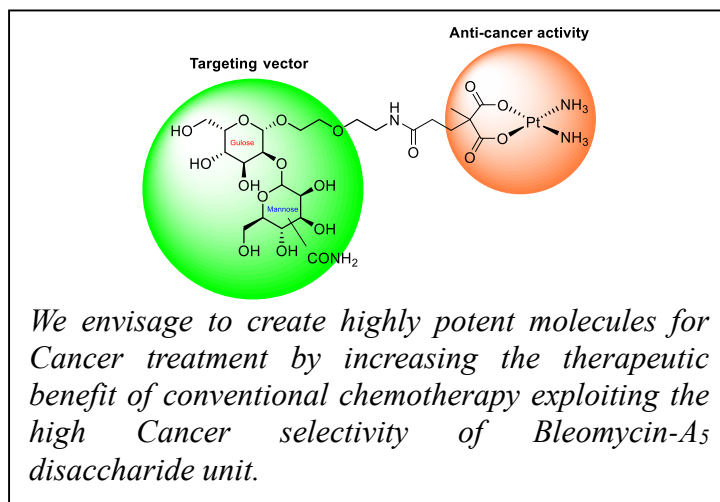
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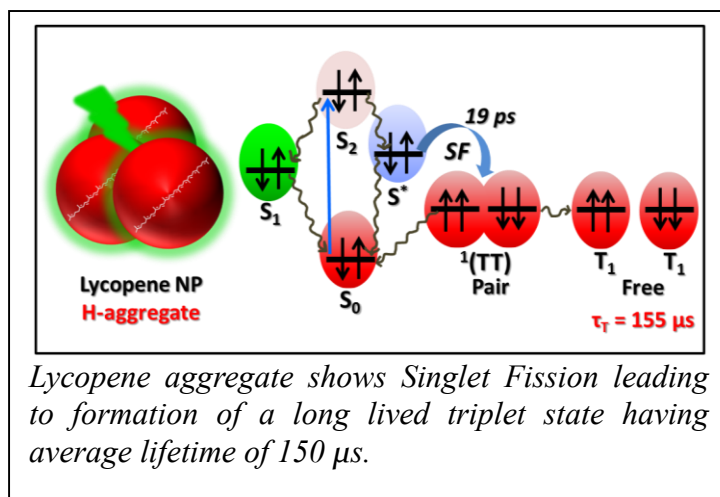
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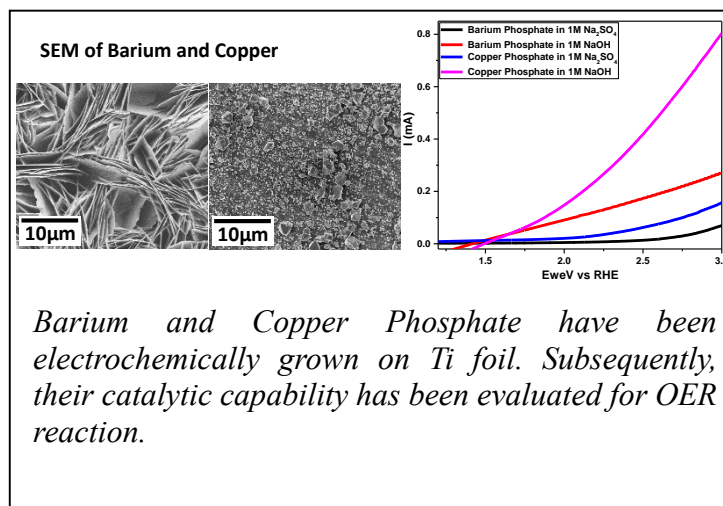
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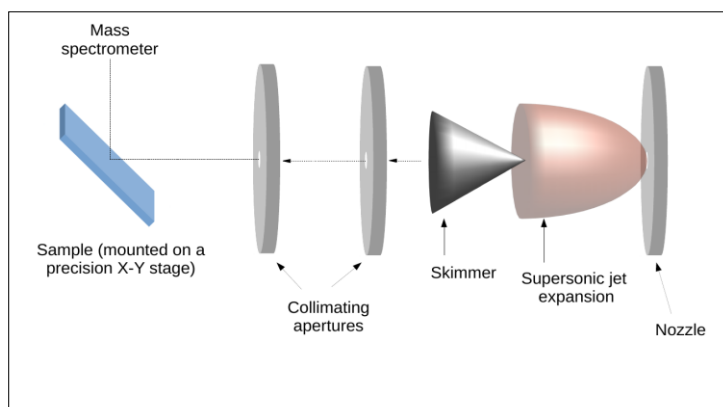
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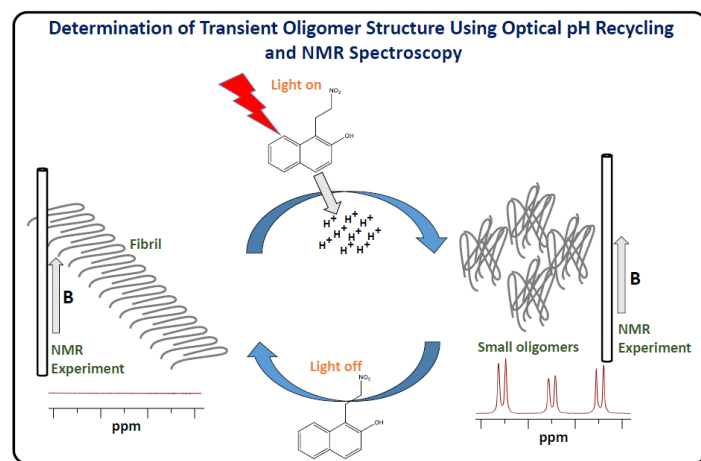
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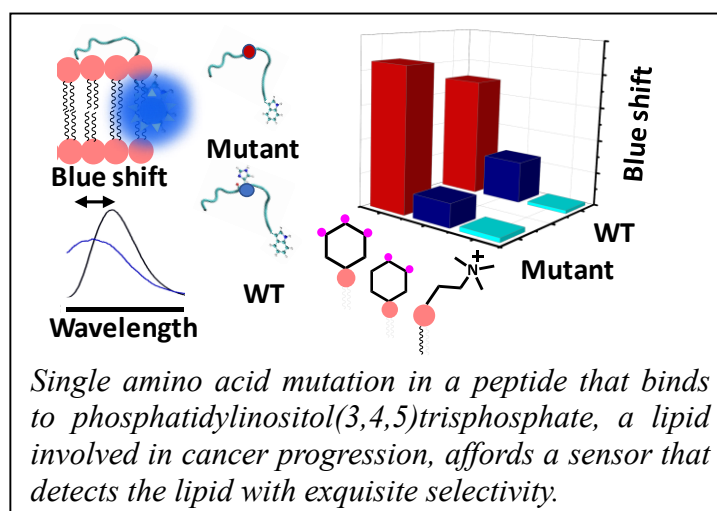
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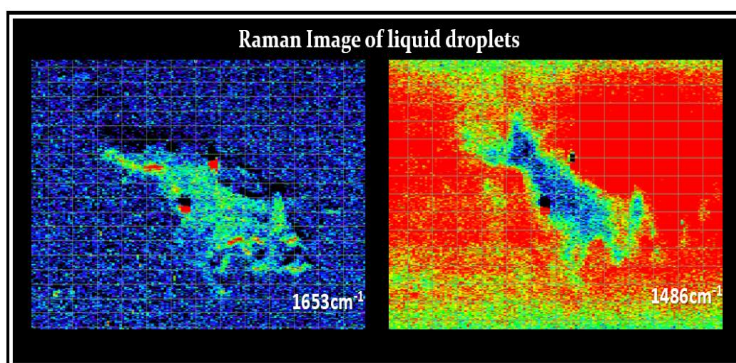
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**Poster Title:** Development of PI (3,4,5)P3 Sensors: Toward a Diagnostic Assay for Cancer Detection.



25) Debsankar Saha Roy (Maiti Group)

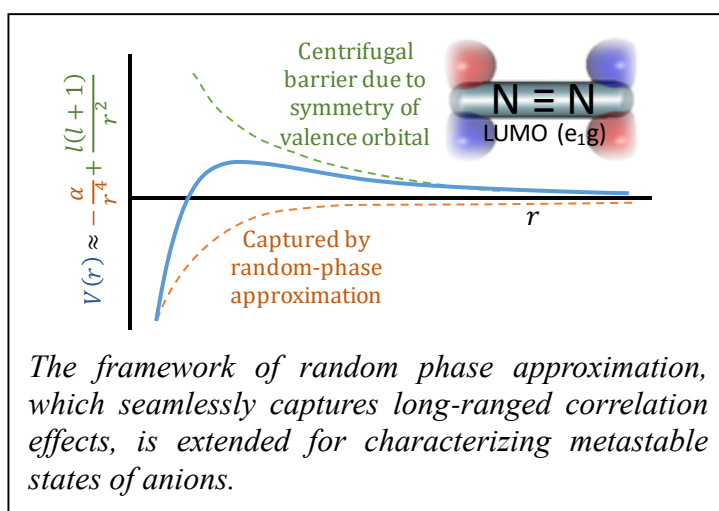
**Poster Title:** Line-Confocal Raman Imaging of Liquid-liquid Phase separation.



We develop a fast line-confocal Raman microscope which can differentiate structures with a micrometer resolution within protein liquid droplets

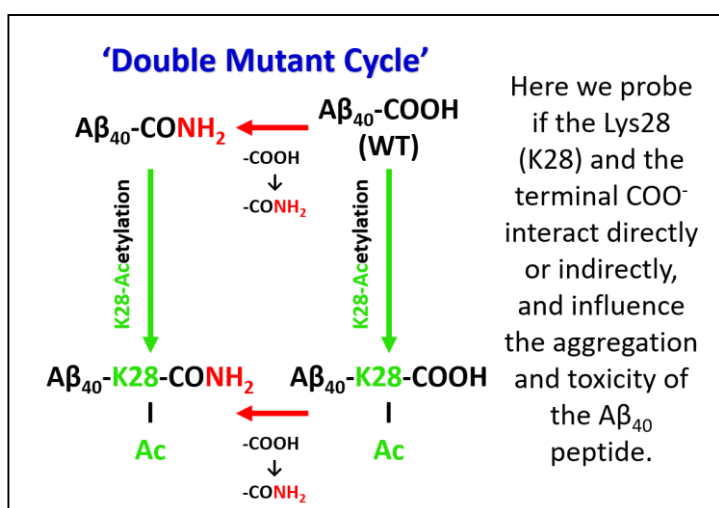
26) Pulkit Joshi (Voora Group)

**Poster Title:** Role of long-range correlation effects on the fate of metastable states.



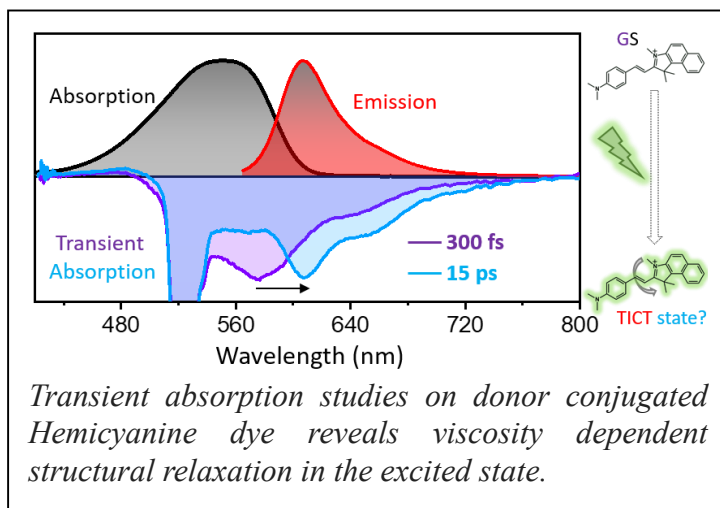
27) Anirban Das (Maiti Group)

**Poster Title:** A Double Mutant Cycle Involving the Charged Residues of Amyloid beta 1-40 shows that Aggregation and Toxicity can be independently controlled.



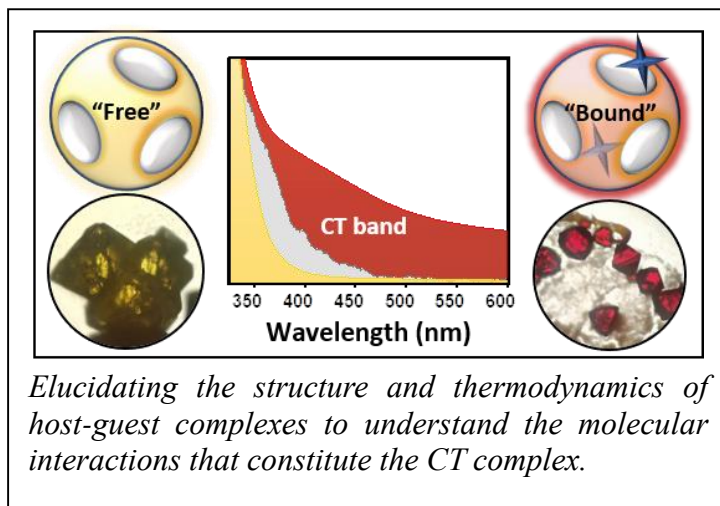
28) Atanu Ghosh (Dasgupta Group)

**Poster Title:** Probing the molecular origin of Stokes shift in donor substituted Hemicyanine dyes.



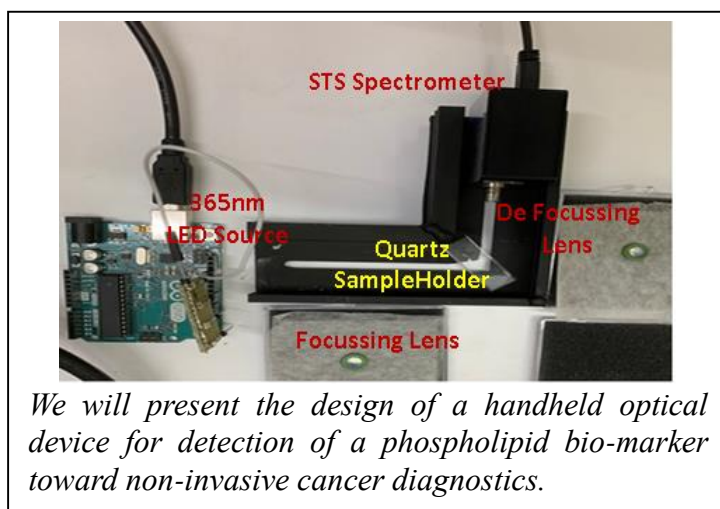
29) Dipin Tomar (Dasgupta Group)

**Poster Title:** Towards the quantification of donor-acceptor interactions in host-guest CT complexes.



30) Thulasi Ram K V (Datta Group)

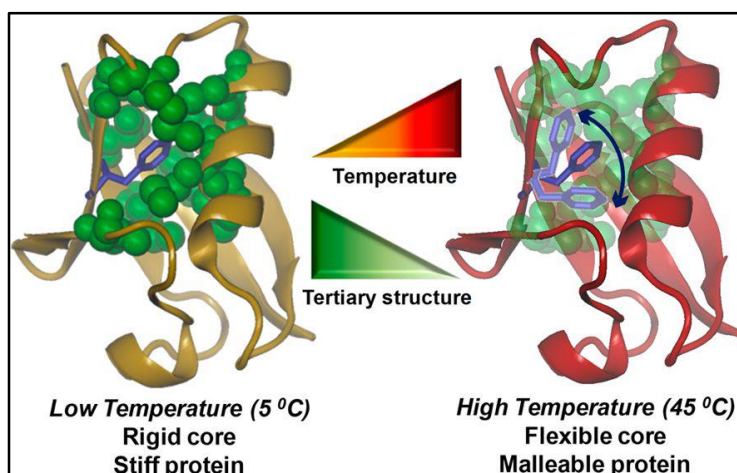
**Poster Title:** Design and Development of a Handheld Cancer Detection System Based on a Ratiometric Phospholipid Detection Assay.





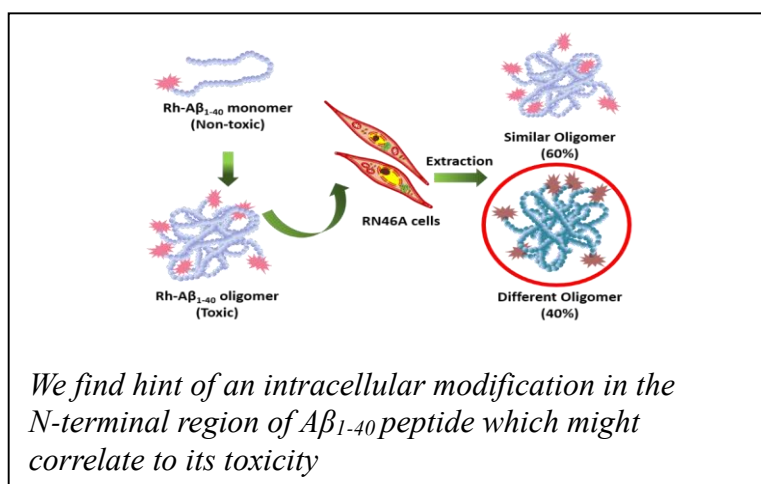
### 31) Shrabasti Bhattacharya (Koti Group)

**Poster Title:** A tale of two proteins: Similar structure but different dynamics.



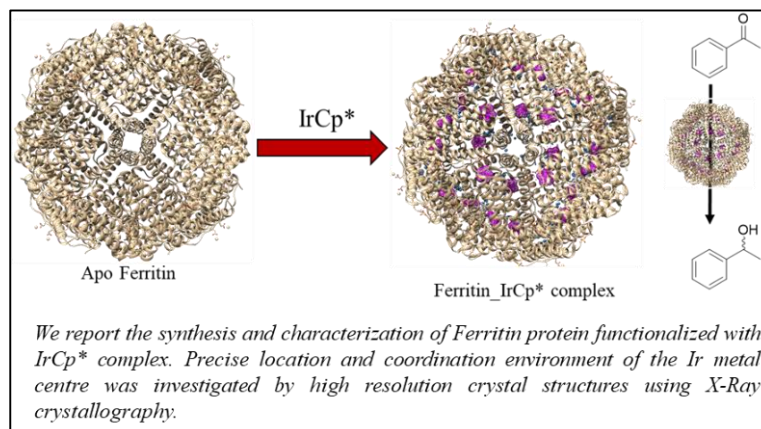
### 32) Arpan Dey (Maiti Group)

**Poster Title:** Hint of an intracellular modification being the key to Abeta toxicity



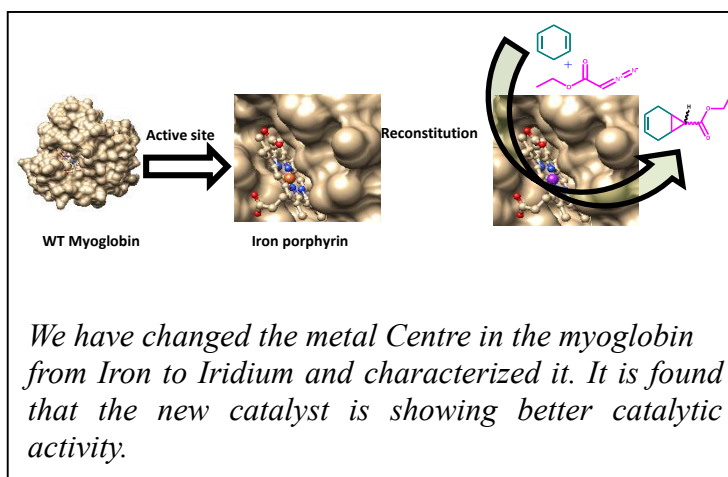
### 33) Mohd Taher (Mazumdar Group)

**Poster Title:** Synthesis and characterization of Ferritin Protein based metalloenzyme for asymmetric reduction of carbonyl compound



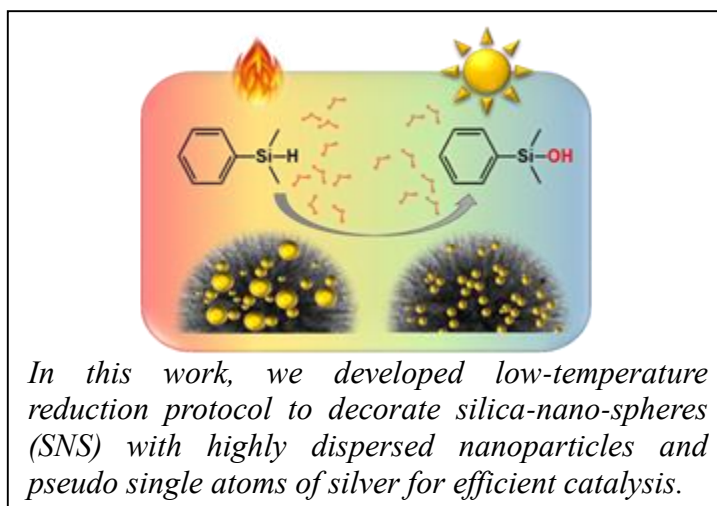
### 34) Vijay Kumar Singh (Mazumdar Group)

**Poster Title:** Cyclopropanation reaction catalyzed by Iridium Myoglobin.



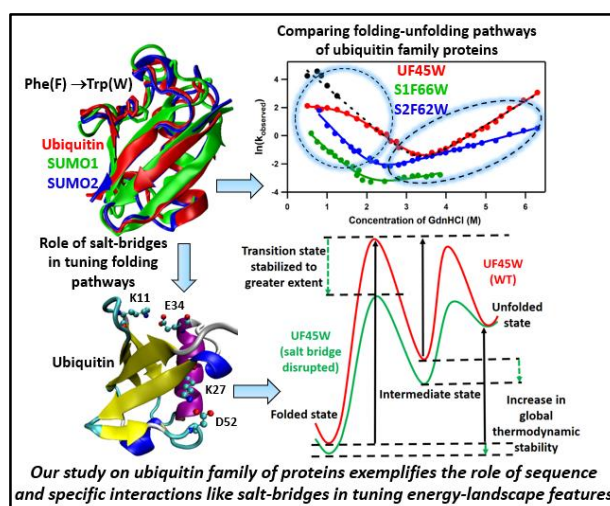
### 35) Rishi Verma (Polshettiwar Group)

**Poster Title:** Combining Plasmonic Nanoparticles and Pseudo Single Atoms of silver for Efficient Catalysis.



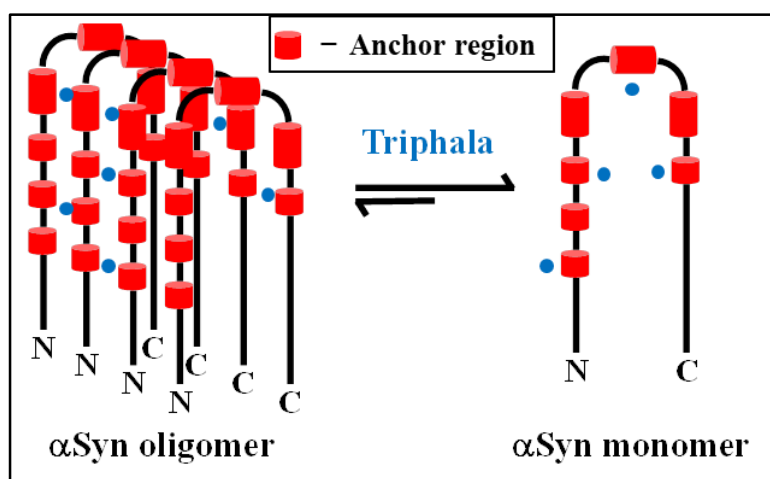
### 36) Tathagata Nandi (Koti Group)

**Poster Title:** Energy landscape of ubiquitin family proteins - elucidating the role of protein sequence and specific interactions such as salt-bridges in dictating folding pathways.



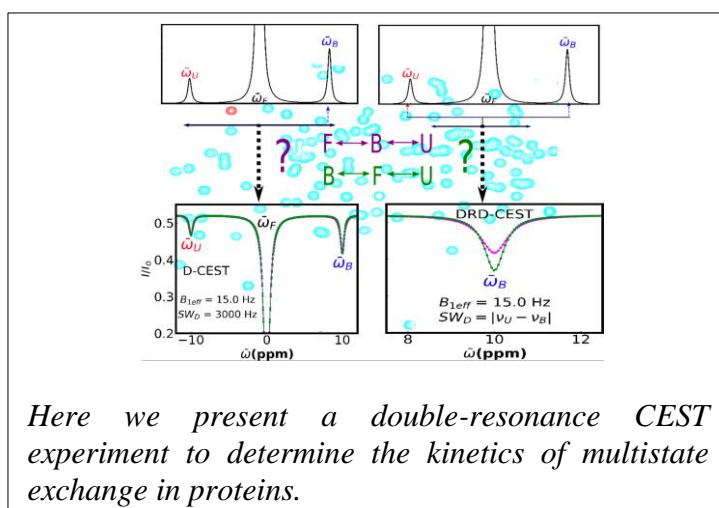
### 37) Mandar Bopardikar (Koti Group)

**Poster Title:** Triphala inhibits alpha-synuclein fibrilization and their interaction study by NMR provides insights into the self-association of the protein.



### 38) Ved Prakash Tiwari (Vallurupalli Group)

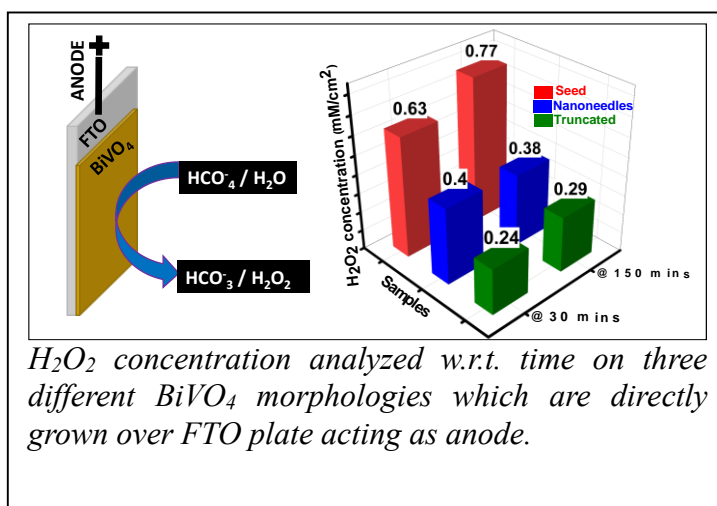
**Poster Title:** Studying Multistate Conformational Exchange of Proteins Using a Double-Resonance CEST Experiment: An Application to T4-lysozyme Folding.



*Here we present a double-resonance CEST experiment to determine the kinetics of multistate exchange in proteins.*

### 39) Ashish N Nadar (Khushalani Group)

**Poster Title:** BiVO<sub>4</sub>: An efficient electrocatalyst for water oxidation reaction.

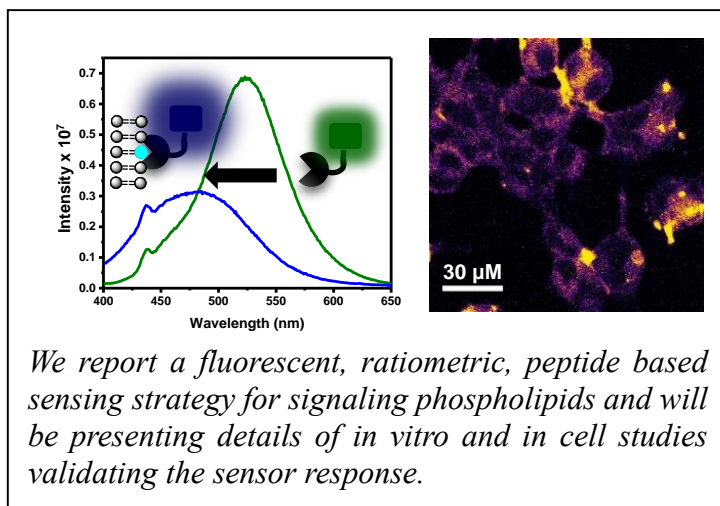


*H<sub>2</sub>O<sub>2</sub> concentration analyzed w.r.t. time on three different BiVO<sub>4</sub> morphologies which are directly grown over FTO plate acting as anode.*



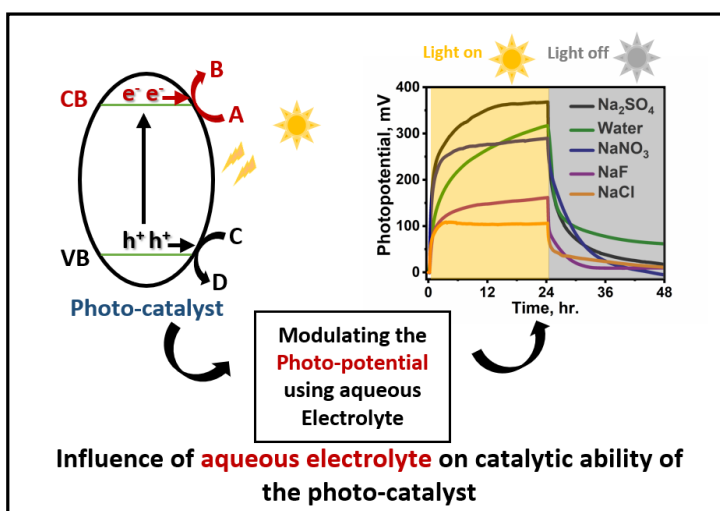
#### 40) Amitava Chandra (Datta Group)

**Poster Title:** Optical Probes for Imaging Signal Mediating Phospholipids.



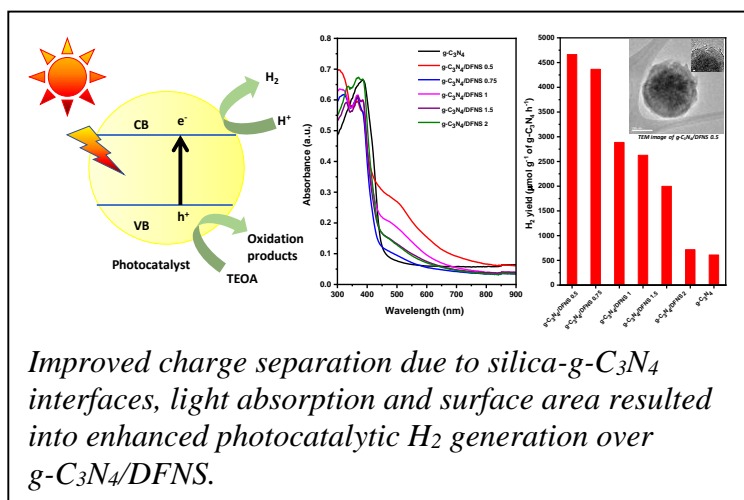
#### 41) Rohit (Khushalani Group)

**Poster Title:** Endeavoring to modulate the catalytic ability of a photocatalyst via aqueous electrolyte.



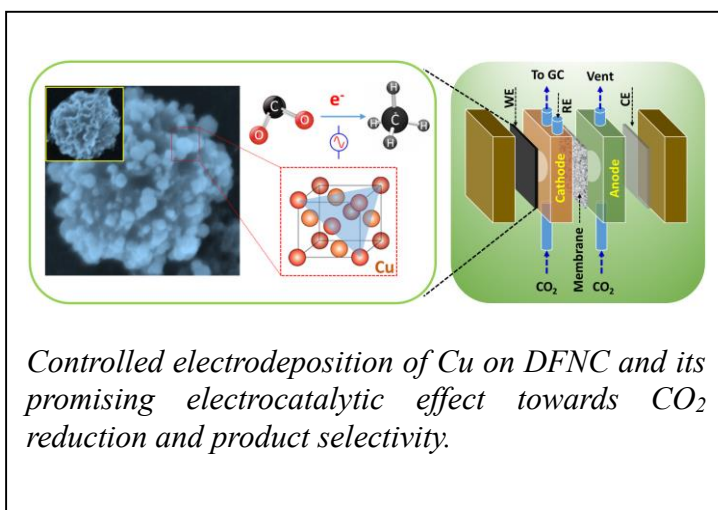
#### 42) Sushma Rawool (Polshettiwar Group)

**Poster Title:** Photocatalytic  $H_2$  generation over g- $C_3N_4$  decorated DFNS



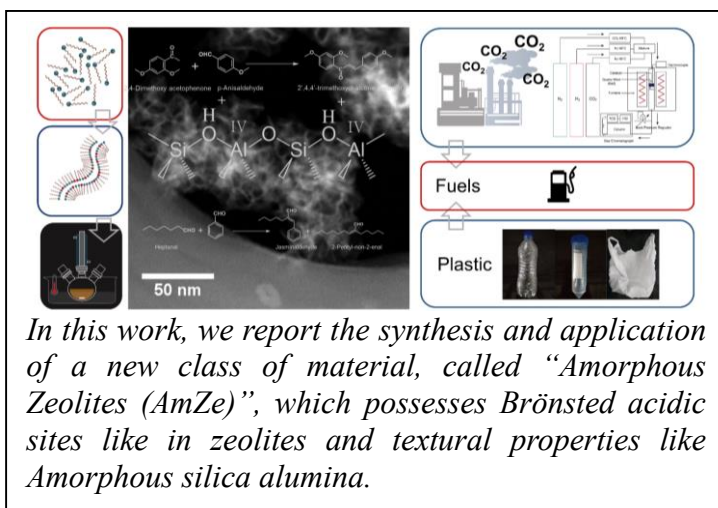
43) Chandan Das (Polshettiwar Group)

**Poster Title:** Controlled growth of electrodeposited Cu on dendritic fibrous nano-porous carbon (DFNC) and its electrocatalytic effect towards CO<sub>2</sub> reduction.



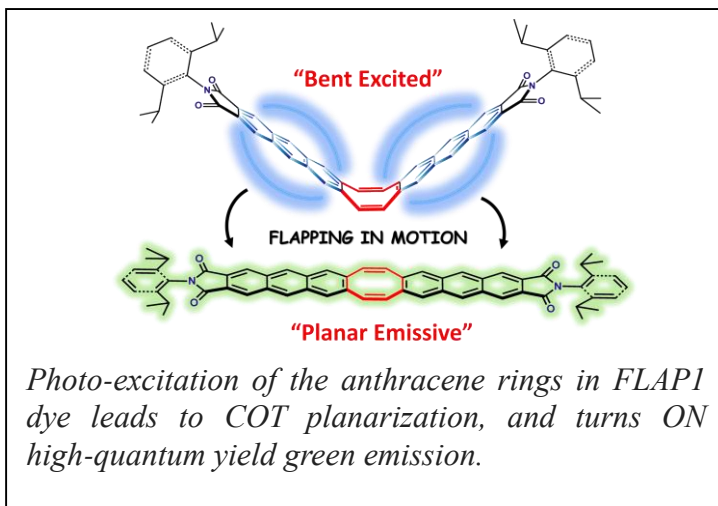
44) Ayan Maity (Polshettiwar Group)

**Poster Title:** Active and Stable Amorphous Zeolites Nanosponges for Catalysis, Plastic Degradation and CO<sub>2</sub> to Fuel Conversion.



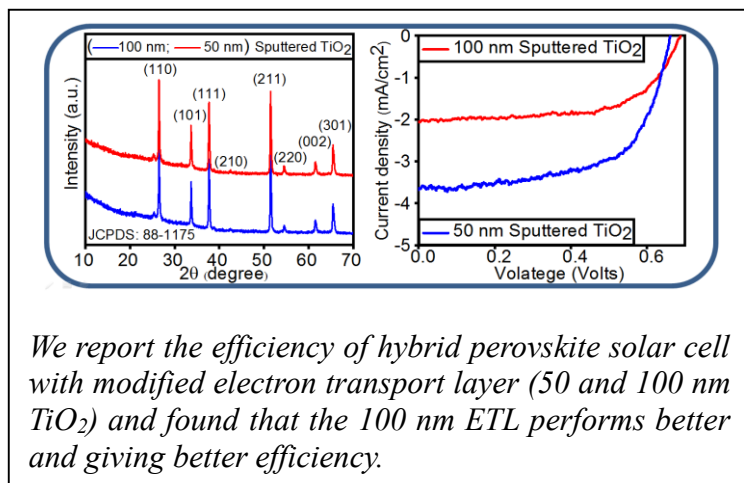
45) Sunandita Paul (Dasgupta Group)

**Poster Title:** Tracking Excited State Planarization in Anthracene-fused Cyclooctatetraene.



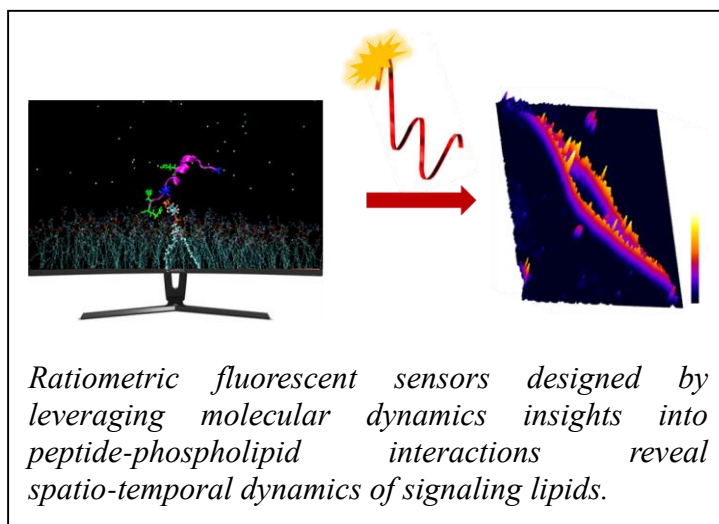
46) Deepak Kumar Dinkar (Khushalani Group)

**Poster Title:** Performance analysis of radio frequency magnetron sputtered TiO<sub>2</sub> electron transport layers on hybrid perovskite solar cell.



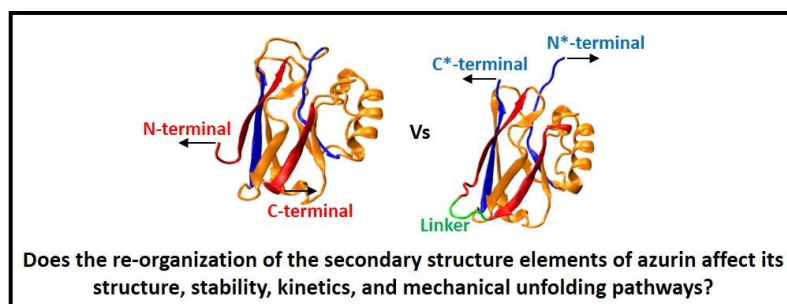
47) Rajasree Kundu (Datta Group)

**Poster Title:** Molecular Dynamics Guided Design of Phosphoinositide Selective Probes.



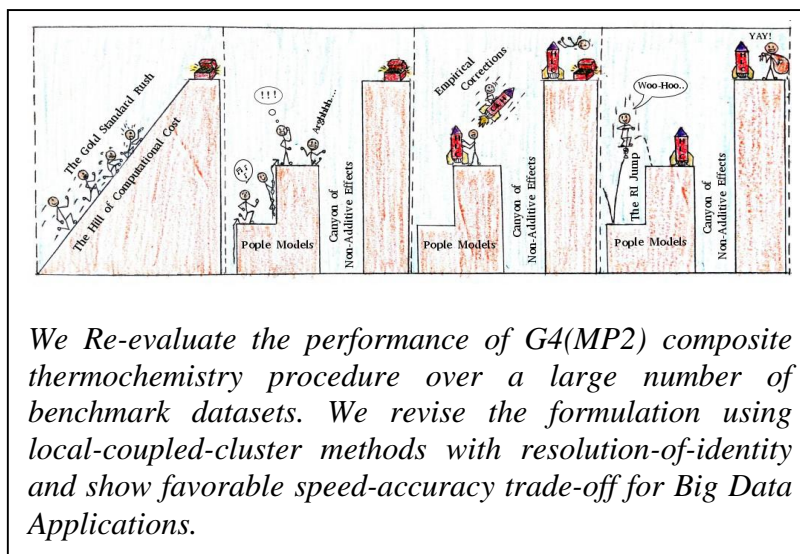
48) Priya Yadav (Koti Group)

**Poster Title:** The response of a blue copper protein to changes in  $\beta$ -sheet connectivity.



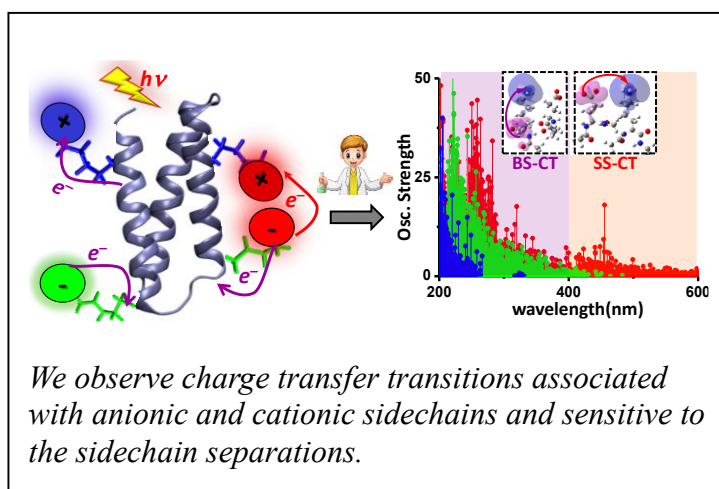
#### 49) Sambit Kumar Das (Ramakrishnan Group)

**Poster Title:** Rapid and accurate composite *ab initio* models for high-throughput computation of molecular thermochemistry across chemical space.



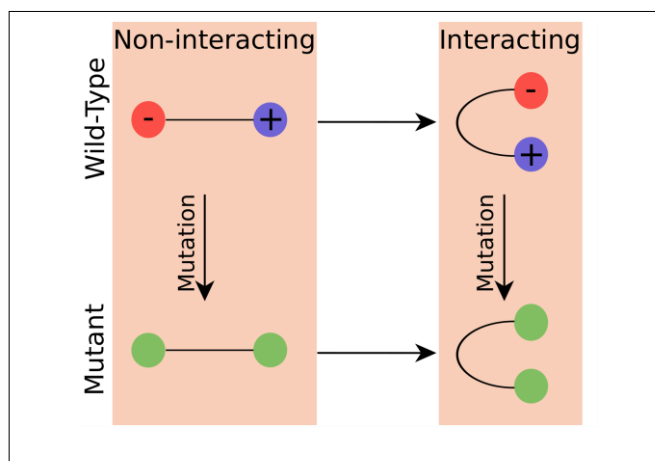
#### 50) Imon Mondal (Venkatramani Group)

**Poster Title:** Photoinduced Charge Transfer Transitions in Charged Amino Acids: New Label free Spectroscopic Marker to Probe Protein Structure and Dynamics.



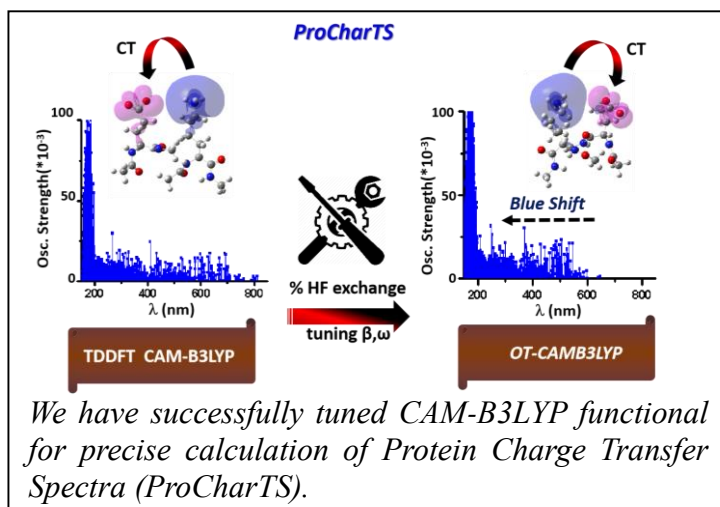
#### 51) Sabyasachi Chakraborty (Ramakrishnan Group)

**Poster Title:** A Thermodynamic cycle for intramolecular ion-pair interactions.



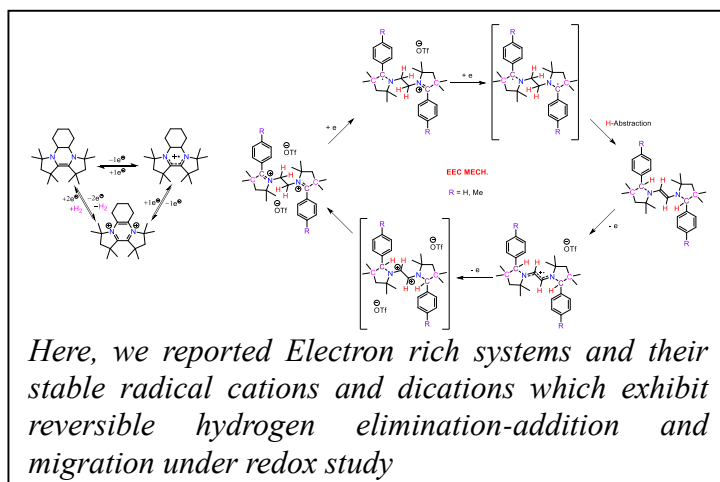
## 52) Sutanuka Manna (Venkatramani Group)

**Poster Title:** Refining Protein Charge Transfer Spectra (ProCharTS) using Optimally tuned CAM-B3LYP Functional.



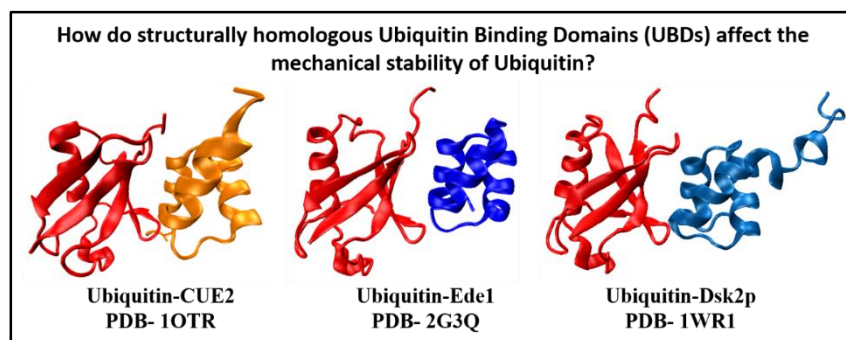
## 53) Mithilesh Kumar Nayak (Jana Group)

**Poster Title:** A Novel Access to Bis-Pyrrolinium Dications and their Transition Metal-Like Properties in Reversible Multi-Redox Coupled Bond Activation Reactions.



## 54) Mona Gupta (Koti Group)

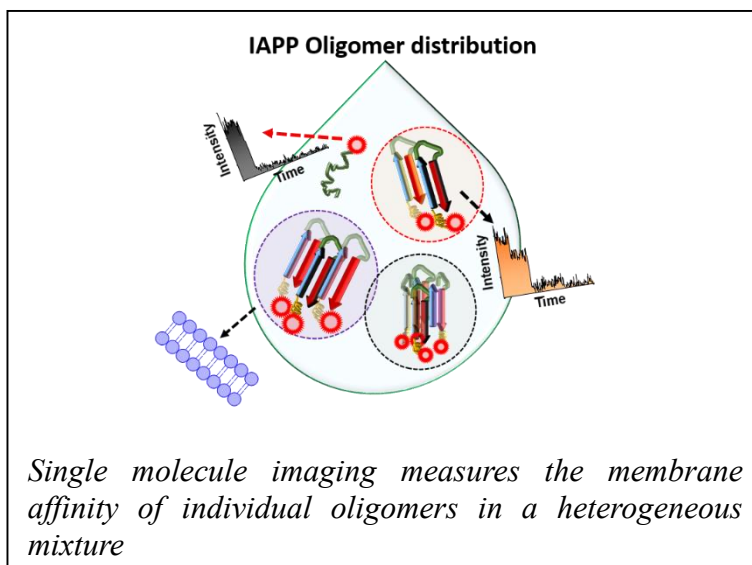
**Poster Title:** Mechanical properties of ubiquitin complexed with structurally homologous ubiquitin-binding domains.





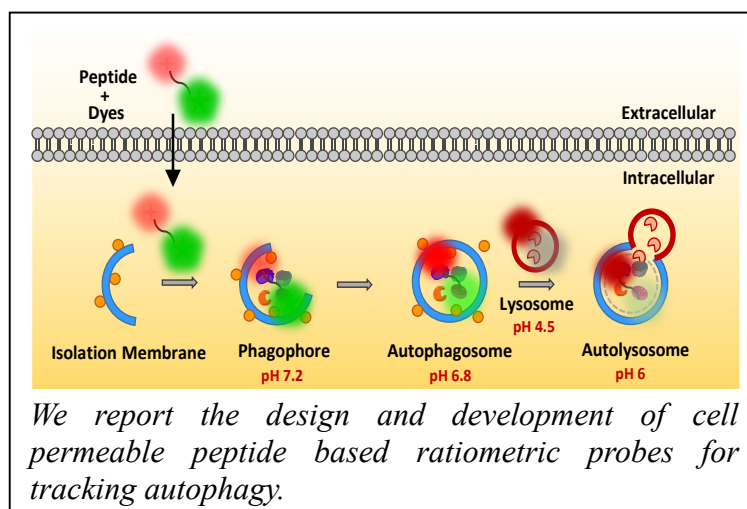
55) Simli Dey (Maiti Group)

**Poster Title:** Membrane affinity of individual IAPP oligomers measured by single molecule photo-bleaching.



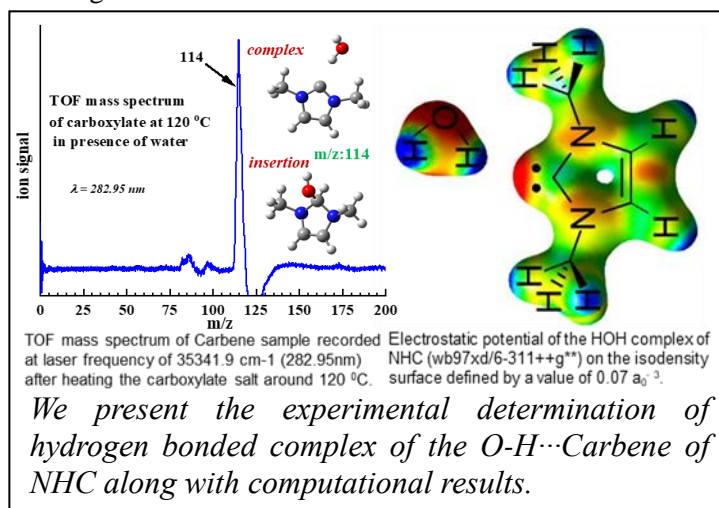
56) Sayani Das (Datta Group)

**Poster Title:** Cell Permeable Ratiometric Probes for Tracking Autophagy.



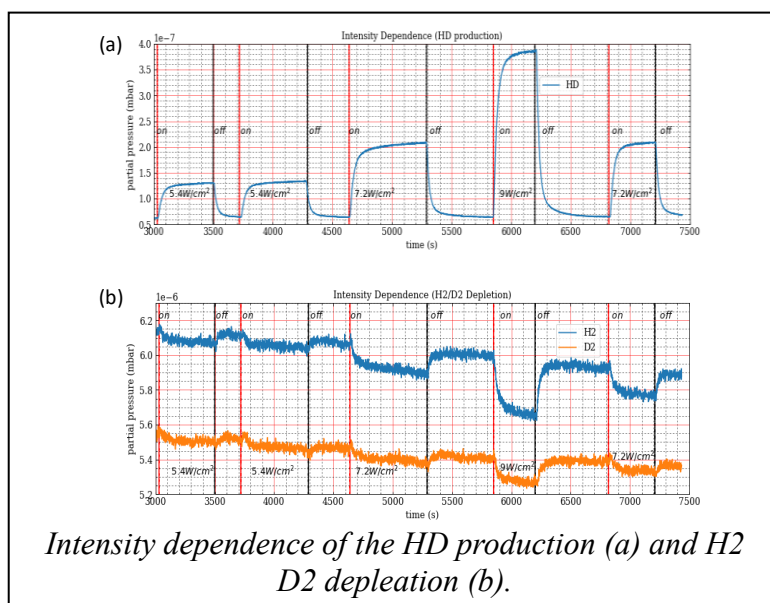
57) Pritam Eknath Kadam (Wategaonkar Group)

**Poster Title:** Hydrogen Bonding Interaction of Carbenes.



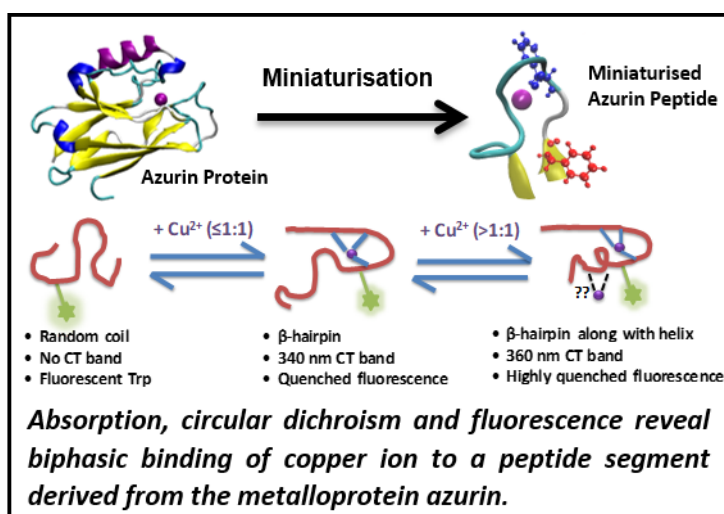
58) Amaraja Taur ( Shirhatti Group)

**Poster Title:** Towards Understanding the Hot electron Chemistry of Plasmonic Nanoparticles.



59) Debanjana Das (Koti Group)

**Poster Title:** Copper-Binding Induced Structural Transitions in Small Peptides derived from Azurin.



60) Subhendu Pandit (Vallurupalli Group)

**Poster Title:** Studying Dynamics of Hyberantion Promoting Factor Using Solution NMR Spectroscopy.

