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MAF 2024 8-11 September, Valencia, Spain

Venue

Universidad de Valencia
Auditorium/Assembly Hall
of the Research Centre "Institute of Molecular Science (ICMol)"
Catedrático José Beltrán n° 2, 46980 Paterna, Spain Valencia.
It can be conveniently reached by tram and walking in 20 min.
A tram stop is located at the back of Palacio de Congresos.
From here, a tram (line 4, direction "Mas del Rosari") can be taken and then getting off at "A Punt" stop, which is 3 minutes from ICMol.

Acknowledgements

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PicoQuant

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FRET Satellite Workshop @ MAF2024

Organizing commitee: Don Lamb, Thorben Cordes, Claus Seidel

Wed. 11.09.2024	
After MAF2024 closing at 13:45	Change of venue (Valencia Conference Centre) to our new venue (Universidad de Valencia, Auditorium/Assembly Hall)
Session 1a: *Structural modeling with FRET*	
16:00 - 17:30 Chair: D. Lamb	Niko Hildebrandt (McMaster University CA; 30 min+5) Richard Börner (HS Mittweida DE; 30 min+5) Bianca Reschke (HHU Düsseldorf DE; 15 min+5)
17:30 - 17:50	Coffee Break + Posters
Session 1b: *Structural modeling with FRET*	
17:50-19:15 Chair: R. Börner	Thomas Peulen (TU Dortmund DE; 30 min+5) Veronika Frank (U. Freiburg DE; 15 min+5) Claus Seidel (HHU Düsseldorf DE; 15 min+5) PicoQuant (Berlin DE; 10 min)
19:15 - 19:45	Poster session and drinks
19:45- 20:30	Discussion Rounds / Ask the Experts
21:15 Joint Workshop Dinner at the Restaurante Vinoteca La Dehesa (Carrer de la Vall d'Aiora, 6,46015, Benicalap, 46015 València, ES)	
Thurs. 12.09.2024	
Session 2a: *Cellular FLIM and FRET measurements*	
9:30 - 11:00 Chair: T. Cordes	Elizabeth Hinde (University of Melbourne, Australia; 30 min+5) Dorus Gadella University of Amsterdam NL; 30 min+5) Rory Cunnison (Warwick, UK; 15 min+5)
11:00 - 11:20	Coffee Break + Posters
Session 2b: *Cellular FLIM and FRET measurements*	
11:20-12:35 Chair: T. Peulen	Katharina Hemmen (U Würzburg DE; 30 min+5) Christoph, Nocker (U Frankfurt DE; 15 min+5;) Claus Seidel (HHU, Düsseldorf DE; 15 min+5)
12:35-14:00 **Lunch Break** (you are on your own)	
Session 3: *Instrumentation and probes*	
14:00-16:00 Chair: C. Seidel	Thorben Cordes (TU Dortmund DE; 30 min+5) Viktoria Glembockyte (MPI Med. Research Heidelberg DE; 20 min+5) Lars Richter (LMU München DE;20 min+5) Don Lamb (LMU München DE;20 min+5) Concluding remarks

Session 1a: *Structural modeling with FRET*

Niko Hildebrandt - nanofret.com, McMaster University, Hamilton, Canada

FRET as a biomolecular research tool — understanding its potential while avoiding pitfalls

Börner, Richard - Biophotonics, Laserinstitut Hochschule Mittweida, Mittweida University of Applied Sciences

FRET-guided integrative modelling of ncRNA - from single structures to a structural ensemble

The functional diversity of RNA is encoded in their innate conformational heterogeneity. The combination of single-molecule FRET and computational modelling offers new opportunities to map structural transitions within RNA ensembles. We developed a streamlined workflow, which integrates de novo structure prediction through FARFAR2 paired with MD simulation using GROMACS followed by in silico FRET predictions with FRETraj as a FRET-guided integrative modelling approach to capture RNA structural dynamics and to gain RNA folding pathways. FRETraj enables to compute the accessible-contact volume (ACV) of the fluorescent dyes along MD trajectories or de novo generated structural ensembles (multi-ACV) without the need of explicit dye labeling in silico. FRETraj uses experimental measures such as fluorescence QY, detection efficiency and intensity burst size distribution for FRET predictions yielding an exceptional agreement with the experimental derived FRET distribution. We use multi-ACVs and thus FRET as a post-hoc scoring method for fragment-assembly and we demonstrate that FRET effectively refines de novo RNA structure prediction.
We benchmark our FRET-assisted modeling approach on double-labeled DNA strands and validate it against an intrinsically dynamic Mn(II)-binding riboswitch and a Mg(II)-sensitive ribosomal RNA tertiary contact. We show that already one FRET coordinate allows to recapitulate the global fold and significantly reduces the de novo generated RNA ensemble.

Bianca Reschke - Molecular Physical Chemistry, Heinrich-Heine University Duesseldorf

FRET-assisted structural modeling of dynamic protein ensembles

Förster Resonance Energy Transfer (FRET) experiments provide information on the structure, dynamics and conformational transitions of biomolecules. FRET experiments combined with computational methods in integrative approaches allow to generate dynamic ensembles and to resolve static and dynamic heterogeneities with high accuracy and precision. Utilization of single-molecule FRET measurements using a diffusion-based confocal microscope and FRET observables together with molecular simulations and FRET-restrained structural modeling enables screening and scoring of an ensemble of conformations against experimental FRET data to identify conformers with the best agreement to experimental data. Integrative structural models obtained from various experimental data can be deposited in the archiving system PDB-Dev.
One system of interest is the carbohydrate-binding module 56 (CBM56), a C-terminal subunit of the enzyme Glucan endo-1,3-D-glucosidase from the organism Bacillus circulans. As a target protein for the CASP 13 competition, its structure has not yet been experimentally elucidated by X-ray crystallography. The structure proposed with the help of homology modeling consists of two domains, which are primarily composed of beta-sheets, connected by a linker unit.
Another system of interest is the lysozyme of the bacteriophage T4 (T4L), which structurally consists of two interconnected subdomains (N- and C-terminal) and a long alpha-helix between them. T4L undergoes a dynamical exchange between two states, an open (C1) and a closed (C2) state, which occurs in the course of substrate binding and conversion. The newly-defined compact state C3 is thought to play an important role in the formation of the enzyme-product complex and the subsequent release of the product.
The generation of structural ensembles combined with single-molecule FRET experiments for the respective informative FRET pair networks enables the investigation of the structure ensemble and dynamic behaviour of CBM56 as well as the structure ensemble for the C3 state of T4L.

Session 1b: *Structural modeling with FRET*

Peulen, Thomas - Heinze Group, Rudolf-Virchow Centre Integrative Microscopy

Towards in-situ structural biology: Integrative modeling resolves FRET-based structures and conformational ensembles

Förster Resonance Energy Transfer (FRET) combined with integrative modeling is used to resolve protein structures, dynamics, and conformational ensembles. FRET provides crucial nanometer-scale distance measurements between labeled sites on biomolecules, capturing real-time conformational changes and dynamic transitions.
To resolve structures and dynamics, we employ an integrative approach combining FRET data with Bayesian modeling and the Maximum Entropy method to capture structures, model conformational ensembles and dynamic. Showcasing how FRET can effectively resolve a wide range of biomolecular conformations and their associated dynamics.
Combining microscopy and single-molecule spectroscopy through integrative modeling, we aim to resolve the structures of biofilm components in situ. Using RuvA as a probe to target Holliday junctions of extracellular DNA (eDNA), we capture in situ single-molecule FRET data. This data, combined with atomistic cryoEM data, allows us to infer the structural organization of biofilm constituents in their native, complex environments, advancing our understanding of biomolecular structures in living systems.

Veronika Frank - Hugel Group, Institute of Physical Chemistry, Albert-Ludwigs-Universität Freiburg

Dynamic structure of a multi-domain protein quantified by single-molecule FRET based methods

For decades protein structures were the main reference for researchers to explore fundamental biology, biophysics and biomedicine including computer-aided drug design. As more and more different structures (conformations) for one and the same protein were determined, it became clear that structural ensembles, their connectivity and their kinetics are crucial for an understanding of protein function. Here we present approaches that enable us to simultaneously access structure and dynamics of the multi-domain protein machinery and heat shock protein Hsp90 in solution. First, we recapitulate how structural ensembles can be obtained from single-molecule (sm) FRET networks [1]. Then, we show how a comparison of FRET distributions from simulations and smFRET experiments can be the basis to delineate allosteric structural changes [2]. Furthermore, we show how FRET and nanosecond fluorescence correlation spectroscopy (FRET-nsFCS) in combination with full-atom MD simulations and neutron scattering can be used to determine structural ensembles, including their kinetics in the form of principal components (eigenmodes) [3]. Altogether, we demonstrate how smFRET can enrich the determination of structural ensembles and their dynamics. [1] B. Hellenkamp, P. Wortmann, F. Kandzia, M. Zacharias & T. Hugel; Multidomain structure and correlated dynamics determined by self-consistent FRET networks; Nat Methods, 14 (2), 174 (2017). https://doi.org/10.1038/nmeth.4081. [2] S. Wolf, B. Sohmen, B. Hellenkamp, J. Thurn, G. Stock & T. Hugel; Hierarchical dynamics in allostery following ATP hydrolysis monitored by single molecule FRET measurements and MD simulations; Chem. Sci. 12, 3350 (2021). https://doi.org/10.1039/D0SC06134D. [3] Sohmen, B., Beck, C., Frank, V., … Hugel, T. (2023). The Onset of Molecule-Spanning Dynamics in Heat Shock Protein Hsp90, Advanced Science, 10(36). https://doi.org/10.1002/advs.202304262

Seidel, Claus - Molecular Physical Chemistry, Heinrich-Heine University Duesseldorf

Advanced Multiparametric Image Spectroscopy and Super-resolution Microscopy Reveal a Minimal Model of CD95 Receptor Signal Initiation

Unraveling the concentration dependent spatiotemporal organization of receptors in the plasma membrane is crucial to understand cell signal initiation. A paradigm of this process is the oligomerization of cluster of differentiation 95 (CD95) during apoptosis signaling, with different oligomerization models being discussed. Here, we establish the molecular sensitive approach cell lifetime FRET image spectroscopy (CELFIS) to determine CD95 configurations in live cells. This data is corroborated by STED microscopy, confocal photobleaching step analysis, and FCS. We probed CD95 interactions for ~10 - 1000 molecules/µm2 concentrations, over ns to hours, and molecular to cellular scales. Quantitative benchmarking was achieved establishing high-fidelity monomer and dimer controls. While CD95 alone is primarily monomeric (~96%) and dimeric (4%), the addition of ligand induces oligomerization to dimers/trimers (~15%) leading to cell death. This study highlights molecular concentration effects and oligomerization dynamics.

Session 2a: *Cellular FLIM and FRET measurements*

Hinde, Eliszabeth - University of Melbourne, Australia

Histone FRET of chromatin architecture

Inside the nucleus of an intact cell, DNA is folded around histone proteins into nucleosomes and compacted into a multi-layered three-dimensional chromatin network. The nanometre spacing between nucleosomes positioned throughout this structural framework is known to locally modulate local DNA template access and regulate genome function. However, given that this structural feature occurs on a spatial scale well below the diffraction limit of optical microscopy, real time observation of nucleosome proximity in live cells has proven technically difficult, despite recent advances in live cell super resolution imaging. Thus, in recent work, we have been exploring a powerful alternative solution that is based on fluorescence lifetime and anisotropy imaging microscopy (FLIM and FAIM) of Förster resonance energy transfer (FRET) between fluorescently labelled histones – the core protein of a nucleosome. Here we present recent findings from application of this technology to the study of live cell chromatin network dynamics, which demonstrate local ensemble nucleosome proximity, spatiotemporally oscillates between different spacings that are ‘invisible’ to diffraction limited microscopy.

Dorus Gadella - University of Amsterdam, NL

Latest News on fluorescent proteins

Cunnison, Rory - Robb Group, Warwick Medical School, University of Warwick

Using smFRET to elucidate viral protein structure and function

smFRET is a powerful tool which can be used to explore the distances between fluorescently labelled molecules of interest, informing structure and function. We have utilised this technique in the Robb lab to understand the mechanisms governing interactions between viral proteins and RNA in multiple systems. First, we have developed an in vitro system to directly visualize replication as carried out by the SARS-CoV-2 RNA polymerase. By displacing a self-annealed strand of double-labelled RNA, the primer elongation can be monitored at a single-molecule level. We have further applied this approach to known inhibitors of SARS-CoV-2 replication, validating inhibition and differentiating between inhibition mechanisms of action, and we expect that this technique can be used to screen novel inhibitory compounds. The Robb group is now applying this technique to other priority diseases to further understand their replication and transcription cycles and provide a new platform for RNA polymerase-specific antiviral compound screening.

Session 2b: *Cellular FLIM and FRET measurements*

Hemmen, Katherina – Rudolf-Virchow-Center for Translational & Integrative Bioimaging

PIE-FLIM-FRET and High content image analysis reveal molecular interactions in living cells

Biomolecular interactions are fundamental processes critical for signaling and gene regulation - understanding them is a crucial step towards developing therapeutic interventions. FRET by polarization-resolved Fluorescence Lifetime Imaging Microscopy in Pulsed Interleaved Excitation mode has shown to be powerful to elucidate these interactions. Even if the experiments are accompanied by technical and analytical complexities, we show that the effort is worthwhile, especially when combined with fluorescence anisotropy. Our automated and integrated PIE-FLIM-FRET approach provides a pipeline for image segmentation and spectroscopic analysis. We demonstrate the utility of this approach with three examples:
1. Dimerization of the G Protein-Coupled Receptor MC4R: This receptor is linked to puberty onset in X. nigrensis and obesity in humans.
2. Differentiation of PSD95-Binding Peptides in Neurons: This is achieved through fluorescence anisotropy, allowing insights into neuronal interactions.
3. Dimerization and Interaction of Forkhead-Box Transcription Factors: These interactions are critical for the proper regulation of gene expression, influencing metabolism and disease related processes.

Nocker, Christoph - Tampé group, Institute of biochemistry, Goethe university Frankfurt

Peptide transport across membranes visualized at single-molecule level

ABC transporters such as transporter associated with antigen processing (TAP) have a key role in the cellular immune defense. TAP and its structural and functional homolog Thermus thermophilus multidrug resistance proteins A and B (TmrAB) use the energy of ATP hydrolysis to transport peptides across lipid bilayers. To understand the transport process in detail without ensemble averaging, single-molecule methods enable the ability to follow the transport of single substrates through individual transporters. Here, we developed a single-molecule FRET (smFRET) sensor based on the substrate-binding proteins OppA from Nontypeable Haemophilus influenzae (NthiOppA) and Lactococcus lactis (LlOppA) to follow the transport of peptide by ABC transporters on a single-molecule level and reveal mechanistic insight into the transport process. In addition, the effect of inhibitors on the transport kinetics of TmrAB can be studied. We demonstrated the functionality of the sensor by tracing the arrival of a single peptide after transmembrane translocation and uncover sequential power stroke events of the ATP turnover reduced TmrAE523QB variant. The approach will provide new insights into the stoichiometries of membrane transport processes of ABC transporters and will reveal a mechanistic and detailed understanding of their transport behavior.

Seidel, Claus - Molecular Physical Chemistry, Heinrich-Heine University Duesseldorf

Making fluorescence-based integrative structures and associated kinetic information accessible

In integrative structure modeling approaches, data from different experimental and theoretical techniques are combined to maximally utilize method-specific advantages and complementary information. Making these results publicly available following the FAIR (Findable, Accessible, Interoperable, Reusable) principles, e.g. in structural biology model repositories, is crucial for advancing science. The prototype PDB-Dev repository (https://pdb-dev.wwpdb.org/) offers a framework for this. For seamless interoperation of fluorescence-based integrative structure models in PDB-Dev, we present flrCIF (https://github.com/ihmwg/flrCIF), as an extension of PDBx/mmCIF data standard with extensions for Integrative/Hybrid Models (IHMCIF). Moreover, we extended the IHMCIF dictionary to introduce descriptions of complex kinetic schemes connecting multiple states, exchange

kinetics, and intrastate dynamics characterizing flexibility. Overall, these tools contribute towards dynamic structural biology by enabling standardized deposition, archiving, and dissemination of information on biomolecules in their functional context: from static structures towards dynamic structural networks and connecting structures with energy landscapes and real time motions.

Session 3: *Instrumentation and probes*

Thorben Cordes - Biophysical Chemistry, Faculty of Chemistry and Chemical Biology, Technische Universität Dortmund

From accurate FRET studies to systematic assay design and benchtop experiments

Single-molecule FRET (smFRET) has become an established tool to study biomolecular structure and dynamics in vitro and in vivo. We recently performed an international blind study in collaboration with the Seidel and Lamb labs[1] to assess the uncertainty of FRET experiments for proteins with respect to the measured FRET efficiency histograms, determination of distances, and the detection and quantification of structural dynamics. While this provided confidence in the use of smFRET for both mechanistic biochemical studies and structural biology, the design of smFRET assays and the selection of suitable labelling positions remains rather unsystematic. Based on a large literature screen and bioinformatics analysis, we identified a set of four parameters to rank residues for their suitability as label site. The “labelizer” package performs an analysis of a pdb-structure (or structural models), label score calculation, and FRET assay scoring in a script or via publicly available webserver (https://labelizer.bio.lmu.de/) to conveniently apply our approach.[2] I show the predictive power of our labelizer score for analysis of literature data and new experiments and outline our recent efforts to conduct smFRET experiments on the biochemistry bench.[3]
[1] Agam, Gebhardt, Popora et al., Nature Methods 20 (2023) 523-535
[2] Gebhardt, et al., https://www.biorxiv.org/content/10.1101/2023.06.12.544586.abstract
[3] Moya et al., https://www.biorxiv.org/content/10.1101/2023.12.29.573596v2

Viktoria Glembockyte LMU Munich

Modular DNA-Mediated Photostabilization for Extended Single-Molecule and Superresolution Imaging

Single-molecule fluorescence imaging methods have expanded tremendously in the last decades and led to many exciting experiments observing interactions between individual biomolecules. Meanwhile one of the main bottlenecks in any fluorescence imaging experiment remains the premature photobleaching of fluorescent labels. In this contribution, we show how we can exploit the self-assembly nature of a DNA origami based fluorescent labels to first establish dynamic self-repair mechanisms. By dynamically exchanging bleached labels with intact analogues from solution, we are able to recover the designed brightness of DNA origami reference structures even after complete photodamage. Nevertheless, even the imaging strategies that rely on the exchange of bleached labels are still limited by the photochemical processes in the excited states. Every time the fluorescent label enters the triplet excited state it has a probability to produce singlet oxygen and other reactive oxygen species (ROS). While the photodamaged fluorescent label can be dynamically replaced, ROS-induced photodamage to the target molecule or binding site is not mitigated and can also be detrimental imposing the need for millimolar concentrations of photostabilization additives. Keeping these limitations in mind, we developed a DNA-mediated strategy to to achieve photostabilization comparable to solution-based approaches at several orders of magnitude lower concentrations of additives.

Richter, Lars - LMU Munich

Immobilizing Nucleic Acids on Graphene: Possibilities and Limitations Compared to Single-Molecule FRET

Single-molecule FRET is a powerful technique that has been pushing dynamic structural biology. Yet, its application is partially limited by the requirement for double labeling, an about 6 nm-wide dynamic range, as well as photobleaching and complex acceptor photophysics. We employ graphene energy transfer (GET), where the two-dimensional material acts as an unbleachable broadband energy transfer acceptor up to 40 nm distance, and introduce a novel strategy for immobilizing nucleic acids, called GETvNA. This strategy enables us to study DNA bending or enzyme translocation with unprecedented precision for confocal, fluorescence microscopy. Furthermore, we visualize the translocation of the tumor relevant MGMT protein with Ångström spatial resolution on a confocal microscope.

The talk aims at discussing the possibilities and limitations of GETvNA with respect to single-molecule FRET. A special focus is set on the analysis of structural changes of DNA, when investigated with both methods. Overall, it will be shown that GETvNA can provide a simple and robust tool that complements FRET and is promising the widespread adaption for single-molecule fluorescence studies.

Lamb, Don - LMU Munich

FRET: It's all in the labels

Förster Resonance Energy Transfer (FRET) is the radiationless transfer of energy between two dipoles. Typically, fluorophores are used due to their high absorption cross-sections and high fluorescence quantum yields. When using FRET to measure distances and dynamics in biomolecules, the challenge often becomes how to place the labels at the correct locations. In this talk, I will discuss two different unconventional approaches we have used to label proteins to study their folding and dynamics. The first experiments involved the heat shock protein Hsp90. Hsp90 forms a dimer, so for intermolecular FRET, it is only necessary to label each monomer specifically with a single dye. While the yeast variant of Hsp90 does not contain cysteine residues, making it easy to introduce single cysteines for specific labeling, the human variant of Hsp90 contains a large number of accessible cysteines. To specifically label human Hsp90, we expressed the protein in two parts. The N-terminal domain was expressed separately from the middle and C-terminal domains. The N-terminal domain was modified with a single cysteine and then labeled. Afterwards, it was ligated with the remainder of the protein. As a second example, we labeled the Maltose Binding Protein specifically with three fluorophores for monitoring the order of domain folding. For labeling, we used a combination of a non-natural amino acid residue and two cysteines, one of which can be protected from labeling in the presence of maltose.

Posters

Salama, Noah - Seidel group, Molecular Physical Chemistry, Heinrich-Heine-University

Performing and Analyzing FRET Nanoscopy on DNA-Origami Platforms with sub-Nanometer Precision

Super-resolution microscopies enable the study of larger cellular structures and molecular assemblies with high precision by overcoming the diffraction limit. They provide an invaluable tool due to being minimally invasive and highly selective to the molecule of interest, with nanometer resolution. However, the currently achieved spatiotemporal resolution cannot resolve distances on the size of individual molecules, thus dynamics and conformational fine structure on the scale of single molecules remain concealed.

It is therefore desirable to additionally resolve intra- and inter-molecular distances with Ångström precision by overcoming the resolution limit of fluorescence nanoscopy alone. We achieve this through the combination of multiparameter FRET-spectroscopy and colocalization stimulated emission depletion (cSTED) microscopy, giving a versatile and readily available tool for investigation of structure and dynamics on a single-molecule level.[1]

We demonstrate the feasibility and accuracy of our approach by using standardized DNA origami platforms with two dye pairs in a distance of 75 nm as a benchmark sample. We simultaneously localize donor and acceptor dyes of single FRET pairs with nanometer resolution and quantitatively measure intramolecular distances with sub-nanometer precision over a large dynamic range.

The analysis of FRET parameters yields the Euclidean distance with Ångström precision while colocalization provides the distance projected onto the image plane. Consequently, the combined information of FRET and cSTED analysis allows for the determination of 3D-orientations via Pythagoras' theorem. We established an easy-to-follow workflow for performing and analyzing FRET nanoscopy measurements and obtain inter-dye distances with sub-nanometer precision. We demonstrate the potential of FRET nanoscopy to unravel the interplay between spatial and local molecular organization of biomolecules. The concept will further be extended to modified DNA origami constructs containing a dynamic element to probe the capabilities of obtaining kinetic information via FRET nanoscopy.

Saurabh, Rai - Ultrafast and Molecular Spectroscopy Lab, Indian Institute of Science Education and Research Bhopal, India

Fluorescence Resonance Energy Transfer in a Supramolecular Assembly of Luminescent Silver Nanoclusters and Cucurbit[8]uril Based Host-Guest System

The exploration of interactions between organic chromophores and biocompatible luminescent noble metal nanoclusters (NCs) has revealed a promising avenue for harnessing energy transfer processes with diverse applications in materials science. We present a photoluminescent supramolecular assembly, fabricated through a two-stage process, leveraging the energy transfer mechanism between silver (Ag) NCs as donors and a host-guest system as acceptors.
Our investigation delves into the host-guest, employing advanced spectroscopic techniques to finely tune the fluorescence properties of the acceptor. Through a non-covalent strategy, this study advances the development of Fluorescence Resonance Energy Transfer (FRET) pairs featuring blue-emitting NCs and host-guest complexes. Our non-covalent approach holds promise for sustainable materials in light harvesting, white light emission, and anti-counterfeiting applications. This research signifies a significant step in harnessing supramolecular assemblies' potential in photonics and materials science.

Nivedita Pan - Prof. Samir Kumar Pal's group (S. N. Bose National Centre for Basic Sciences), Department of Nanoscience and Nanotechnology, University of Calcutta

Plasmon-Coupled Donor−Acceptor Based Organic Sensitized Photoanodes for Improved Photovoltaic Performance: Unraveling an Ultrafast Electron Transport and FRET Mechanism

Challenges such as back electron-hole recombination, rapid electron injection, broad-spectrum light harvesting, and environmental concerns are critical factors influencing advancements in this field. Organic photosensitizers, which feature a delocalized π-electron system capped with electron acceptors (A) and donors (D), offer simple synthesis, excellent solar energy capture, and highly tunable absorption properties. These attributes, combined with semiconductor-metal (plasmonic) nanohybrids, have the potential to address these challenges. In this study, we report enhanced photovoltaic performance using organic D-π-A type photosensitizer (RK1)-based plasmonic Au nanoparticle-decorated hybrid mesoporous TiO2 photoanodes in dye-sensitized solar cells (DSSCs) and dye-sensitized photoelectrochemical water splitting (DSPEC). The plasmonic material not only reduces back electron-hole recombination but also enhances device performance through the spectral overlap of its localized surface plasmon resonance (LSPR) band with that of the RK1 organic sensitizer near the TiO2 surface, enabling Förster resonance energy transfer (FRET). A femtosecond resolved fast electron transfer has been reported when photosensitizer RK1 has been attached to the surface of the semiconductor nanoparticle, which in turn plays a crucial role in the development of an efficient light harvesting material.

Mondal, Susmita – S.N. Bose National Centre for Basic Sciences (West Bengal, Indien)

A combined spectroscopic and computational study of functionalized hybrid-nanomaterials to validate their efficacy in nano-theranostics

Functionalization of an inorganic nanoparticle with an organic ligand mostly predominates its interaction of the functionalized nanoparticles (NPs) with various cellular components leading to therapeutic effect diminishing the adverse side effects. Apart from the therapeutic effect of the nanoparticles other physical properties of the organic-inorgaic complex (nanohybrid) including fluorescence, x-ray or MRI contrast offer diagnosis of the anomalous target cell. Here we have functionalized Mn3O4 nanoparticles with organic citrate (C-Mn3O4) and folic acid (FA-Mn3O4) ligand and investigated their antimicrobial activities using Staphylococcus hominis as a model bacteria, which can be remediated through their membrane rupture. While, HRTEM, XRD, DLS, absorbance and fluorescence spectroscopy have been used for the structural characterisation of the functionalised nanoparticles, zeta potential measurement, temperature dependent ROS generation reveal the drug action of the NPs. We have used high end density functional theory (DFT) calculation to rationalise the specificity of the drug action of the NPs. Pico-second resolved FRET studies confirm the enhanced affinity of FA-Mn3O4 to the bacteria compared to C- Mn3O4 leading to enhanced anti-microbial activity. We have shown that the functionalised nanoparticles offer significant x-ray contrast in in-vitro studies indicating the FA-Mn3O4 NPs to be a potential theranostic agent against bacterial infection.

Participants of FRET Satellite Workshop @ MAF2024

Name, Surname	poster/talk	Group, Institute, Organization
Ahmed, Zainab		Jamia Millia Islamia
Bagheri, Niusha		KTH Royal Institute of Technology
Börner, Richard	talk	Biophotonics, Laserinstitut Hochschule Mittweida, Mittweida University of Applied Sciences
Caneva, Sabina		TU Delft
Chenyuan, Yan		Philip Tinnefeld Group, Faculty of Chemistry and Pharmacy,Ludwig Maximilian University of Munich
Cordes, Thorben	talk	Biophysical Chemistry, Faculty of Chemistry and Chemical Biology, Technische Universität Dortmund
Cunnison, Rory	talk	Robb Group, Warwick Medical School, University of Warwick
Czeslik, Claus		TU Dortmund, Physical Chemistry
Dineshbabu, Takkella		IIT Hyderabad
Fayad, Nour		Universite de Rouen- NanoFRET group
Francés Soriano, Laura		Photoreactivity group, ICMOL, UVEG
Frank, Veronika	talk	Hugel Group, Institute of Physical Chemistry, Albert-Ludwigs-Universität Freiburg
Gadella, Dorusi	talk	University of Amsterdam, NL
Giulia Micolonghi		University of Granada
Glembockyte, Viktorija	talk	LMU Munich
Hemmen, Katherina	talk	Rudolf-Virchow-Center for Translational & Integrative Bioimaging
Hildebrandt, Niko	talk	nanofret.com, McMaster University, Hamilton, Canada
Hinde, Elizabeth	talk	University of Melbourne, Australia
Karakani, Ali		University of Toronto
Kirti		Indian institute of technology guwahati
Kramm, Kevin		PicoQuant
Kulkarni, Abhilash		Experimental Biomolecular Physics, KTH Royal Institute of Technology
Lamb, Don	talk	Physical Chemistry, Department Chemistry, LMU Munich
Lars Richter	talk	LMU Munich
Martins, Catarina		Faculty of Pharmacy of University of Porto, REQUIMTE
Micolonghi, Giulia		University of Granada
Mondal, Susmita	poster	S. N. Bose National Centre for Basic Sciences
Nocker, Christoph	talk	Tampe´ group, Institute of biochemistry, Goethe University Frankfurt
Ortmann, Uwe	poster	PicoQuant GmbH
Paez Larios, Francisco		Eggeling Lab, IAOB, Jena FSU

Pan, Nivedita	poster	Prof. Samir Kumar Pal's group (S. N. Bose National Centre for Basic Sciences), University of Calcutta
Peulen, Thomas	talk	Heinze, Rudolf-Virchow Centre Integrative Microscopy
Rai, Saurabh	poster	Ultrafast and Molecular Spectroscopy Lab, Indian Institute of Science Education and Research Bhopal, India
Reschke, Bianca	talk	Molecular Physical Chemistry, Heinrich-Heine-University Düsseldorf
Richter, Lars	talk	LMU Munich
Salama, Noah	poster	Molecular Physical Chemistry, Heinrich-Heine-University Düsseldorf
Salto-Giron, Carmen		FAM-247 (Ángel Orte Gutierrez's Group), Univerdad de Granada
Seidel, Claus	talk	Molecular Physical Chemistry, Heinrich-Heine-University Düsseldorf
Sudhanshu, Sharma		LBCS, IIT Hyderabad