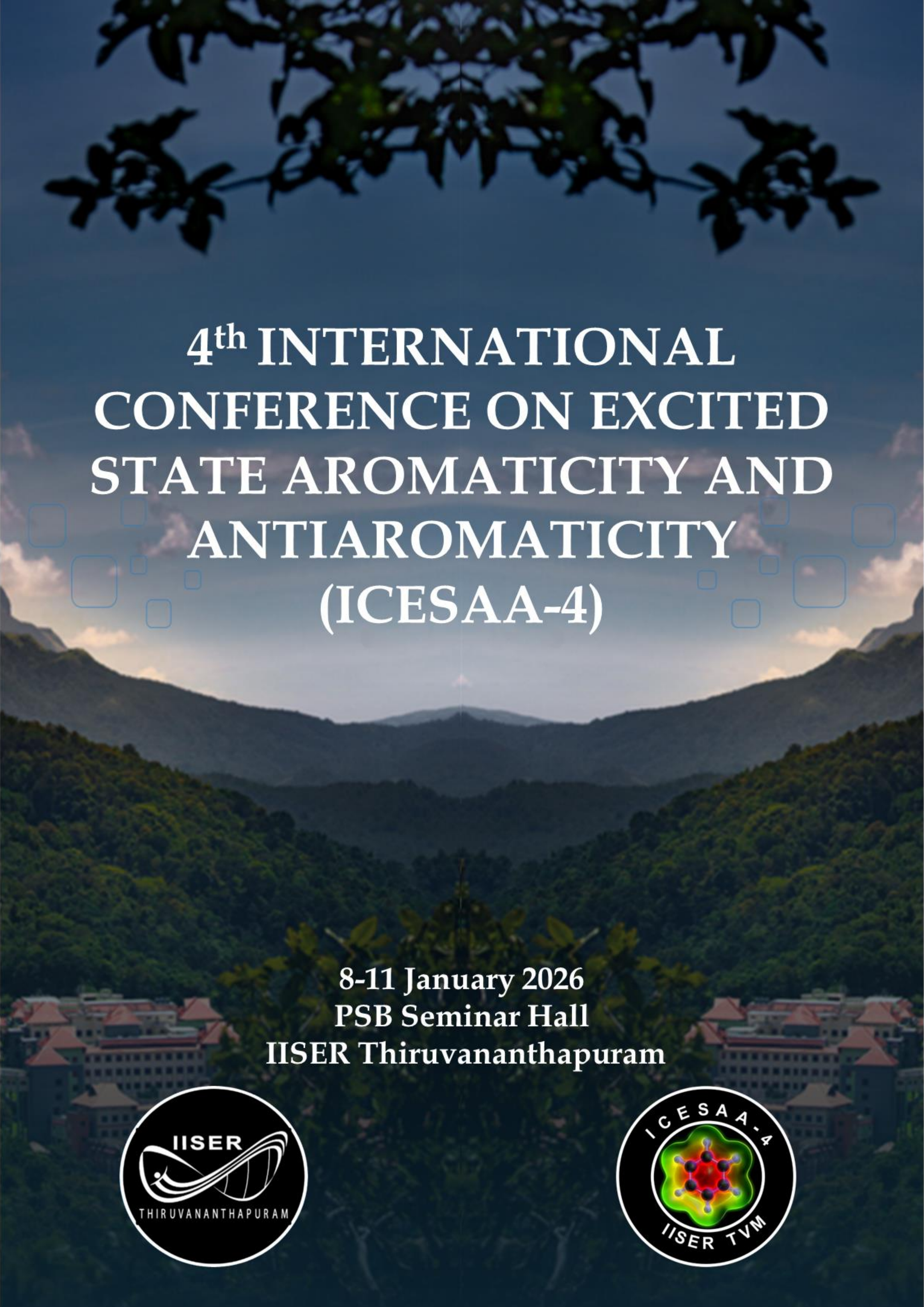

4th INTERNATIONAL CONFERENCE ON EXCITED STATE AROMATICITY AND ANTIAROMATICITY (ICESAA-4)

8-11 January 2026
PSB Seminar Hall
IISER Thiruvananthapuram

SCHEDULE FOR ICESAA-4 WINTER SCHOOL

DAY 1 (08/01/2026)

Session-I		
08:40 AM – 09:00 AM	Opening Remarks	Prof. J N Moorthy Director, IISER TVM
	Welcome Remarks	Prof. R. S. Swathi
09:00 AM – 10:00 AM	Fundamentals of aromaticity	Prof. Henrik Ottosson
10:00 AM – 10:40 AM	Electronic aromaticity descriptors	Prof. Irene Casademont
(10:40 AM – 11:10 AM) Coffee Break		
Session-II		
Chairperson		
11:10 AM – 11:50 AM	Magnetic aromaticity descriptors	Prof. Igor Roncevic
11:50 AM – 12:20 PM	Geometric aromaticity descriptors	Prof. Bo Durbeej
12:20 PM – 01:20 PM	Fundamentals of excited state calculations	Prof. Debashree Ghosh (Online)
(01:20 PM – 02:50 PM) Lunch Break		
Session-III		
Chairperson		
02:50 PM – 03:20 PM	Energy-based descriptors	Prof. Mercedes Alonso Giner (Online)
03:20 PM – 04:20 PM	Fundamentals of photochemistry	Prof. Victor Gray
04:20 PM – 05:20 PM	Ultrafast spectroscopy	Prof. Juwon Oh
(05:20 PM – 05:50 PM) Coffee Break		
Session-IV		
Chairperson		
05:50 PM – 06:25 PM	Research Talk	Prof. Juwon Oh
06:25 PM – 06:55 PM	Excite state surface features	Prof. Josene Toldo
06:55 PM – 07:25 PM	Organic photochemistry	Prof. Igor Alabugin
07:25 PM – 07:55 PM	Pitfalls of excited state (anti)aromaticity	Prof. Henrik Ottosson
07:55 PM – 08:00 PM	Concluding Remarks	Prof. Mahesh Hariharan
Dinner		

SCHEDULE FOR ICESAA-4

DAY 2 (09/01/2026)

Session-I		
Chairperson		
09:00 AM – 09:05 AM	Welcome remarks	
09:05 AM – 09:40 AM	IL1	Prof. Henrik Ottosson
09:40 AM – 10:15 AM	IL2	Prof. Cate Anstöter
10:15 AM – 10:50 AM	IL3	Prof. Scott C. Blanchard (Online)
(10:50 AM – 11:20 AM) Coffee Break		
Session-II		
Chairperson		
11:20 AM – 11:55 PM	IL4	Prof. Debashree Ghosh
11:55 PM – 12:15 PM	CL1	Dr. Matthew Johnson
12:15 PM – 12:35 PM	CL2	Dr. Kannan Subburaj
(12:35 PM – 02:30 PM) Lunch Break		
Session-III		
Chairperson		
02:30 PM – 03:05 PM	IL5	Prof. Nikola Basaric
03:05 PM – 03:40 PM	IL6	Prof. Bern Kohler
03:40 PM – 04:00 PM	CL3	Dr. Peter Sebej
(04:00 PM – 05:30 PM) Coffee Break and Poster Session Part 1		
Session-IV		
Chairperson		
05:30 PM – 06:05 PM	IL7	Prof. Anna Gudmundsdottir
06:05 PM – 06:25 PM	CL4	Dr. Peter Mayer (Online)
06:25 PM – 06:45 PM	CL5	Dexter Gordon
06:45 PM – 07:20 PM	IL8	Prof. Yoshimitsu Itoh
Dinner		

DAY 3 (10/01/2026)

07:00 – 10:30 AM	Excursion (Options 1, 2 and 3)	
(10:30 AM – 11:00 AM) Coffee Break		
Session-V		
Chairperson		
11:00 AM – 11:35 AM	IL9	Prof. Florian Glöcklhofer
11:35 AM – 12:10 PM	IL10	Prof. Jyotishman Dasgupta
12:10 PM – 12:30 PM	CL6	Dr. Tanveer Rasool
(12:30 PM – 02:00 PM) Lunch Break		
Session-VI		
Chairperson		
02:00 PM – 02:35 PM	IL11	Prof. Manabu Abe
02:35 PM – 03:10 PM	IL12	Prof. Ryohei Kishi
03:10 PM – 03:45 PM	IL13	Prof. Josene M. Toldo
(03:45 PM – 05:30 PM) Coffee Break and Poster Session Part 2		
Session-VII		
Chairperson		
05:30 PM – 06:05 PM	IL14	Prof. Igor Alabugin
06:05 PM – 06:40 PM	IL15	Prof. Jishan Wu (Online)
06:40 PM – 07:00 PM	CL7	Dr. M. A. Rather
07:00 PM – 07:20 PM	CL8	Dr. M. S. Charoo
Dinner		

DAY 4 (11/01/2026)

Session-VIII		
Chairperson		
09:00 AM – 09:05 AM	Welcome remarks	
09:05 AM – 09:40 AM	IL16	Prof. Prasun Mandal
09:40 AM – 10:15 AM	IL17	Prof. Martin Peeks
10:15 AM – 10:50 AM	IL18	Prof. Shohei Saito
(10:50 AM – 11:20 AM) Coffee Break		
Session-IX		
Chairperson		
11:20 AM – 11:55 PM	IL19	Prof. Ori Gidron
11:55 PM – 12:15 PM	CL9	Dr. Moumita Gangopadhyay
(12:15 PM – 02:00 PM) Lunch Break		
Session-X		
Chairperson		
02:00 PM – 02:35 PM	IL20	Prof. Jinquan Chen (Online)
02:35 PM – 03:10 PM	IL21	Prof. Igor Roncevic
03:10 PM – 03:45 PM	IL22	Prof. Yusuke Yoneda
03:45 PM – 04:20 PM	IL23	Prof. Gokulnath Sabapathi
(04:20 PM – 04:50 PM) Coffee Break		
Session-XI		
Chairperson		
04:50 PM – 05:25 PM	IL24	Prof. Tomas Slanina
05:25 PM – 06:00 PM	IL25	Prof. Bo Durbeej
06:00 PM – 06:35 PM	IL26	Prof. Irene Casademont Reig
06:35 PM – 07:10 PM	IL27	Prof. Daniele Leonori (Online)
07:10 PM – 07:20 PM	ICESAA-5 Announcement	
Conference Dinner (07:30 PM-11:00 PM)		

Effect of Excited-State Antiaromaticity on the Ligand-to-metal Charge Transfer

Juwon Oh

Department of Chemistry, Kyuongpook National University, Daegu, 41566, Korea

Aromaticity is one of the key fundamental concepts in organic chemistry. As cyclic π-conjugated molecules increase in size, local or global cyclic π-conjugation can form, which has a significant effect on their π-electron structures and aromaticity. This further provides important information for understanding the characteristics and designing functional macrocyclic compounds. From this perspective, we explored how excited-state antiaromaticity influences ligand-to-metal charge transfer (LMCT) in metallohexaphyrins.[1] In line with Baird's rule, metallohexaphyrins that are aromatic in the ground state acquire antiaromatic character upon excitation to the S_1 state. Given the redox-like interaction between the metal center and the ligand framework during LMCT,[2] this process effectively alleviates the energetic penalty associated with excited-state antiaromaticity. A clear relationship is observed between the degree of ground-state aromaticity and the characteristic time scales of LMCT, indicating that antiaromatic destabilization at the Franck–Condon region serves as a key driving force for charge transfer. Overall, this study clarifies the role of excited-state antiaromaticity in governing excited-state dynamics and offers new perspectives on the photochemical behavior of organic molecular systems.

1. J. Kim, H. Kim, J. Oh, D. Kim, Bull. Korean Chem. Soc. 2022, 43, 508-513.
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Deciphering the astrophotochemical inertness of H_3^+ at molecular level

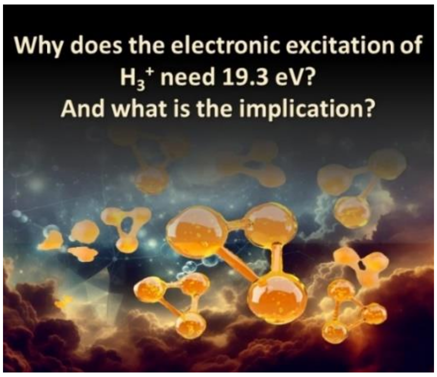
Josene Toldo,[1-3] Jakob Staab,[1,4] ,Eduard Matito,[5,6] Cina Foroutan-Nejad,[7] Henrik Ottosson [1]*

[1] Department of Chemistry – Ångström, Uppsala University, Sweden. [2]Aix-Marseille University, CNRS, ICR, Marseille, France; [3] Université Claude Bernard Lyon 1, ENS de Lyon, CNRS, LCH, UMR 5182, Lyon, France; [4] Department of Chemistry, The University of Manchester, Oxford Road, Manchester, UK; [5] Donostia International Physics Center, 20018 Donostia, Euskadi, Spain; [6]Ikerbasque, Basque Foundation for Science, 48009 Bilbao, Spain; [7] Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, Poland.

E-mail: Henrik.Ottosson@kemi.uu.se

Abstract:

The trihydrogen cation, H_3^+, is unique in the Universe.[1] It serves as the primary proton reservoir, driving essential astrochemical reactions,[2] and functions as a thermostat for giant gas planets.[3] H_3^+ has also a remarkably low photodissociation rate, explained by its exceptionally high first electronic excitation energy (19.3 eV).[4] We now reveal the key factors behind this high energy: (*i*) aromatic stabilization in its electronic ground state, (*ii*) antiaromatic destabilization in its first excited state, and (*iii*) a high nuclear-to-electronic charge ratio (+3 *versus* -2).[5] Through comparisons with analogous π-conjugated carbocations, we find that ground state aromatic stabilization plus excited state antiaromatic destabilization raise the excitation energy of H_3^+ by 4.8 - 6.0 eV. Only with this increase can it fulfil its unique functions in space. Although our study focuses on H_3^+, it unravels that excited state antiaromaticity also impacts on the excited state properties other species of astrochemical importance, *e.g.*, the cyclopropenium cation.[6]



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Same, Same, but Different: Aromaticity and Metastability in Anionic PAH Isomers

Chiara Beldì & **Cate S. Anstöter***

*Cate.anstoter@glasgow.ac.uk

Aromaticity and antiaromaticity are central organising principles in ground- and excited-state chemistry, yet their role in governing the stability of transiently bound anionic states remains comparatively unexplored. Carbon-rich molecules, and in particular polycyclic aromatic hydrocarbons (PAHs) and related isomers, provide an ideal platform for probing this interplay, as subtle changes in connectivity can lead to markedly different aromatic signatures across electronic states.

In this work, we explore how differences in (anti)aromaticity between structural isomers influence their propensity to bind an extra electron and form molecular anions. While ground-state aromaticity is often invoked to rationalise molecular stability, electron attachment frequently populates electronically excited or metastable states that are embedded in the autodetachment continuum. In such cases, conventional aromaticity/excited state descriptors may no longer provide a complete picture of stability.

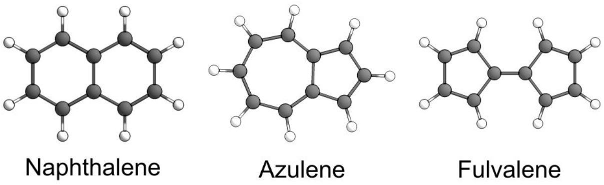

Figure 1. The three relevant isomers of $C_{10}H_8$.

Focusing on small carbon-based isomers with identical stoichiometry but distinct ring connectivities, we will discuss how their aromatic character evolves upon electron attachment, and how this evolution correlates with the energies, lifetimes, and decay pathways of the resulting anionic states. By combining insights from advanced electronic structure calculations with concepts from excited-state aromaticity theory, this work highlights how aromatic stabilisation and antiaromatic destabilisation manifest in transient anionic resonances.

Self-healing fluorophores in biological research

Maxwell Martin, Sukanta Bar, Rakesh Paul, Roger Altman, **Scott Blanchard**

St. Jude Children's Research Hospital, Department of Structural Biology
Memphis, TN 38104

Organic fluorophores serve as powerful tools in biomedical research due to their absorption and emission properties spanning the visible spectrum. Our team has leveraged the Baird aromatic properties of cyclooctatetraene, combined with principles of intra-molecular chemistry, to mitigate excitation-induced accumulation of chemically distinct organic fluorophores fluorophores in triplet excited states to dramatically enhance their performance. Through collaborative investigations, we have used "self-healing" cyanine-class organic fluorophores spanning the visible spectrum to reveal previously obscured rate-limiting processes underpinning function in diverse biological systems. Through these studies, we empirically observed that organic fluorophores exhibit order-of-magnitude reductions in performance on proteins compared to nucleic acids. Using chemical, photophysical and single-molecule imaging methods, we show that the mechanism of protein-induced fluorophore photobleaching is driven by hydrogen atom transfer (HAT) from the peptide-backbone to excited-state fluorophores, resulting in the termination of fluorescence (photobleaching). We further show that HAT-mediated fluorophore photobleaching is general to both cyanine- and rhodamine-class fluorophores – the most widely utilized classes in biomedical research. With this knowledge, we are actively pursuing strategies to overcome this general limitation to thereby advance both existing and future single-molecule, super-resolution, and live-cell imaging applications.

Quantum chemistry methods to study strongly correlated systems – from variational to machine learning approaches

Debashree Ghosh, School of Chemical Sciences, Indian Association for the Cultivation of Science

Polyaromatic hydrocarbons (PAHs) such as acenes have long been studied due to its interesting optical properties and low singlet triplet gaps. Earlier studies[1,2] have already noticed that use of complete valence active space is imperative to the understanding of its qualitative and quantitative properties. Since complete active space based methods cannot be applied to such large active spaces, we have used density matrix renormalization group (DMRG)[3] based approaches. Further small modification to the PAH topology shows interesting new phases of behaviour in its optical gaps. We have understood the effect of these effects based on spin frustration due to the presence of odd membered rings. In this talk, I will discuss these observations from molecular and model Hamiltonian perspectives.[4]

Further developments based on artificial neural network based configuration interaction for strongly correlated systems will also be discussed.[5] The similarities between the ANNs and the MPS wavefunctions will be leveraged for 2D systems.

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4. In the quest for a stable triplet state in small polyaromatic hydrocarbons: an in silico tool for rational design and prediction, M. Rano, S.K. Ghosh, D. Ghosh, *Chemical Science*, **10**, 9270 (2019).
5. Configuration interaction trained by neural networks : Application to model polyaromatic hydrocarbons, S.K. Ghosh, M. Rano, D. Ghosh, *J. Chem. Phys.*, **154**, 094117 (2021).

Does the antiaromaticity in the excited state always drive the elimination of small molecules from aryl derivatives?

Nikola Basarić, [1]* Jiani Ma, [2] Ivana Antol, [1] and Nađa Došlić [1]
*[1]*Presenting Author-NB*
[1] Affiliation: Ruđer Bošković Institute, Zagreb, Croatia
[2] School of Chemistry and Chemical Engineering, Shaanxi Normal University, Xi'an, China
E-mail: nbasaric@irb.hr

Photodehydration of *o*-hydroxymethylphenol (**1**) gives rise to quinone methide (QM) **2** intermediate in an adiabatic reaction occurring on the singlet excited state surface.[1] The similar mechanism for the photoelimination of ammonium salt was reported also for phenol **3** (Figure 1).[2] However, structurally modified molecules undergo photoelimination via different mechanistic pathways, in some cases via a conical intersection delivering QMs directly in their ground state. It is known that phenols in the singlet excited state exhibits antiaromatic character, which is relieved in photochemical reactions.

More complex substrates such as naphthols or anthrols undergo the H_2O elimination to QMs via entirely different mechanism involving a photoionization and deprotonation to a phenoxyl radical, followed by an elimination of the OH·.[3] Furthermore, we have studied the photoelimination of H_2O or acetic acid from the suitably substituted anilines, such as **4**, and found out that the mechanism is non-adiabatic and involves higher excited nσ* states.[4] In these examples some straightforward conclusions about the antiaromaticity as a driving force are not so evident. The detailed computational and experimental investigation of the elimination reactions will be disclosed.

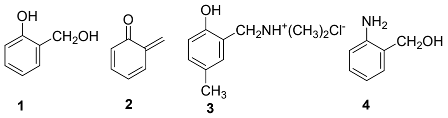

Figure 1: Molecules undergoing photoelimination in the singlet excited state.

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Toward a Unified Photophysical Framework for Eumelanin and Related Carbon-Based Nanomaterials

Bern Kohler

Department of Chemistry and Biochemistry
The Ohio State University
Columbus, Ohio, USA

Eumelanin is the ubiquitous brown-black pigment found in nearly all organisms, including humans, that provides coloration, sunscreening, metal ion chelation, and radical scavenging. Many biological pigments are small molecules, but eumelanin is a natural nanomaterial with hierarchical structure. Understanding structure-function-property relationships in eumelanin is primitive because the underlying molecular structures are obscure despite more than a century of study. Although it is still frequently referred to as a biopolymer, growing evidence indicates that eumelanin is composed of modestly sized covalent units that undergo extensive aggregation. Eumelanin furthermore has remarkably similar properties to other carbon-based nanomaterials such as asphaltenes and natural organic matter. These materials have typically been viewed through a molecular lens, but our femtosecond and steady-state spectroscopic studies provide evidence of extensive interactions among chromophores. By disassembling synthetic eumelanin nanoparticles into smaller subunits, we explore the morphological and supramolecular origins of its photoproperties. Using atomic force microscopy (AFM) imaging, we have obtained evidence that the fundamental chromophores of eumelanin are ultrasmall, few-layer stacks that resemble molecular nanographenes. Our emerging model explains how common photoproperties that include transient spectral hole burning and excitation-wavelength dependent emission arise in eumelanin and other carbon-based nanomaterials from the ensemble behavior of these ultrasmall units. Because similar interactions among polycyclic aromatic hydrocarbon-type building blocks recur in other carbon-based nanomaterials, this model provides a framework for tailoring their photophysical properties, offering promising opportunities in photocatalysis, energy capture and storage, and bioelectronics.

Anna D. Gudmundsdottir, University of Cincinnati, Ohio, USA

Photophysical Characteristics, Photoreactivity, and Photodynamic Behavior of Coronene, Corannulene, and Phenyl Azido Derivatives in Solution and the Solid State

Over the past two decades, corannulene and its derivatives have found numerous applications in host–guest chemistry, metal–organic frameworks, and porous organic polymers. Despite these advances, a detailed molecular-level understanding of how molecular curvature influences photophysical behavior and photochemical reactivity remains limited. Corannulene provides a curved aromatic platform that contrasts sharply with the well-studied chemistry of planar polycyclic aromatic hydrocarbons and aryl nitrenes, enabling systematic investigation of curvature-dependent excited-state properties and reaction pathways.

Herein, we present a comparative study of the photophysical properties, photoreactivity, and photodynamic behavior of corannulene, coronene, and phenyl azido derivatives in solution and in the solid state. Upon irradiation, the azido derivatives undergo nitrogen extrusion to form the corresponding singlet nitrenes, which intersystem cross to their triplet configurations. The resulting triplet nitrenes were characterized using ESR spectroscopy and laser flash photolysis, and their photoreactivity was evaluated. Analysis of the aromaticity of the triplet states of the corannulene, coronene, and phenyl nitrene derivatives provides insight into how molecular curvature and planarity modulate electronic structure, excited-state stabilization, and photochemical reactivity. The photodynamic behavior of these azido derivatives in the solid state will also be discussed.

Amide-Embedded π-Systems: Novel Interface that Connects Electronic Function and Molecular Assembly

Yoshimitsu Itoh

Affiliation: Department of Chemistry and Biotechnology
E-mail: itoh@chembio.t.u-tokyo.ac.jp

Abstract:

Amide group is one of the most common hydrogen-bonding (H-bonding) motifs and play crucial roles in protein folding, high-strength polyamides, and functional supramolecular polymers. One important feature of the amide group is its partial C=N double bond character, which arises from resonance effect. In this study, we introduce a new strategy of “amide-embedding” by substituting C=C double bonds of polycyclic aromatic hydrocarbons (PAHs) with amide groups. Such molecular design allows amide groups to be utilized not only for assembling molecules through 1D H-bonding but also for rationally designing higher-order 2D molecular assembly. Moreover, as the amide bond is not simply appended but “embedded” in the PAH framework, molecular assembly through H-bonding would directly perturb the π-conjugation network of the molecules to tune optoelectronic functions of the parent molecule. In the presentation, we present an example of tuning T1 state energies by a simple covalent and non-covalent modification of the amide group. Our new molecular design expands the utility of the amide bond for novel functional molecular design.

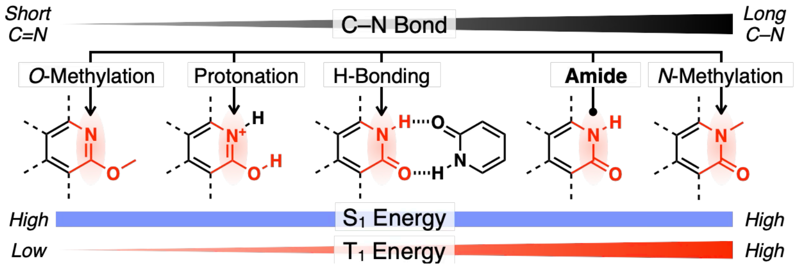

Figure 1: Selective tuning of T1 state energy by amide modification.

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Exploiting excited-state aromaticity for two-photon polymerisation

Florian Glöcklhofer (TU Wien)

Institute of Applied Synthetic Chemistry, TU Wien, Getreidemarkt 9/163, 1060 Vienna, Austria

Two-photon polymerisation (2PP) is a powerful technique for 3D printing at the micro- and nanoscale, enabling high-resolution fabrication of structures and devices for various applications, including in photonics, soft robotics, and biomedical systems. The development of next-generation 2PP resins for these applications depends on photoinitiators that offer efficient radical generation, high optical transparency, and straightforward synthesis and formulation. However, 2PP photoinitiators designed by traditional approaches usually rely on donor–acceptor chromophores that introduce visible colouration, involve multistep syntheses, or show limited solubility in common monomers, motivating the search for alternative molecular frameworks and design approaches.

In my talk, I will present paracyclophanetetraene (**PCT**) as a fundamentally distinct photoinitiator framework. PCT is a heteroatom-free, high-symmetry conjugated macrocycle that is accessible in a single synthetic step from commercially available precursors and is notable for its chemical and thermal stability and high solubility in organic solvents compared to its linear structural analogues.[1] PCT has been described as a molecule with concealed antiaromaticity;[2] it features a formally antiaromatic macrocyclic conjugated system with $4n$ (24) π-electrons, but its properties in the ground state are dominated by the four locally aromatic units with $4n+2$ (6) π-electrons, which conceal the antiaromaticity and impart the molecule with high stability. Despite the presence of these Hückel aromatic subunits, PCT still shows increased macrocyclic, global aromaticity in the excited S_1 and T_1 states, a feature known as excited-state or Baird aromaticity that is normally attributed to molecules with antiaromatic ground states.[3] Owing to PCT's symmetry, the lowest-energy $S_0 \rightarrow S_1$ transition for accessing these Baird aromatic states is one-photon forbidden,[4] appearing experimentally only as a weak absorption shoulder near 390 nm. This weak absorption in the visible range of the spectrum means excellent transparency (and minimal colouration) while simultaneously providing a two-photon allowed transition that can be accessed with 780 nm excitation, a wavelength commonly used in commercial 2PP printers. Based on these structural, electronic and photophysical features, we anticipated that a long-lived Baird aromatic dark S_1 and T_1 state might act as a reactive, initiating species under two-photon excitation.

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Triplet conformation in acene-fused cyclooctatetraene dyes

Jyotishman Dasgupta
[1] *Affiliation: Tata Institute of Fundamental Research, Mumbai, India 400005*
E-mail: dasgupta@tifr.res.in

Abstract:

Cyclooctatetraene (COT) has a tub-shaped conformation in its ground non-aromatic state, while it is predicted to have a planar aromatic triplet state. [1,2, 4] However, COT possesses a non-vertical triplet state and therefore its detection has remained elusive through direct photoexcitation.[3] Recently, fluorescent dyes synthesized by fusing COT with anthracene and phenazine “wings” have shown a large Stokes shift [5, 6] implying a significant conformational change in their excited singlet manifold. Here, using broadband transient absorption spectroscopy supported with electronic structure calculations, we demonstrate that intersystem crossing occurs in the planar COT conformation in these flapping dyes.[7] We confirm that such a planar conformation in the triplet state does not impart aromaticity to the COT backbone, as previously predicted. In addition using femtosecond stimulated Raman spectrosocopy (FSRS) we could observe Raman signatures of planarization as the molecule relaxes on the excited singlet surface [8]. Our work therefore provides the basis for the requisite structural design principles that would allow for triplet formation from excited singlet states in COT-based functional molecules.

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2-(4-Nitrophenyl)-1*H*-indolyl-3-methyl Chromophore: A Versatile Photocage

Manabu Abe
Department of Chemistry, Hiroshima University, Japan
E-mail: mabe@hiroshima-u.ac.jp

Abstract:

Photolabile protecting groups (PPG) allows us to deprotect functional groups under neutral and mild conditions. Furthermore, the deprotection can be controlled in spatiotemporal manners. In our previous study, a new PPG, i.e. *p*-nitrophenyl indole derivative (NPIM), was developed to release not only acids but also amines and alcohols [1]. Although radical intermediates were detected [2], the reaction mechanism has not been well elucidated. In this study, the photoinduced deprotection reaction was investigated using product analysis and transient absorption spectroscopy of compound **1a** under various reaction conditions. In the transient absorption spectroscopy in benzene, the triplet excited state and radical species from **1a** were observed. In the presentation, the reaction mechanism will be discussed in detail.

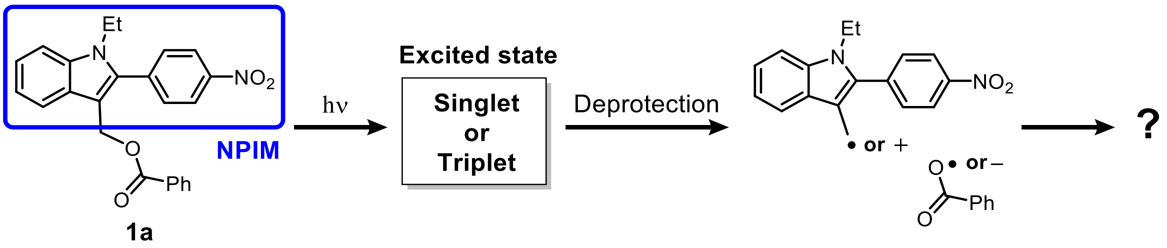

Figure 1:

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Relationship between Stacked-Ring Aromaticity and Baird’s Rule

Ryohei Kishi,[1,2,3,4,*] Kenji Okada,[1] Ryota Sugimori,[1] Kosei Nishino,[1]
Kohei Tada,[1,2] and Yasutaka Kitagawa.[1,2,3,4,5]
[1] Graduate School of Engineering Science, The University of Osaka,
[2] RCSEC, The University of Osaka, [3] QIQB, The University of Osaka,
[4] ICS-OTRI, The University of Osaka, [5] OTRI-Spin, The University of Osaka
E-mail: kishi.ryohei.es@osaka-u.ac.jp

Abstract:

Recent theoretical and experimental studies have indicated that closely π-stacked dimers of several $4n\pi$ antiaromatic molecules tend to exhibit structures, electronic states, and magnetic response properties similar to those of $4n+2$ π systems.[1,2] This phenomenon is sometimes called stacked-ring aromaticity. The mechanisms behind stacked-ring aromaticity have primarily been explained using molecular orbital (MO) theory and related computational results, including the magnetic response properties of each monomer.

This paper presents our recent theoretical research on interpreting stacked-ring aromaticity and related phenomena, combining ideas from both MO and valence-bond (VB) theories with high-precision quantum chemical calculations.[3] Our work links stacked-ring aromaticity with other rules and chemical concepts, such as Baird’s rule, diradical character, selection rules, and chemical bonding.

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Molecular Design Strategies for Ultrafast Photoisomerization

Josene M. Toldo,[1]* Mariana T. do Casal,[2] and Mario Barbatti[2]
*[1]*Presenting Author and Corresponding author*
[1]Université Claude Bernard Lyon 1, LCH, ENS de Lyon, UMR 5182, Lyon, France
[2]Aix-Marseille Université, CNRS, ICR, Marseille, France
E-mail: josene.toldo@univ-lyon1.fr

Abstract:

Understanding and controlling ultrafast nonradiative decay pathways is crucial for designing efficient photoprotective and photothermal materials. Sinapate esters and cinnamate derivatives, archetypal systems used as UV filters, serve as playground for exploring ultrafast excited-state relaxation through photoisomerization. In these molecules, photoisomerization is strongly influenced by steric and electronic modifications.

Here, we investigate the photophysics and photoisomerization of a series of sinapate and cinnamate derivatives by combining transient absorption spectroscopy, quantum chemical calculations, and mixed quantum–classical nonadiabatic dynamics.[1-5] To elucidate their excited-state behavior, we employ a range of theoretical approaches, including TDDFT, DFT/MRCI, CASSCF/CASPT2, and surface hopping dynamics. Our results reveal that molecular symmetry, steric effects, and electronic substitution play decisive roles in governing the access to conical intersections and photoisomerization efficiency.

We show that symmetric derivatives exhibit, in general, faster nonradiative decay due to readily accessible conical intersections, whereas asymmetric analogues show slower relaxation dynamics. Moreover, isomerization yields are strongly influenced by the local topography of the potential energy surface in the vicinity of these intersections. Finally, our results provide a mechanistic framework for tailoring excited-state dynamics guiding the design of next-generation of photoprotective and photothermal materials, such as molecular heaters.

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Photoredox Paradox: How Upconversion and Electron Catalysis Unlock "More-Than-Perfect" Chemistry

Igor V. Alabugin

Department of Chemistry and Biochemistry, Florida State University, Tallahassee, Florida 32306, USA
E-mail: ialabugin@fsu.edu

Although photoredox catalysis looks simple from a mechanistic point of view, a closer look reveals something counter-intuitive: many widely used photoredox reactions are *too efficient*. Measured quantum yields frequently exceed 1, and in some cases a single photon produces more than 100 product molecules. In other words, these reactions appear to outperform the fundamental photon-to-product limit, hinting at hidden mechanisms that propel them beyond simple light absorption.

In this lecture, I will uncover the origin of this "photoredox paradox." We will trace how chain processes contribute to unusual reactivity, and explore where the thermodynamic driving force sustaining these catalytic cycles actually comes from. I will show how combining radical and polar reactivity opens unrecognized reaction manifolds, giving rise to electron and hole catalysis - high-energy pathways powered not by strong reagents, but by redox upconversion.

Finally, I will discuss recurring mechanistic motifs, emphasizing how 2-center–3-electron ("half-bond") interactions serve as the structural gateway for upconversion. These insights allow us to rationally design catalytic systems where electron flow is amplified rather than consumed, enabling productive chemistry that looks "more than perfect" only until its logic is revealed.

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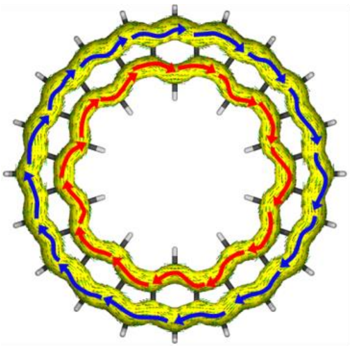
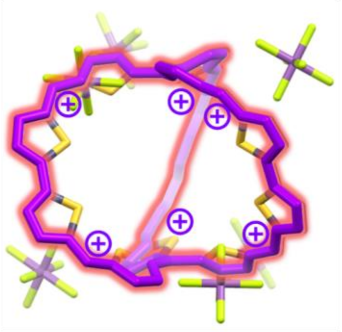
Aromaticity in 2D Open-shell Macrocycles, 3D Full π-Conjugated Cages, and Mechanically Interlocked [2]Catenanes

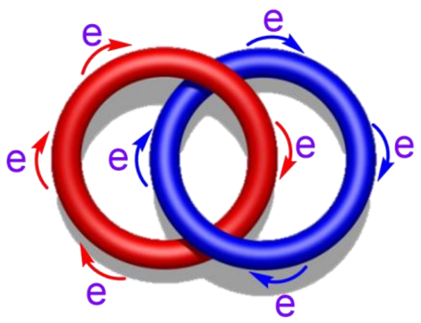
Jishan Wu

Department of Chemistry, National University of Singapore, 3 Science Drive 3, 117543, Singapore
E-mail: chmwuj@nus.edu.sg

This lecture will primarily delve into the aromaticity of 2D open-shell macrocycles,[1] 3D fully π-conjugated molecular cages and mechanically interlocked molecules. Notably, three-dimensional global aromaticity has been achieved in thiophene-based molecular cages.[2] This phenomenon can be elucidated by the two-dimensional Hückel/Baird aromaticity observed in the individual constitutional macrocycles in their respective singlet or triplet states. We also observed unique through-space electronic coupling between two globally (anti)aromatic rings in a [2]catenane structure.[3]







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Meta-Fluorophores: An Uncharted Ocean

Prasun K. Mandal*[a,b]

Affiliation: [a]Department of Chemical Sciences, [b]Centre for Advanced Functional Materials, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, West Bengal, India – 741246.

E-mail: prasunchem@iiserkol.ac.in

Abstract:

Meta-Fluorophores (*MF*s) are a new class of fluorophores in which the charge-transfer (*CT*) donor and acceptor moieties are located in *meta*-orientation in a single benzenic molecule.[1] Contrary to the basic understanding/knowledge that *CT* does not happen when the donor and acceptor moieties are in meta-orientation,[2,3] we have observed that based on suitable choices of donor and acceptor moieties, *CT* in *MF*s can be even stronger than the corresponding para-analogues.[1,4,5]

Thus, a large Stokes shift (as high as 260 nm (8965 cm^{-1})),[1,4,5] and solvatochromic shift (as high as 175 nm)[1,4,5] are observed for the *MF*s. Red emission (say 600 nm or higher) could be achieved with tiny *MF*s having a molecular weight (*MW*) of only 255 g mol^{-1} (in a non-polar medium) and only 177 g mol^{-1} (in a polar medium).[1,4,5] Such *MW*s are extraordinarily low in comparison to not only popular red emitting fluorophores but also para-fluorophores emitting in red.[6] These *MF*s are reasonably bright with the highest photoluminescence quantum yield achieved so far to be 63%.[1,4] Moreover these *MF*s, exhibit comparatively much larger excited state lifetime than the corresponding para-analogues.[1,4,5] Suitably chosen *MF*s exhibit rarely observed *CT*-mediated *J*-aggregation in the crystal state.[7]

All these results will be elaborated.

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Unusual properties of aromatic and antiaromatic molecules

Stephen D. S. Bortolussi, Auguste McNally, Martin D. Peeks

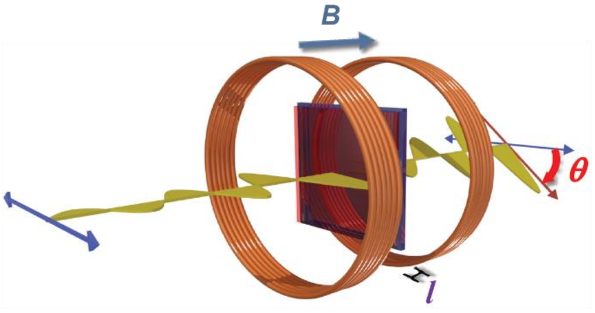
School of Chemistry, University of New South Wales, UNSW Sydney NSW 2052 Australia
E-mail: m.peeks@unsw.edu.au

Ever since the olfactory meaning of the term was supplanted by chemists, debates around the definition and identification of aromaticity, and its siblings, have persisted.[1,2] Recent years have seen a proliferation of computational techniques which have allowed chemists to develop nuanced understandings of the electronic implications of aromaticity. Far from being purely semantic matters, these debates and advances offer pathways toward identifying practical applications of (anti)aromatic systems.

In this talk, I will present our recent research related to two questions:

(1) How is aromaticity manifested in oxidized and reduced states of molecules,[3] with particular emphasis on the applicability and limitations of Mandado's rules?[4]

(2) How are the optical properties of (anti)aromatic molecules affected by magnetic fields?[5,6] We discuss Faraday rotation and magnetic circular dichroism as probes of (anti)aromaticity, and introduce potential applications.



Schematic of Faraday rotation.

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Aromaticity for the design of dynamic molecules and materials

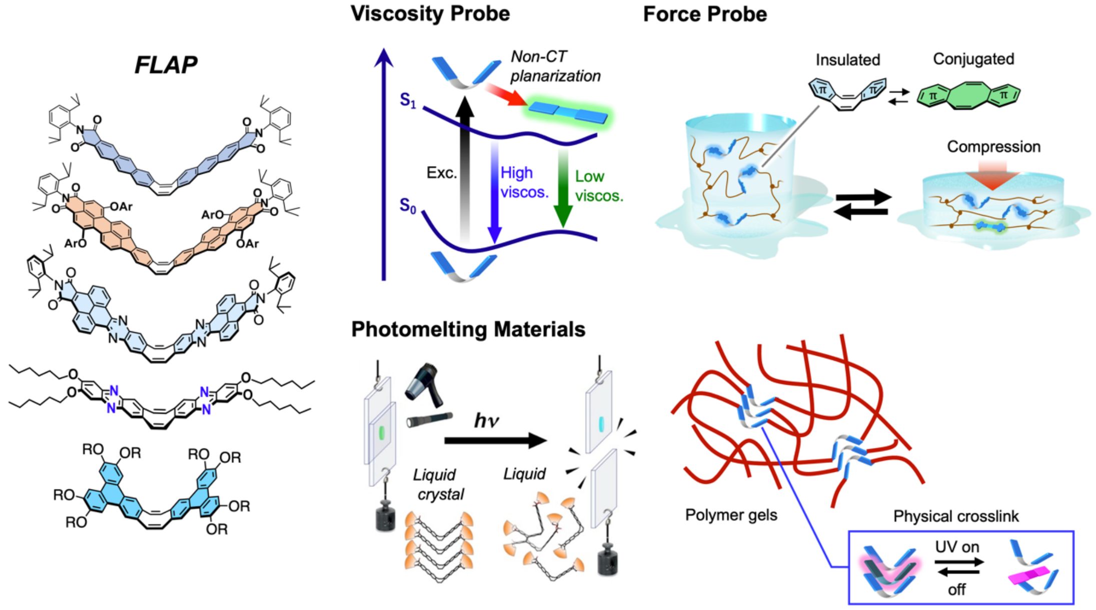
Shohei Saito[*]
The University of Osaka
*E-mail: saito.shohei@chem.sci.osaka-u.ac.jp

Flexible and aromatic photofunctional system (FLAP) has been developed based on the design of flapping molecules, in which a central flexible ring is fused with multiple rigid wings. A series of FLAPs demonstrated diverse functions as below.

1) Viscosity probe: A molecular flapping motion feels nanoscale viscosity more sensitively than a conventional twisting motion. Dynamics of single free volume in polymeric materials can be also monitored by the flapping motion.

2) Force probe: Dual emissive force probes explore quantitative mechano science. The ratiometric fluorescence analysis monitors mechanical polymer chain stretching.

3) Photomelting materials: Twofold π-stacking of V-shaped molecules exhibits high cohesive force of materials, while excited-state planarization plays a key role for photoinduced melting. The control of assembly develops light-melt adhesives and photomelting gels on demand.


Viscosity Probe

Force Probe

Photomelting Materials

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Size and Curvature Dependent Excited State Aromaticity

Ori Gidron

Institute of Chemistry and the Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Edmond J. Safra Campus, 9190401, Jerusalem, Israel

Size and shape play a crucial role in determining the electronic and optical properties of π-conjugated backbones. Here, I will discuss how size and shape determine excited-state properties in general, and excited-state aromaticity in particular.

In the first part, I will discuss the excited-state properties of macrocyclic furans with alternating (anti)aromatic global ring current.[1] Excited-state dynamics indicate that the alternation in size persists not only for the $S_0 \rightarrow S_1/T_1$ transitions but also for the $T_1 \rightarrow T_2$ and $S_1 \rightarrow S_2$ transitions. In the second part, I will show how bending aromatic acceptor-donor-acceptor molecules affects their exciton localization: we found that increasing the bend of the donor moiety results in excited-state symmetry breaking, a process crucial for effective charge separation in organic solar cells.[2]

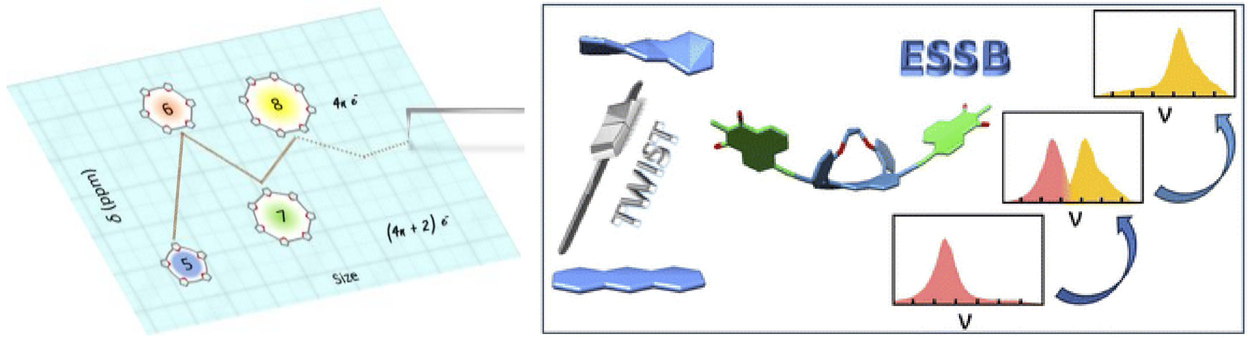

Figure: Right: Size-dependent excited-state aromaticity. Left: The effect of distortion on excited-state symmetry breaking (ESSB).

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Excited State Chirality Revealed by Ultrafast Time-resolved Chiral Spectroscopy

Jinquan Chen*

***** State Key Laboratory of Precision Spectroscopy, East China Normal University, Shanghai 200241, China

Email: jqchen@lps.ecnu.edu.cn

Abstract:

Chirality is one of the universal phenomena in nature. Research on the mechanisms governing the generation, transmission, amplification, and regulation of molecular chirality is currently evolving from traditional macroscopic steady-state investigations to emerging microscopic transient-level studies. To address this, we have developed ultrafast time-resolved chiral spectroscopic techniques and analytical methods, establishing a technical foundation for elucidating the origin and evolution mechanisms of excited-state chirality in molecular systems. By using the femtosecond time-resolved circular dichroism (fs-TRCD) and femtosecond-nanosecond circularly polarized luminescence (TR-CPL) spectroscopy technologies, we achieved simultaneous analysis of molecular excited-state dynamics and the generation/evolution processes of excited-state chirality [1-5]. This revealed the mechanisms by which picosecond-scale excited-state chirality in molecular and supramolecular systems cooperatively evolves through intersystem crossing, electron spin polarization, and energy transfer. Finally, focusing on the structure-activity relationship between DNA chiral secondary structures and their triplet excited states/photochemical properties, we designed and constructed a series of DNA-targeting photosensitizer molecules based on excited-state chiral engineering. This work unveils their reaction mechanisms in biological chiral environments.

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Conjugated π-systems and how to describe them

Igor Roncevic

This talk will discuss the electronic structure of various π-conjugated systems in terms of simple (tight-binding) models. We will explore the relationship between aromaticity, coherence, and electronic structure, using cyclocarbons, annulenes, and porphyrin nanorings as examples.

Cyclo[*n*]carbons (Fig. 1a) are loops of *n* carbon atoms. Recent advances in scanning probe microscopy (SPM) have enabled the on-surface synthesis and characterisation of these unusual molecular carbon allotropes, which have long served as a playground for theoretical approaches.[1,2] We will compare SPM resonance images with high-level *ab initio* calculations, showing that the electronic structure of cyclocarbons can be captured by a particle-on-a-ring model, and revealing unusual topologies.[3]

Conjugated porphyrin nanostructures (Fig. 1b) display remarkable properties such as quantum interference and length-independent conductance, which make them excellent candidates for molecular electronics.[4] These properties stem from the coherent delocalisation of the wavefunction through the whole molecule, which becomes weaker as the molecule become larger. By analysing the ways in which π-systems can distort, we will estimate the maximum size at which edge-fused porphyrin nanorings (Fig. 1b) can still be expected to exhibit quantum behaviour.[5,6]

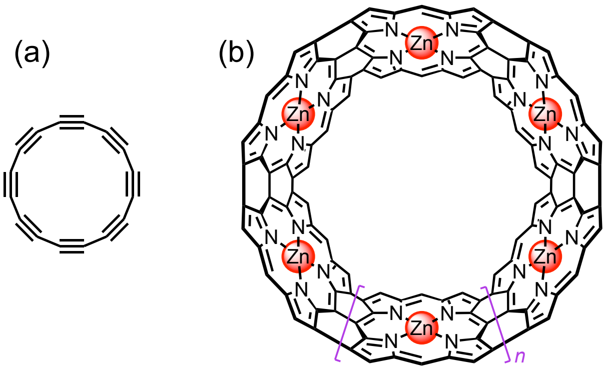

Fig. 1. *(a) Cyclo[16]carbon. (b) Edge-fused porphyrin nanoring.*

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Nonequilibrium planarization dynamics triggered by the onset of excited-state aromaticity revealed by time-domain vibrational spectroscopy.

Yusuke Yoneda.[1,2*]
[1]*Institute for Molecular Science, National Institutes of Natural Sciences*
[2]*Graduate Institute for Advanced Studies, SOKENDAI*
E-mail:yyoneda@ims.ac.jp

Abstract:

Excited-state aromaticity is one of the most widely applied concepts in the field of chemistry. Yet, the details of the relationship between the corresponding photoinduced electronic and structural dynamics remain unexplored. Here, we investigated the excited-state dynamics of one in a series of “flapping” molecules (FLAP), TP-FLAP bearing cyclooctatetraene and triphenylene moieties, by time-resolved time-domain Raman spectroscopy (Fig. 1) [1, 2]. The results provide a direct experimental observation of non-equilibrium planarization dynamics accompanying the onset of excited-state aromaticity.

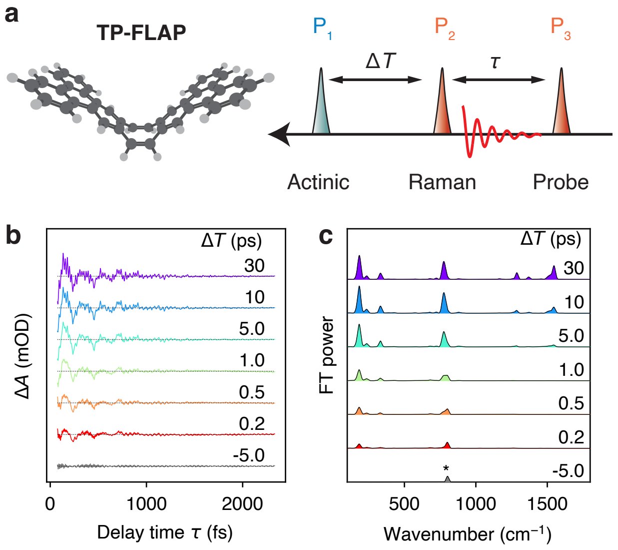

Figure 1: (a) Pulse sequence for TR-ISRS experiment. (b) Time-domain oscillation signals. (c) Frequency-domain time-resolved Raman spectra.

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Novel Synthetic Methods Using Triplet Nitroarenes

Daniele Leonori[*,1]
[1] *Affiliation: Institute of Organic Chemistry, RWTH Aachen University, Aachen, Germany*
E-mail: daniele.leonori@rwth-aachen.de

Abstract:

Nitroaromatics are widely available feedstocks that are routinely used for the preparation of anilines upon reduction. I will present our most recent work that demonstrates how these species can be used, upon blue light irradiation, to promote the ozonolysis-style cleave of olefins[1] and also allow preparation of complex and highly functionalised saturated heterocycles.[2] Furthermore, I will present our recent work where modulation of the excited configuration of these species has enabled the currently elusive ozonolysis of aromatics in the presence of olefins.[3] This discussion will also highlight how aspects of excited-state antiaromaticity relief might be used to rationalize the observed reactivity.

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Aromaticity *vs.* Antiaromaticity in Large Macrocyclic Structures: Unprecedented Formation of Stable Antiaromatic Systems

Dr. Sabapathi Gokulnath
Affiliation: School of Chemistry, IISER Thiruvananthapuram
E-mail: gokul@iisertvm.ac.in

Expanded porphyrinoids have gained immense attention due to their unique optical, electrochemical and coordination properties. Due to their extended conjugation and larger ring size, they often show potential applications such as near-IR dyes, contrast agents in photodynamic therapy (PDT) and non-linear optical devices etc. In this talk, I will disclose the unique antiaromatic macrocyclic systems with altered optical and varied conformational properties.

We prepared two key “hybrid” diheterole precursors consisting of pyrrole/(furan or thiophene) rings for the target macrocycles through acid-catalyzed condensation. Lewis acid catalyzed self-condensation of these key building blocks precursors produced novel planar antiaromatic 24π hexaphyrin(1.0.1.0.1.0) and 32π octaphyrin(1.0.1.0.1.0.1.0) with no β-annulated bridges. Single-crystal X-ray diffraction analysis of the hybrid porphyrinoids revealed planar conformation. These antiaromatic macrocycles revealed the characteristic optical feature and further undergo reversible two-electron reduction to Hückel aromatic 26π and 34π electron species, respectively as evident from the spectroscopic and theoretical studies. Depending on the physical properties of the diheterole subunits, the structure, optical/ electrochemical properties and antiaromaticity of the resulting $4n\pi$-conjugated macrocycles were varied as inferred from spectroscopic data. Surprisingly, the antiaromatic systems were deemed to be more stable than the aromatic ones.

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Aromaticity as a Design Variable

Irene Casademont-Reig,[1*] Roger Monreal-Corona,[2] Tatiana Woller,[2] Eline Desmedt,[2] *Freija De Vleeschouwer,*[2] Miquel Torrent-Sucarrat,[1] Julia Contreras-García,[3] Eduard Matito,[1] and Mercedes Alonso[2]
[1] Donostia International Physics Center (DIPC), 20018 Donostia, Euskadi, Spain
[2] Research group of General Chemistry (ALGC), Vrije Universiteit Brussel (VUB), Pleinlaan 2, 1050 Brussels, Belgium
[3] Laboratoire de Chimie Théorique, Sorbonne Université and CNRS, F-75005, Paris, France
e-mail: irene.casademont@dipc.org

Aromaticity is a fundamental molecular property[1] that can guide the rational design of functional materials. Singlet Fission (SF) chromophores provide a concrete example, they can surpass the Shockley-Queisser limit in solar cells by converting one singlet exciton into two triplet excitons. However, the scarcity of stable chromophores that satisfy the energetic requirements limits the development of SF-enhanced devices.

In this talk, I will illustrate how control over π-electron delocalization enables molecular design. Using fulvene derivatives[2] as an example, we combined their electronically flexible π-systems with an efficient inverse design algorithm to identify promising SF candidates and derive design rules linking substitution patterns and electronic structure.[3] I will then discuss how understanding the impact of delocalization error in larger π-conjugated systems, such as expanded porphyrins, is essential for extending these strategies.[4] Together, these studies demonstrate aromaticity as a powerful, yet method-sensitive, design variable for molecular discovery.

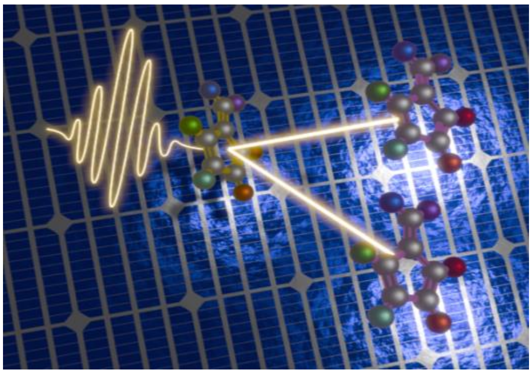

Figure 1: Schematic representation of studied fulvenes.

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Simultaneous Optimization of Both Electrocyclization and Cycloreversion Reactions of Diarylethene Photoswitches through Aromaticity Considerations for Ground and Excited States

Bo Durbeej,[1*] D. Sravanakumar Perumalla,[1,2] Thillaiarasi Sukumar,[3] Jun Wang[4] and Baswanth Oruganti[3,5]

[1] Division of Theoretical Chemistry, IFM, Linköping University, Sweden
[*]E-mail: bo.durbeej@liu.se

[2] Department of Applied Sciences and Humanities, Sasi Institute of Technology & Engineering, India

[3] Department of Chemistry, SRM University-AP, India

[4] School of Chemistry and Chemical Engineering, Huaiyin Normal University, China

[5] School of Mathematics and Natural Sciences, Chanakya University, India

Abstract:

Diarylethene (DAE) photoswitches featuring an aromatic π-linker as the bridge between the two aryl groups convert between ring-open and ring-closed forms through photochemical electrocyclization and thermal cycloreversion reactions. Owing to this ability, DAEs are widely considered as potential solar thermal fuels,[1] where absorbed solar energy is stored as chemical energy in the ring-closed isomer, and is released as heat when the ring-open isomer is reformed. In this talk, I will describe results from quantum chemical calculations and non-adiabatic molecular dynamics simulations that have helped show how the use of polycyclic π-linkers makes it possible to simultaneously optimize both the electrocyclization and the cycloreversion reactions of DAEs for solar-energy storage, by appropriately tuning the ground- and excited-state aromatic character of the individual rings of such π-linkers.[2–5]

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Photodynamics and Aromaticity of Azulene and Pseudoazulenes

Tomáš Slanina, [1]* David Dunlop, [1] Henrik Ottosson, [2]
[1] *IOCB Prague, Flemingovo nám. 2. Prague 6, 160 00, Czech Republic*
[2] *Department of Chemistry, Ångströmlaboratoriet, Uppsala University, Lägerhyddsvägen 1, Uppsala, 751 20, Sweden*
E-mail: tomas.slanina@uochb.cas.cz

Abstract:

Azulene is one of the most peculiar small hydrocarbons. Being isoelectronic with colourless naphthalene, its blue colour has attracted the attention of chemists and was theoretically explained by Michl and Thulstrup already in 1976.[1] In addition, azulene disobeys Kasha's rule, which states that emission occurs exclusively from the lowest excited state of a given multiplicity. It has a strong emission from the S_2 state while the excitation by the visible light leads to the dark S_1 state. Unlike the absorption, anti-Kasha emission of azulene is understood merely on a phenomenological basis, which presents a fundamental obstacle in the generalization of the observed behaviour for rational design and property-tuning of analogical systems.

In this combined experimental and theoretical contribution, we propose a model for the description of photophysical properties of the prototypical anti-Kasha fluorophore, azulene, based on its ground and excited state (anti)aromaticity. Our model reveals that the anti-Kasha properties of azulene are a consequence of a) the contrasting aromaticity and electron configurations of the S_1 and S_2 states and b) the highly accessible unimolecular antiaromatic relief pathway of the S_1 state.[2]

Moreover, we extend this approach to a series of pseudoazulene (thialene) derivatives and their benzannulated analogues, highlighting the specificity of azulene-type aromaticity. We compare their electronic properties with other regioisomers, such as benzo[*b*/*c*]thiophene. Ultimately, we study their photodynamics and compare the isoelectronic and isoaromatic derivatives to set general rules for their ground- and excited-state behaviour.

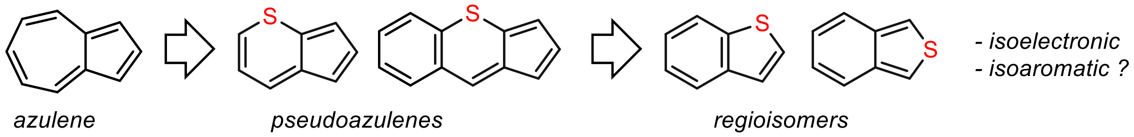

Figure 1: Azulene and its analogues

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Search for improved triplet-state quenchers for fluorescence imaging: A computational framework incorporating excited-state Baird-aromaticity

Matthew A. Johnson,[1*] Ouissam El Bakouri,[1,2] Joshua R. Smith,[1,3] Avik K. Pati,[4,5] Maxwell I. Martin,[4] Scott C. Blanchard,[4] and Henrik Ottosson [1*]

[1] *Affiliation: Department of Chemistry –Ångström, Uppsala University, Uppsala, Sweden.*
E-mail: matthew.johnson@kemi.uu.se
[2] *Affiliation: Institut de Química Computacional i Catàlisi (IQCC), Departament de Química, Universitat de Girona, C/Maria Aurèlia Capmany 6, 17003 Girona, Catalonia, Spain*
[3] *Affiliation: Department of Chemistry & Biochemistry, Cal Poly Humboldt, Arcata, CA 95501, USA*
[4] *Affiliation: Department of Structural Biology, St. Jude Children's Research Hospital, Memphis, USA*
[5] *Affiliation: Department of Chemistry, Birla Institute of Technology and Science, Pilani, Rajasthan 333031, India*

Abstract:

Triplet state quenchers (TSQs) offer a method to improve fluorophore performance in fluorescence imaging by reducing triplet-state accumulation of the fluorophore, thereby enhancing fluorophore brightness and mitigating the formation of reaction with molecular oxygen.[1] Cyclooctatetraene (COT) is an 8π-electron species which displays strong excited-state Baird-aromaticity and is among the most effective TSQs.[2,3] However, COT has a long-lived triplet state, which significantly reduces its performance as a TSQ. To identify alternative TSQs, we computationally screened other analogous species and compared their computed photophysical properties to COT.[4] Specifically, we evaluated photostability, singlet-triplet energy gaps, reorganization energies, spin-orbit coupling, and phosphorescence intersystem (ISC) crossing rates. We identify several 7 and 8-membered ring species which are predicted to have favorable TSQ performance with a range of singlet-triplet energy gaps compatible with a diverse range of fluorophores. Additionally, several candidates exhibit ISC rates up to 10^6 times faster than COT. Finally, we examine whether structural modifications of COT can tune the underlying problem of long-lived triplet states and enable fast ISC rates.

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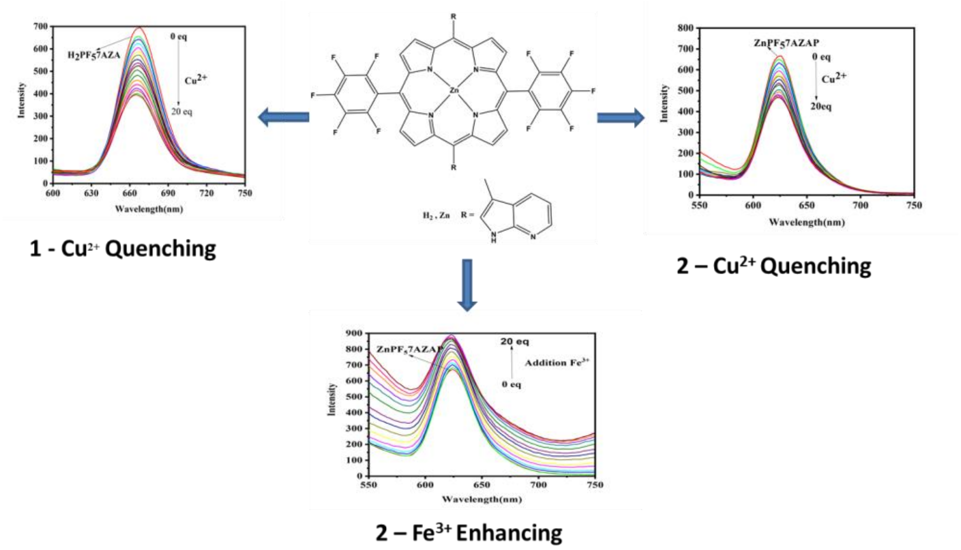
MESO-ARYL 7-AZA INDOLE SUBSITTED PORPHYRIN AND THEIR ZINC (II) COMPLEX FOR CHEMOSENSING Cu^{2+} and Fe^{3+} PHOTODYNAMIC ANTICANCER ACTIVITY

Kannan Subburaj,[1] Subashini Mohan,[1] Rahul Soman [2] and Nallathambi Sengottuvelan.[1]*
[1] *Presenting Author:* **Kannan Subburaj**
[1,] Department of Industrial Chemistry, Alagappa University Karaikudi – 630003.
[2] Department of Pharmaceutics, School of Pharmacy, Kochi - 682041
E-mail: svelann@alagappauniversity.ac.in, kannanraj527@gmail.com

Abstract:

The Lindsey method was used to synthesis 5,15-(7-azaindole-3-yl)-10,20-(2,3,4,5,6-pentaflurophenyl)porphyrin (H_2PF7AP)(**1**) using (2,3,4.5,6-pentafluorophenyl)dipyrromethane as the precursor with 7-azaindole-3-carbox aldehyde and their Zinc(II) Complex 5,15-(7-azaindole-3-yl)10,20-(2,3,4,5,6-pentaflurophenyl) porphyrinato zinc(II) (ZnPF7AP) (**2**) was synthesized using the compound **1** (H_2PF7AP) with Zinc(II) acetate.The produced compounds 1 and 2 were analyzed using by mass spectrometer compound confirmed by :free base 875.17 Zinc complex 937.08.,^{1}H NMR spectroscopy interestingly free base –NH proton observed by -2.9 ppm 7-azaindole –NH peak observed at -12.7ppm Zinc complex –NH proton not observed 7-azaindole –NH peak observed at -12.6ppm, fluorescence and UV-Visible spectral techniques. The Chemo sensing activity of 1 and 2 were studied. The chemo sensor 1 and **2** displayed quick sensitivity and selectivity towards Cu^{2+} & Fe^{3+} ions. Interestingly, the probe **1** and **2** exhibits "Turn-Off" fluorescence response to Cu^{2+} ion and 2 displayed the "Turn-On" fluorescence signals to Fe^{3+} ions. The photo dynamic anti-cancer studies of compounds 1 and 2 performed and the IC_{50} values of these compounds in presence of light were found to be 38.54 μg/ml and 32.42 μg/ml.



1 - Cu^{2+} Quenching

2 – Cu^{2+} Quenching

2 – Fe^{3+} Enhancing

Scheme 1: ***Meso*-Aryl substituted 7-azaindole porphyrin**

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Substituent Effects on Cyanines: The Role of Chain Length and Position

David Dunlop,[1,2] Rebecca Strada,[3] and Peter Šebej[3,*]
[1] Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo náměstí 542/2, Prague 6, 160 00 Czech Republic; [2] Dept. of Inorg. Chem., Faculty of Science, Charles University, Hlavova 2030, Prague 2, 128 40, Czech Republic;
[3] RECETOX, Fac. of Science, Masaryk University, Kamenice 5, 611 37 Brno, Czech Republic
E-mail: sebej@recetox.muni.cz

Abstract:

Cyanines' properties are typically tuned by prolonging the polymethine chain chromophore and leveraging the auxochrome end groups, both influencing energies and separation of their HOMO and LUMO. However, the substituents on non-terminal positions of the chromophore are almost neglected degree of freedom in these dyes.[1] We build a model to semiquantitatively assess the structure-properties relationships in substituted cyanines (Fig. 1a) to tackle this gap (Fig. 1b). Then we validated our approach with empirical spectral data of such cyanines from representative publications[2,3] and found a clear correlation of the absorption and emission bands' maxima with the electronic properties of the chain substituents (Figure 1c).[4]

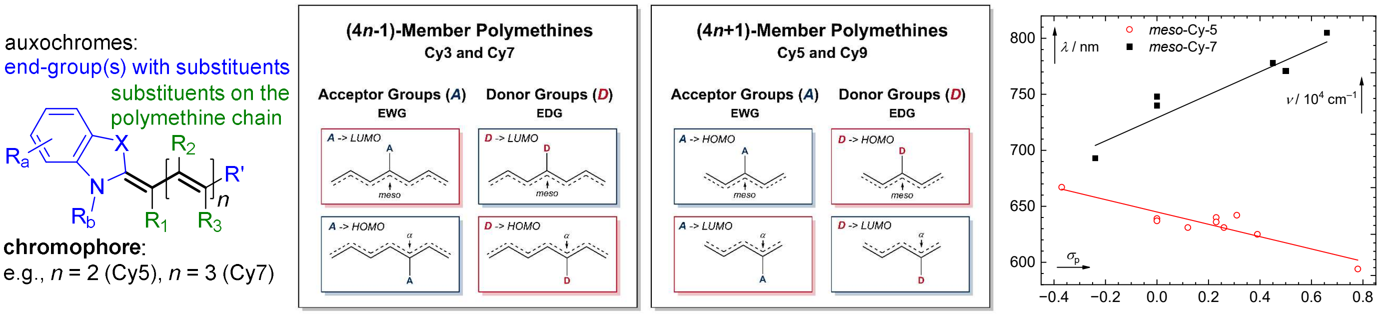

Figure 1: a) general structure of cyanines substituted on the polymethine chain (left); b) substituents effects on cyanine spectral properties vary with chain length and substituent position (middle); and c) LFER of absorption maxima of meso-substituted Cy-5 and Cy-7 (right).

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Can Small Changes Address the Major Issue of Pentalenes?

Péter J. Mayer, [1*] Kangwei Wang, [1] and Henrik Ottosson. [1]
*[1]*Presenting Author-*
[1] Affiliation: Department of Chemistry − Ångström Laboratory, Uppsala University, Box 530, 751 20 Uppsala, Sweden
E-mail: kangwei.wang@kemi.uu.se

Abstract: It was earlier proposed by us that 4*n*π-systems can be of interest as singlet fission (SF) chromophores due to their highly stable aromatic first excited states.[1] Since both first excited singlet (S_1) and triplet (T_1) states are essential in the SF process, this could provide a route to photovoltaics that break the Shockley–Queisser limit.[2] We already proposed pentalenes as potential SF chromophores, however, a major issue was identified as the S_1 state is photophysically unavailable.[3] It was also found that substituents are only able to "fine-tune" the availability of the S_1 state.[3] Herein, we investigate whether heteroatoms can "coarse-tune" said property.

A family of heteroaromatic pentalenes was investigated, generated by replacing a C atom with a N or a C=C bond with an O, S, or NH (Figure 1). Through this replacement, the 8π-electron number was maintained while changing the electronic properties of the cycle. Firstly, we checked the planarity of these molecules and found that two 4-membered heterocycles do not prefer a planar structure, while the others are mostly planar. Next, we examined the excited-state aromaticity and found that they acquire significant aromatic character upon excitation. One can also "coarse-tune" the availability of the S_1 state by these replacements. Even though not all motifs are accessible experimentally, we suggest investigating their synthesis in the future.

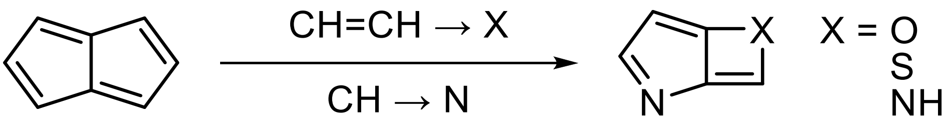

Figure 1: The investigated molecular family generated by heteroatomic replacements in pentalene.

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The physical organic chemist's toolbox for designing singlet fission chromophores

Dexter J. Gordon,[1]* Damon M. de Clercq,[1] Timothy W. Schmidt,[1] and Martin D. Peeks.[1]
*[1]*Presenting Author*
[1]School of Chemistry, University of New South Wales, Sydney, Australia
E-mail: d.gordon@unsw.edu.au

Abstract:

Singlet fission (SF), a photophysical process where the energy of an incident photon is divided across multiple excitons, promises a substantial increase in efficiency of photovoltaic devices.[1] As such, the search is on for organic molecules that undergo singlet fission efficiently and are stable to UV radiation. Our research leverages aromaticity concepts to understand known SF chromophores such as DKPP[2] and DPND[3] and to identify new compounds with SF potential, then exploits organic reactivity to assemble and functionalise these structures.

Here, we explore the spectroscopic properties of 'isopyrocoll', an underexplored π-system that was discovered in 1968.[4] Using microwave-assisted thionation followed by silver(I)-mediated malononitrile condensation, the excited-state photophysics of this molecule as measured by ultrafast transient absorption spectroscopy can be radically altered. We also describe synthetic progress towards a modular, adaptively aromatic π-system with predicted SF capability.

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Extraction and characterisation of type-I collagen from the fish skin waste

M.A.Rather[1]* , Massarat Majeed, [2]
[1]**Presenting Author-*
[1,2] NATIONAL INSTITTUTE OF TECHNOLOGY SRINAGAR- KASHMIR.
E-mail: marather@nitsri.ac.in

Abstract:

Fish skin waste is a fish processing waste generated globally and in India at present over 2 million metric tons of it is generated annually. This waste poses environmental challenges which can be mitigated by repurposing it into valuable products. Present research considered the extraction of fish collagen from locally available Rohu fish (*Labeo rohita*) skin waste, characterized the product and studied its biocompatibility .Type-I collagen contains aromatic amino acid residues like phenylalanine and tyrosine within its polypeptide chains. Type I collagen was successfully extracted from the Rohu fish (*Labeo rohita*) skin waste with maximum extracted yield of 74.45% of the total collagen available. The extracted collagen was found to be Type I, with a preserved triple-helical structure. UV-Vis absorption at ~230 nm and SDS-PAGE profiles (α1, α2, and β chains) validated purity of extracted collagen. The extracted collagen exhibited good thermal stability, with a high denaturation temperature of 97.80 °C, which compared well with the previously documented fish collagens. Amino Acid Profile of the extracted fish collagen was rich in glycine, proline, alanine, and glutamic acid. Biocompatibility Evaluation by 100% mesenchymal stem cell viability after 72 hours was validated by in vitro cytotoxicity assays with Trypan Blue and MTT, demonstrating the nontoxic nature of Rohu-derived collagen. The collagen produced from Rohu fish skin waste exhibited high thermal stability, excellent purity, and significant biocompatibility, proving its suitability for use in biomedicine.

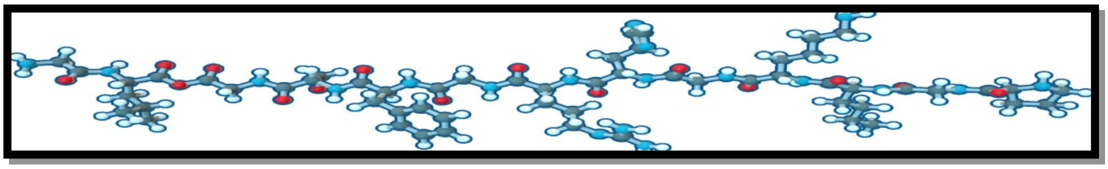

Figure 1: Structure of type-I collagen which contains aromatic amino acid residues .

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Tribological and Chemical Characterisation of Epoxidised *Peganum harmala* L. Oil as a Sustainable Bio-Lubricant

Afan Masoodi[1], M.S.Charoo[2*]

[2*]*Presenting Author-*

[1,2] Mechanical Engineering Department, National Institute of Technology Srinagar

E-mail:shaficharoo123@nitsri.ac.in

Abstract:

Epoxidised *Peganum harmala* L. Oil has been known for its key aromatic ring compounds β-carboline alkaloids (indole.pyridine fuded rings), quinazoline alkaloids and many phenoloc polyphenolic compounds possessing many pharmacological and practical applications.However present study of *Peganum harmala* L. oil demonstrates that a single-step chemical modification, i.e, epoxidation, transforms *Peganum harmala*L. seed oil into a high-performance lubricant base stock with properties comparable to a commercial SAE 5W-30 synthetic oil.Physicochemical analysis confirms the successful transformation: epoxidation increased the flash point from 220°C to 245°C, more than doubled the kinematic viscosity at 40°C (from 20.9 to 46.5 mPa·s), and virtually eliminated acidity, with the total acid number falling from 5.47 to 0.07 mg KOH g^{-1}. Thermogravimetric analysis showed the onset of thermal degradation increased by 15°C to 300°C, expanding the oil's operational safety window.Tribologically, the epoxidised *Peganum harmala*L. oil (EPHL) exhibited superior performance. In low-load reciprocating tests, EPHL achieved an ultra-low friction coefficient of 0.0079, a 43% reduction compared to the SAE 5W-30 reference. Under high-stress, extreme-pressure conditions, four-ball tests revealed a 74% contraction in the mean wear-scar diameter relative to the native oil (from 1.97 mm to 0.52 mm). Surface analysis via Raman spectroscopy suggests these gains are attributable to the formation of a duplex tribofilm, comprising a durable iron-phosphate foundation overlaid with a low-shear, polymerised oxirane layer. This mechanism explains the observed combination of low friction and high wear resistance. FTIR Spectra: Confirm disappearance of C=C bonds (1650 cm^{-1}) & appearance of Oxirane groups (845 cm^{-1}).

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Fluorescent Nanoprobes for Volatile Organic Compound (VOC)-Guided Photodynamic Therapy (PDT)

Vaishnavi Mekkeparambath,[1] Pragya,[2] M M Sreejaya,[1] Reshmi,[1] Avijit Jana,[2*] P D Pancharatna,[1*] Moumita Gangopadhyay[1*]
[1*] *Presenting Author*-Moumita Gangopadhyay
[1] *Affiliation: Department of Chemistry, Amrita Vishwa Vidyapeetham, Amritapuri, Kollam, Kerala 690525.*
E-mail: moumita@am.amrita.edu

Abstract:

The heterogeneous intracellular environment of tumor cells has always been a topic of interest associated with the design of a controlled treatment method. Concentration of certain volatile organic compounds (VOCs) like ethanol, acetone, etc. are more abundant in cancer-affected cells than in healthy ones.[1] Hence, such VOCs can serve as significant biomarkers for cancer treatment. Fluorescent probes, owing to their site-specificity and non-invasiveness, have been well-explored for application in theragnostic approaches to the treatment of various critical diseases. In our group, we have developed fluorescent probes that can prompt real-time monitoring of cancer treatment. We have exploited intramolecular charge transfer in designing the nanoprobe with tunable emission property. To ensure distinct fluorescence response to the presence of ethanol, the donor and acceptor units were connected via an imine functionality.[2] The effect of imine bond was substantiated by density functional theory calculations using 6-31G+(d,p) basis set. The theoretical calculations and rationally curated photophysical studies revealed selective hydrogen bonding between the imine nitrogen atom and ethanol. For better cellular internalization and retention of the probes, they were made into nanoparticles, exploiting the possible aggregation between two adjacent hydrophobic aromatic rings. The nanoprobes exhibited promising singlet oxygen generation ability for proficient PDT selectively inside cancer cells. In a nutshell, this study features a novel fluorescent nanoprobe for ethanol-guided PDT-mediated selective cancer treatment.

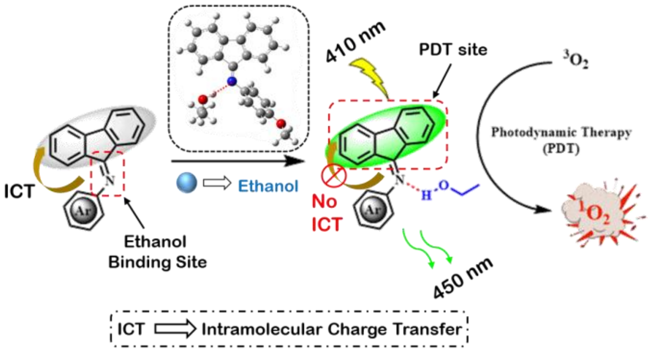

Figure 1: Schematic of fluorene nanoprobes for ethanol-guided PDT

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