



New Molecular Designs for Functionalizable Donor-Acceptor Strapped Macromolecules and Nanographenes

Dr. Santhosh Babu Sukumaran



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12:15 pm - CiQUS Seminar Room

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Abstract

Two important classes of molecules, thiophene and perylene bisimide (PBIs), serve as the foundation for most of the important donor-acceptor-based small molecules and polymers. The synthetic versatility and tunable redox properties made oligothiophenes one of the best donor molecules.^[1] Perylene bisimide is also another most extensively studied fluorescent organic molecule.^[2] Both oligothiophene and PBI-based materials are chemically and thermally stable. The rich photo and electrochemistry provide a wide range of features to explore, such as visible light absorption, tunable emission, quantum yield, and characteristic long-lived excited states, as well as the ability to undergo efficient energy and electron transfer reactions, making them ideal components in donor-acceptor assemblies. Still, there are new opportunities for PBIs to be more functional. One among them is PBI-based functionalizable macrocycles. Donor-acceptor linked π -conjugated macrocycles are inspiring as modular building blocks for the development of new functional materials (1D and 2D polymers) and supramolecular structures that allow both light harvesting and excitation energy transfer and electron transfer. Our recent findings in the area of donor-strapped PBI-based macrocycles revealed the importance of new molecular designs in extending the charge-separated state and opportunities for further functionalization of macrocycles.^[3]

Polycyclic aromatic hydrocarbons with π -extended cores, or nanographenes, have attracted attention since the first experimental demonstration of graphene. Recently, chiral and nonplanar cutouts of graphene have been the favorites due to their unique optical, chiroptical, and electronic properties, and offer high solubility compared with their planar counterparts. Despite the remarkable progress in helicenes, π -extended helical nanographenes have not been widely explored. Our new designs enabled us to explore new redox, optical, and chiroptical properties of nanographenes.⁴



References

1. Chem. Rev. 2009, 109, 1141-1276; 2. Chem. Rev. 2016, 116, 962-1052; Chem. Commun. 2004, 14, 1564-1579; 3. Angew. Chem. Int. Ed. 2023, 62, e202212934; Org. Chem. Front. 2023, 10, 5099-5107. 4. Angew. Chem. Int. Ed. 2023, e202311657..

Biosketch

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Professional and Research Experience

Sep. 2014- Present	Principal Scientist, CSIR-NCL, Pune, India Associate Professor, AcSIR
Sep. 2014- 2022	Senior Scientist, CSIR-NCL, Pune, India Assistant Professor, AcSIR
Sep. 2012- Aug. 2014	Marie Curie-AUL incoming postdoctoral fellow in the research group of Prof. Davide Bonifazi, University of Namur, Belgium
Nov. 2010-Apr. 2012	Postdoctoral fellow in the research group of Dr. Takashi Nakanishi, National Institute for Materials Science (NIMS), Japan
Sep. 2009-Oct. 2010	Postdoctoral fellow in the research group of Prof. Dr. Helmuth Möhwald and Dr. Takashi Nakanishi, Max Planck Institute of Colloids and Interfaces, Germany
Aug. 2004-Aug. 2009	Ph. D. Mentor: Dr. A. Ajayaghosh, Photosciences and Photonics Group, CSIR-NIIST, Trivandrum, India Thesis Title: "Control on Optical and Morphological Properties of Oligo(<i>p</i> -phenylenevinylene) Self-assemblies"

Research Interests

Luminescent Organic Materials

Solvent-free Organic Liquids

Functional π -Assemblies and Nanographenes

2D-Polymers for Catalysis and Energy Applications

Honors and Awards

- ❖ Alexander von Humboldt fellowship for experienced researchers
- ❖ *Chem. Commun.* (RSC), Emerging Investigator 2022
- ❖ Merck Young Scientist Award 2021 (Runner up)
- ❖ *Nanoscale* (RSC), Emerging Investigator 2021
- ❖ Scientist of the Year Award 2018-19, CSIR-NCL Research Foundation
- ❖ Ramanujan Fellow, 2015
- ❖ FNRS "CHARGE DE RECHERCHES" Independent Research Fellowship, Belgium, 2014 (Declined)

Important Publications Since 2015

Angew. Chem. Int. Ed. **2024**, 63, e202402259.
Acc. Chem. Res. **2024**, 10.1021/acs.accounts.3c00670
Angew. Chem. Int. Ed. **2023**, 62, e202311657 ([Hot Paper](#))
Angew. Chem. Int. Ed. **2023**, 62, e202307381
Angew. Chem. Int. Ed. **2023**, 62, e202212934
Chem. Commun. **2022**, 58, 1998-2001. ([Emerging Investigator](#))
Nanoscale **2021**, 13, 10780-10784. ([Emerging Investigator](#))
Adv. Energy Mater. **2023**, 13, 202203326
Chem. Sci. **2021**, 12, 4216-4236.
J. Mater. Chem. A. **2020**, 8, 10767-10771.
Angew. Chem. Int. Ed. **2020**, 59, 13079-13085. ([Hot Paper](#))
J. Am. Chem. Soc. **2019**, 141, 14950-14954.
Angew. Chem. Int. Ed. **2019**, 58, 2284-2288. ([Hot Paper](#))
J. Am. Chem. Soc. **2016**, 138, 11113-11116.

Book Chapters

1. Supramolecular Materialization of Fullerene Assemblies, **S. S. Babu**, H. Asanuma and T. Nakanishi in *Supramolecular Soft Matter: Applications in Materials and Organic Electronics*, T. Nakanishi (Ed), [Wiley VCH](#), Pages: 1-18, **2011**.
2. Nanoscopic Organisation of Fullerenes, **S. S. Babu** and T. Nakanishi, in the 2nd Edition of *Fullerenes: Principles and Applications*, J.-F. Nierengarten and F. Langa (Eds), [Royal Society of Chemistry \(RSC\)](#), Pages: 329-353, **2011**.
3. Supramolecular Chemistry of Fullerene Containing Micelles and Gels, H. Li, **S. S. Babu** and T. Nakanishi, in *Supramolecular Chemistry of Fullerenes and Carbon Nanotubes*, N. Martin and J.-F. Nierengarten (Eds), [Wiley VCH](#), Pages: 159-172, **2012**.

US Patents Granted

Title	Number	Authors
1. Synthesized a new pyrene tetraboronic acid for a use of glucose sensing.	US 2020/0079798 A1	Sukumaran Santhosh Babu and V. C. Wakchaure
2. Process for the preparation of (4,8-bis(5 (trimethylstannyl) as a precursor for the synthesis of	US 2019/0300554 A1	Sukumaran Santhosh Babu and V. C. Wakchaure

thiophene based conjugated 2d polymers and its application in organic photovoltaics.		
3. Photocatalytic splitting of water Using self-assembled metalloporphyrin 2D-sheets	US 2020/0247668 A1	Sukumaran Santhosh Babu and K. C. Ranjeesh
4. Metalloporphyrin 2D-sheets for Efficient Photo- and Electro-Catalytic splitting of water	US 2020/0071458 A1	Sukumaran Santhosh Babu and K. C. Ranjeesh

h-index and Citations*

	All	Since 2019
Citations	5222	2004
h-index	28	17
i10-index	37	28

*From Google Scholar Citations on 05-03-2024