## Parantap Sarkar, PhD

DOB: 21st July 1985, Indian

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### Research:

- 10+ years in Synthetic and Structural organic chemistry.
- Expertise in organic synthesis (mg to kg scale) and functionalization of small aliphatic and aromatic molecules, polyaromatic hydrocarbons and heterocycles, carbon nanostructures, esters and imides, carbon-rich macrocycles.
- Supramolecular synthesis with aliphatic carbonyls and silyl ethers, imines, isopyrazoles, aza-arenes, thia-arenes, arylborates, arylacetylenes, aryl triflets and aryl halides through coupling reactions and their structural investigation.
- Synthesis of carbon-rich nanographene and hetero-nanographene (contain S and N) molecules for organic electronics and photovoltaics.
- Expert in computational modelling through DFT and AFIR for designing molecules with predicted properties and reaction pathway.



# PROFESSIONAL EXPERIENCE & RESEARCH

#### April 2019 - Present: Postdoctoral Researcher at WPI-Institute for Chemical Reaction Design and Discovery (ICReDD), Hokkaido University, Sapporo, Japan.

Area of Research • Modular synthesis of aliphatic carbonyl based flexible molecular ropes with precise chain lengths via

> silylation and oxidation of 1,3-diketones. • Functionalization of flexible oligoketones by chemical transformations or by structural confinement through metal ion chelation or encapsulation. • Structural investigation through X-ray crystallography, Molecular dynamics simulation, AFIR (Artificial Force

Induced Reaction) technique and DFT calculation.

Supervisor Prof. Yashuhide Inokuma

#### Jun 2017 - March 2019: Assistant Professor at Manipal Center for Natural Sciences (MCNS), Manipal University, India.

Area of Research · Synthesis of structurally defined and atomically precise novel carbon nanostructures. • Structural investigation of nanocarbons via computational chemistry.

Teaching Preparation of PhD coursework in chemistry and certificate course on "Building blocks in Chemistry"

Research Associate at WPI-Advanced Institute for Materials Research (AIMR), Tohoku Apr 2014 – Jan 2017: University, Sendai, Japan.

Area of Research • "Bottom-up" chemical synthesis of Carbon nanohoops, as segments of various carbon nanotubes,

> through functionalization and coupling of small aromatic molecules followed by transmetalation and reductive elimination. • Investigation of rotational dynamics in aromatic nanohoops through NMR and computational studies. • Stereochemistry of bent aromatics. • Fullerene and nanohoop based host-guest

assembly and related thermodynamics.

Supervisor Prof. Hiroyuki Isobe

Mar 2013 - Feb 2014: Postdoctoral researcher at Chemistry and Nano Science department at Ewha Womans University, Seoul, South Korea

Area of Research • Synthesis of novel N-heterocyclic carbenes followed by adduct with C60 and C70 fullerenes. • Synthesis

of stable N-heterocyclic bis-carbene.

Prof. Jean Bouffard Supervisor

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### Oct 2012 - Jan 2013:

### Research Associate at IISER-Kolkata, Kolkata, India

Area of Research Supervisor

• Synthesis of Chalcogenophene based conjugated polymers through electrochemical polymerization. Prof. Sanjio S. Zade



## EDUCATIONAL QUALIFICATION

#### Sept 2009 - Jul 2012: Doctoral Student at Centre de Recherche Paul Pascal (CRPP-CNRS UMR5031) Université de

**Bordeaux**, France

Title of Thesis The Ceramidonine and Perkin Approaches to Aromatic Nanoribbons

Area of Research · Synthesis of Nitrogen containing soluble and electronically "acceptor" type azaarene nanoribbons

through Ceramidonine approach.

• Synthesis of Sulfur containing electronically "donor" type thiaarene nanoribbons and partially

rigidified conjugated polymers through modified Perkin Approach.

• Synthesis of homoaromatic GNRs with tailored solubility and tunable electronic properties through

modified Perkin approaches. Study of Liquid Crystal properties and molecular self-assembly.

Supervisor Dr. Harald Bock

Co-supervisors Dr. Fabien Durola, Dr. Rodolphe Clérac

#### Aug 2007 - Jul 2009: Masters in Science (Chemistry) at Jadavpur University, India

Title of Thesis Diastereoisomerically pure Pyrazole-3,5-dicarboxylate bridged dimetallic Ru(II) and Os(II)

complexes of 2,2'-bipyridine: Electrochemical and Spectral studies.

Prof. Sujoy Baitalik Supervisor

#### Aug 2004 - Jul 2007: Bachelors in Science (Chemistry Hons.) at Jadavpur University, India



## **PUBLICATIONS**

1. P. Sarkar, I.-R. Jeon, F. Durola, and H. Bock\*, "Tetraazaarenes by the Ceramidonine Approach" New J. Chem., 2012, 36, 570-574 (IF: 3.3 & citation: 6, selected as Cover Article).

P. Sarkar, P. Dechambenoit, F. Durola, and H. Bock\*, "Carboxy-functionalized polycyclic arenes by oxidative cyclizations of 2,3diarylacrylates", Asian J. Org. Chem., 2012, 1 (4), 366-376. (IF: 3.3 & citation: 11)

P. Sarkar, F. Durola, and H. Bock\*, "Dipyreno- and diperyleno anthracenes from glyoxylic Perkin reaction", *Chem. Commun.* 2013, 49 (68), 7552-7554. (IF: 6.8 & citation: 12)

4. H. Bock\*, D. Subervie, P. Mathey, A. Pradhan, <u>P. Sarkar</u>, P. Dechambenoit, E. Hillard, F. Durola, "Helicenes from diarylmaleimides", *Org. Lett.* 2014, 16 (6), 1546-1549. (IF: 6.7 & citation: 29)

5. E. Girotto, M. Ferreira, <u>P. Sarkar</u>, A. Bentaleb, E. A. Hillard, H. Gallardo, F. Durola, H. Bock\*, "Plank-Shaped Column-Forming Mesogens with Substituents on One Side Only", *Chem. Eur. J.* 2015, 21 (20), 7603-7610. (IF: 5.9, citation: 10)

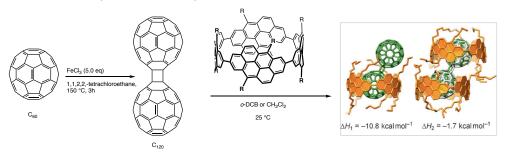
 Z. Sun, <u>P. Sarkar</u>, T. Suenaga, S. Sato, H. Isobe\*, "Belt-shaped cyclonaphthylenes", *Angew. Chem. Int. Ed.* 2015, 54 (43), 12800-12804. (IF: 12.0, citation: 25)

7. P. Sarkar, S. Sato, S. Kamata, T. Matsuno, H. Isobe\*, "Synthesis and dynamic structures of a hybrid nanohoop molecule composed of anthanthrenylene and phenylene panels", *Chem. Lett.* 2015, 44 (11), 1581-1583 (IF: 1.6, citation: 11).

Z. Sun, T. Suenaga, P. Sarkar, S. Sato, M. Kotani, H. Isobe\*, "Stereoisomerism, crystal structures and dynamics of belt-shaped cyclonaphthylenes ", Proc. Natl. Acad. Sci. U. S. A. 2016, 113 (29), 8109-8114. (IF: 9.7, citation: 21)

P. Sarkar, Z. Sun, T. Tokuhira, S. Sato, M. Kotani, H. Isobe\*, "Stereoisomerism in nanohoops with heterogeneous biaryl linkages of E/Z- and R/S- geometries", ACS Cent. Sci. 2016, 2(10), 740-747. (IF: 11.2, citation: 14)

10. T. Matsuno, S. Kamata, S. Sato, A. Yokoyama, P. Sarkar, H. Isobe\*, "Assembly, thermodynamics and structures of a two-wheeled composite of a dumbbell-shaped molecule and cylindrical molecules with different edges", Angew. Chem. Int. Ed. 2017, 56 (47), 15020-15024 (IF: 12.0, citation: 8).



11. P. Sarkar\*, B. K. Das, D. Chakraborty, K. Muthamma, "Carbohelicenes and thiahelicene from phthalaldehydes through Perkin approach", J. Mol. Struct. 2019, 1195, 309-314 (IF: 2.0).

3-step syntheses towards strained and helical polycyclic aromatic hydrocarbons

12. T. Yoneda, C. Kasai, Y. Manabe, M. Tsurui, Y. Kitagawa, Y. Hasegawa, <u>P. Sarkar</u>, Y. Inokuma\*, "Luminescent coordination polymers constructed from flexible tetradentate diisopyrazole ligand and copper(I) halides", *Chem. Asian J. accepted* (DOI: 10.1002/asia.201901682)

13. <u>P. Sarkar</u>, Y. Inaba, T. Yoneda, Y. Inokuma\*, "Modular syntheses of aliphatic polyketones via site-selective monosilylation of 3,3-disubstituted pentane-2,4-diones" *manuscript under preparation. (manuscript in preparation)* 

# **EQUIPMENT EXPERTISE**

Analytical Technique: NMR Spectroscopy (JEOL ECS400 & 600, Bruker DPX 300 MHz), Single crystal XRD (Rigaku XtaLab Synergy), VT-NMR, UV-vis-NIR, CD-spectrometer, DART & ESI-Mass spectroscopy, MALDI-TOF (Bruker microflex), Cyclic Voltammetry, ATR/FT-IR, Multiple preparative HPLC, LC-MS, MPLC, Gel Permeation Chromatography, GC, Column Chromatography, Differential Scanning Calorimetry, Thermogravimetric Analysis, Microscope, Kugelrohr vacuum distillation, Spin Coater, Dry solvent system / Solvent refinery, Karl-Fischer titrator, High-speed cooling centrifuge.

<u>Reaction Technique:</u> Air-free technique (Glovebox, Schlenk line), High-pressure reaction in Autoclave, Immersion well Photo-reactor, Microwave reactor, Cryogenic reactor, Electrochemical Polymerization.

## **Computation and Softwares:**

Calculations: DFT, TD-DFT, AFIR (Artificial Force Induced Reaction), Molecular dynamics simulation, Macromodel, Jmol, Avogadro, Winmostar, GaussView 6 | Chemdraw, ISIC draw, ACD lab 3D, Kaleidagraph | Sci-finder, Reaxys | Origin 8.5, Delta NMR, Topspin, Mestrec, iNMR, OLEX2, Shelxle, CrysAlis-pro| Mercury, Conquest, Chimera | MS office | C, FORTRAN.

<u>Facilities Established:</u> Complete chemistry laboratory setup at Manipal Centre for Natural Sciences via purchasing and installing various equipment like rotary evaporator, UV-cabinet, ultrasonic bath, photo-reactor, reaction fume hoods, Nitrogen line with schlenk facilities, high-speed cooling centrifuge, muffle furnace, oven, UV-spectrophotometer, refrigerator, vacuum pumps, Preparative TLC and column chromatographic setup. In-charge of building software/ computational facilities for chemical drawing and computation at Manipal Centre for Natural Sciences.

Supervised in setting up of glovebox at Ewha Womans University and built solvent distillation facility (laboratory of Prof. Jean Bouffard).

# and COMMUNICATION

- 1. "Towards Heteroaromatic Nanoribbons" at SECO-49, Annecy, France, May, 2012.
- 2. "Synthesis and dynamic structures of a hybrid nanohoop molecule composed of anthanthrenylene and phenylene panels" at CSJ Annual meeting 2016, Kyoto, Japan, March 2016.
- 3. "Nanocarbons With Unique π-surfaces: 'Bottom-up' Fabrication of Graphene Nanoribbons and Carbon Nanotubes" at Jadavpur University, Kolkata, India, February 2018 (Invited Talk)
- 4. "Bottom-up" Synthesis & Structural Chemistry Of Nanocarbons With Unique π-surfaces" at Manipal Research Colloquium, Manipal Academy of Higher Education, Manipal, India, April 2018.

5. "Modular synthesis of aliphatic polyketones via site-selective monosilylation of 3,3-disubstituted pentane-2,4-diones". at CSJ Annual meeting 2020, Tokyo, Japan, March 2020

# POSTER PRESENTATION

- 1. Ceramidonine approach to hetero-nanoribbon, ISNA-14, Eugene, OR, USA, July, 2011.
- 2. Carboxy-functionalized polycyclic arenes by oxidative cyclisations of 2,3-diarylacrylates, ICPOC-21, Durham, UK, September 2012.
- 3. Towards Electronically Tunable Graphene Nanoribbons From Glyoxylic Perkin Reaction, AIMS2015, Sendai, Japan, February, 2015.
- 4. Synthesis and dynamic structures of a hybrid nanohoop molecule composed of anthanthrenylene and phenylene panels, **AIMS2016**, Sendai, Japan, February, 2016.
- 5. Synthesis and dynamic structures of hybrid nanohoops, CURO-Pi-II, Eugene, OR, USA, September, 2016
- 6. Synthesis and Structural Chemistry Of Nanocarbons With Unique π-surfaces, EAS-8, Thiruvanantapuram, India, September 2017
- 7. Modular synthesis of aliphatic polyketones via site-selective monosilylation of 3,3-disubstituted pentane-2,4-diones, **ICReDD Intl Symposium**, Sapporo, Japan, November 2019

## PROJECT SUPERVISION

- 1. Synthesis of [4]cyclo-*peri*-xanthenoxanthene ([4]CX<sub>2,8</sub>); Oxygen containing belt-persistent finite CNT fragment. (Masters Thesis (2015-2017) at Tohoku University. (*Manuscript in progress*)
- 2. Heteroaromatic Graphene Nanoribbons with alternative electron donor and acceptor panels. (M.Sc. Project intern at MCNS, Manipal University March-October 2018) (*Manuscript published, see publication no 11*)
- 3. "Bottom-up" Approach Towards Hetero-nanographenes. (M.Sc. summer research intern from CET Bhubaneswar, June-July 2018).
- 4. Crafting Molecular Giants with Atomic Precision: New Strategies to Construct Gigantic Nanographenes. (M.Sc. summer research intern from NITK-Surathkal, June-July 2018).

## \* AWARDS / ACHIEVEMENTS

- DST SERB-Early Career Research Award in February 2019 (ECR/2018/000185/CS, amount INR 31 lakhs).
- Selected for Leverhulme Fellowship at University of Nottingham, UK in 2019.
- WPI-AIMR Scientist mobility Award for attending conference from WPI-AIMR Tohoku University, Japan in 2016.
- Doctorate degree in Chemistry with "Très honorable" grade [Highest grade in PhD in France] in July 2012.
- Awarded EMMA (Erasmus Mundus External co-operational window with Asia) scholarship for pursuing PhD degree in 2009.
- First class and ranked 4th (71.33%) in Post Graduation. 1st in Analytical chemistry special, Jadavpur University, 2009.
- First class with distinction (67.00%) in Graduation, Jadavpur University, 2007.
- Selected for National merit scholarship scheme by "Ministry of Human Resource Development, Govt. of India" 2004.
- Ranked 2<sup>nd</sup> in West Bengal (state level) in Achievement-cum-diagnostic Test in Mathematics (ADTM) by Centre for Pedagogical Studies in Mathematics, (ADTM) 2001.

## ACADEMIC MEMBERSHIP & RESPONSIBILITIES.

- Active member in organizing committee of conferences in France (Chem on Tubes, Arcachon 2012) and in Japan (25<sup>th</sup> Symposium in Physical Organic Chemistry, Sendai 2014).
- Member of the "Chemical Society of Japan" 2015-present.
- Member of the "Société Chimique de France" (Chemical Society of France), 2010-2012.
- Member of the "Royal Society of Chemistry" (RSC), 2012-2013.
- Member of Jadavpur University Alumni association, lifetime membership.
- Elected Student representative for Campus recruitment, Jadavpur University Science Faculty, 2008-2009.

# H LANGUAGE SKILL

English (Fluent), Bengali (Fluent), Hindi (Fluent), French (Basic), Japanese (Basic)