SYMPOSIUM ON POLYMER SCIENCE - 2019

5TH-6TH JULY, 2019

Abstract Book

Organized by



INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH KOLKATA



Director's Message

I am extremely pleased to learn that the Kolkata Chapter in Society for Polymer Science (SPS), India, under the supervision of Centre for Advanced Functional Materials (CAFM), Indian Institute of Science Education and Research (IISER) Kolkata is organizing a scientific conference, Symposium on Polymer Science, on July 05-06, 2019. It is good to note that the Symposium aims to provide a common platform for the exchange of knowledge among eminent scientists and young researchers

from India and abroad, working in the area of the polymer science.

I am very proud of IISER Kolkata Polymer Community, which has a broad spectrum of interest, including synthesis of polymers, characterization, their applications in diverse fields, along with strong expertise in theoretical area as well. Indeed, today polymer science is central to important interdisciplinary subjects of Chemistry, Physics, Biology and Materials. Polymers have played a key role in the understanding of fundamental aspects of science, apart from their diverse applications.

On behalf of IISER Kolkata and on my own, I welcome all the National and International Speakers who have taken their valuable time for this particular event. I would like to congratulate the organizing committee for taking this initiative to organize a conference on behalf of IISER Kolkata. I wish the organizing committee and all the participants to have a very productive and fruitful discussion for the betterment of the science and society.

Professor Sourav Pal Director

Indian Institute of Science Education and Research (IISER) Kolkata



Message from CAFM Chair

The Centre for Advanced Functional Materials (CAFM) at IISER Kolkata is extremely happy and proud to host the Kolkata Chapter Meeting of the Society for Polymer Science (SPS), India during 5-6 July 2019. CAFM was officially founded on 01 August 2016 to foster collaborative, interdisciplinary research and education in the science and technological applications of solid state and soft materials. At present, 32 faculty members are associated with CAFM, 19 from the Department of Chemical

Sciences, 6 from the Department of Biological Sciences and 7 from the Department of Physical Sciences. The faculty members of CAFM have excellent academic credentials and are highly regarded. Many of them are associate editors and editorial board members of prestigious international journals. Few have already been conferred with prestigious awards and recognitions.

In particular, 11 research groups work in different areas of soft matter namely polymer chemistry, supramolecular chemistry, organic semiconductors and organic materials for biological applications, environmental remediation, gas storage and electronic devices, including theoretical soft condensed matter physics. The research on polymeric materials has been invigorated for nearly a decade at the acclaimed Polymer Research Centre (PRC) by Prof. Raja Shunmugam and Prof. Priyadarsi De, the organizing secretaries of SPS-2019. Besides soft matter, the interdisciplinary research activities at CAFM cover the areas of third-generation photovoltaic cells; batteries; fuel cells; strongly correlated materials; and drug delivery. The rapidly increasing applications of polymer materials encompass all the above areas and many more. Given the high-profile speaker and participant list of SPS-2019 covering diverse areas of polymer research, I hope that you will experience all the sessions of this conference to be scientifically stimulating and highly interactive in nature.

Sincerely, Sayan Bhattacharyya Chair, CAFM

Message from Acting Head, DCS, IISER Kolkata



I am happy to note that Indian Institute of Science Education and Research Kolkata is organizing Society for Polymer Science (SPS), India, Kolkata Chapter, Conference on July 5th and 6th 2019. Polymer science is an important part of material science and mainly deals with the synthetic polymers, plastics, foldamers and elastomers. Also there are large numbers of bio polymers. So, it is a multidisciplinary research including chemistry, biology, physics and engineering. Polymers are now part of our everyday life. But we have to concern and address the issue of pollution due

to non degradable polymers and plastics. The conference will focus on polymer synthesis, morphology, molecular structure and properties. The interaction of small molecules with biopolymers, proteins, synthetic polymers and supramolecular polymers is another important aspect.

I am sure that the conference will unravel new research area in polymer science and stimulate young researcher and technologists.

On behalf of Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, I wish the conference every success and congratulate the organizers for planning and realizing the SPS-2019.

Sincerely

Debasish Haldar 28.06.2019

Programme Schedule

Venue: LHC, IISER Kolkata

Day 1: July 05, 2019

8.30-9.30 AM	Event	Registration at LHC, IISER Kolkata
9.30-9.55 AM	Welcome Address	Prof. Raja Shunmugam, IISER Kolkata
	Inauguration Session	Prof. Sourav Pal, Director, IISER Kolkata
	Chair: Prof. Arindam Kundagrami,	Prof. Debasish Haldar, Acting DCS Chair, IISER Kolkata
	IISER Kolkata	Prof. Sayan Bhattacharyya, Chair, CAFM, IISER Kolkata
		Prof. A. K. Nandi, IACS Kolkata, Secretary, SPSI-Kolkata Chapter
9.55-10:45 AM		Plenary Lecture: Prof. S. Sivaram, IISER Pune
10.45-11.15	High Tea	
AM		
11.15-11.45	Chair: Prof. Suhrit Ghosh, IACS	Dr. Samir Chikkali, NCL-Pune
AM	Kolkata	
11.45-12.15 PM		Prof. Sayam Sen Gupta, IISER Kolkata
12.15-12.35		Prof. Soumyajit Das, IIT Ropar
PM		
12.35-12.55		Dr. Kamal Bauri, Raghunathpur College
PM		
12.55 –3.00 PM	Lunch Break +	Poster Presentation
		Chairs: Prof. Jhuma Ganguly, IIEST, Shibpur
		Prof. Kishor Sarkar, University of Calcutta
3:00-3:30 PM	Chair: Prof. Sudip Malik, IACS Kolkata	Prof. N. K. Singha, IIT Kharagpur
3:30-3:50 PM		Dr. Anindita Das, IACS Kolkata
3.50-4:10 PM		Prof. Sanjib Banerjee, IIT Bhilai
4:10-4:30 PM		Prof. Dhruba Prosad Chatterjee, Presidency University
4:30-4:50 PM	Tea break	· · · · · · · · · · · · · · · · · · ·
4:50-5:20 PM	Chair: Prof. Dipankar Chattopadhyay	Mr. Raj Datta, Haldia Petrochemicals Limited
5:20-5:50 PM	University of Calcutta	Dr. Tapan Kumar Dhar, Berger Paints
5:50-6:20 PM		Mr. Sandip Mitra, Wacker Metroark Chemicals Pvt. Ltd.
6.30 PM		Dinner at LHC

Day 2: July 06, 2019

8.30-9.00 AM	Event	High Tea	
9:00-9.40 AM	Chair: Prof. Abhijit Bandyopadhyay	Prof. Nicolay V. Tsarevsky, Southern Methodist University, USA	
9.40-10.20 AM	University of Calcutta	Prof. Mihaela C. Stefan, The University of Texas at Dallas, USA	
10.20-10.50 AM	1	Dr. Souvik Maiti, CSIR-IGIB, New Delhi	
10.50-11.15 AM	Tea/Coffee Break		
11:15-11:45 AM	Chair: Prof. Dibakar Dhara	Prof. R. Dhamodharan, IIT Madras	
11:45-12:15 PM	IIT Kharagpur	Prof. Sagar Pal, ISM Dhanbad	
12.15-12:45 PM		Prof. Sandanaraj Britto, IISER-Pune	
12:45-1:05 PM		Dr. Shivshankar Mane, NCL-Pune	
1:05-2:00 PM	Lunch Break		
2:00-2:30 PM	Chair: Prof. Tarun Kumar Mandal	Dr. Debmalya Roy, DRDO, Kanpur	
2:30-3:00 PM	IACS Kolkata	Prof. Tushar Jana, University of Hyderabad	
3:00-3:20 PM]	Prof. Chanchal Chakraborty, BITS Pilani, Hyderabad	
3:20-3:40 PM		Dr. Beauty Das, University of Calcutta	
3:40-4:00 PM	Chair: Prof. Sanjio S. Zade,	Concluding Session	
	IISER Kolkata		
	Prof. Priyadarsi De,		
	IISER Kolkata		

Poster Session – TRC

Poster No.	Presenting Author	Title
P1	Sayan Basak	Development of a Neoteric Melt-Processable Thermoresponsive Self-Healable Elastomer, its Characterization, and its Quantification by a Novel 'Software
P2	Udayan Basak	Imaging' Technique Synthesis of PVDF based Graft Copolymers for the Fabrication of Affinity
P3	Kapil Dev	Membrane Cyclic Hypervalent Iodine(III) Reagents as Inimers for the Synthesis of Branched
	Sayala	Polymers
P4	Kapil Dev Sayala	Chemical Modification of Polyisoprene using Tetrazole containing Hypervalent Iodine(III) Reagents
Р5	Tapas Ghosh	Controlled Synthesis of Nano Structured Polyaniline on Graphene Oxide Sheets for Efficient Energy Storage Application
P6	Anwesha Chakraborty	Organobase Triggered Controlled Supramolecular Ring Opening Polymerization and 2D Assembly
P7	Ranjit Das	Synthesis of Covalently Connected Graphene Oxide-g-Chiral Polyaniline
P8	Ranajit Barman	Nanocomposite with Improved Energy Storage Antimicrobial Polyurethane with Selective Activity against <i>E. coli</i>
P9	Neha	Tryptophan-Based Polymeric chemosensor for sensing and removal of Cu(II) and
17	Choudhury	Hg(II) from aqueous media
P10	Subhadip Roy	A Simple Strategy for the gram-scale Synthesis of Graphene Quantum Dot with Unique Optical Property
P11	Tuhin Ghosh	Synthesis of Living poly (2-Dimethylaminoethyl Methacrylate) by Solvent Free
		ATRP in Ambient Temperature
P12	Ranita Samanta	Multitasking single-crystal-to-single-crystal /solid state photopolymerization
P13	Priyapratim Patra	Modified starch-based graft copolymeric flocculant for treatment of blast furnace effluent
P14	A. Jamadar	Supramolecular Assembly by Orthogonal Hydrogen and Halogen Bonding
P15	Krishna Gopal Goswami	Modulation of Side Chain Crystallinity in Fatty Acid and MethoxyPoly(ethylene glycol) Containing Alternating Copolymers
P16	Krishanu Ghosal	Dendron Conjugated Carbon Quantum Dot for Selective detection of Breast Cancer and Gene Therapy
P17	Rima Saha	RAFT Polymerized Amino Acid Based Cationic Polymer for Excellent Gene Transfection Efficiency in Triple Negative Breast Cancer
P18	Priyatosh Sarkar	Carbon Dot Functionalized Nanoengineered Template for Targeted Doxorubicin Delivery to Triple Negative Breast Cancer
P19	Shuvam Ghosh	Targeted Gene Therapy for Hepatocellular Carcinoma by Gelatin Based Silver Nanoparticle
P20	Tapan K. Dash	Design of Malonic Acid Based Linker and ConjugatedAmphiphilic Theranostic
P21	Sayantani	System for Effective Cancer Therapy A Study on the Effect of PEG in the Thiol-norbornene Crosslinked Network for the Remarked of Tavia Cationia Due
P22	Bhattacharya Sourav Mete	the Removal of Toxic Cationic Dye The Role of Aliphatic chains on Crystallinity of Fatty Acid Containing Styrenic
BAA	T	Polyperoxides
P23	Tapendu	Poly-Norbornene coupled Rhodamine-B derivative as an excellent Fe(III) ion
	Samanta	chemodosimeter in semi-aqueous medium: a colorimetric and fuorimetric approach
P24	Sujay K. Nandi	Schellman Loop from small α-Peptides: Hydrogen bond arrangements
P25	Pousali Samanta	Arm First Approach Towards Synthesis of Core Cross-Linked Star Polymer with Hydrophobic Corona Via Click Chemistry
P26	Puja Poddar	Synthesis of Temperature, Redox, pH Triple Responsive Amphiphilic Block Copolymers for Potential Drug Delivery Applications
P27	Satyagopal	Cationic Block Copolymers with Different Architectures and their
	Sahoo	Capability towards DNA Condensation and De-condensation
P28	Neha Rani Kumar	2,4,6-Tri(thiophen-2-yl)-1,3,5-triazine Based Conjugated Porous Polymers for Reversible Dye Adsorption and CO_2 Capture

P29	Subhajit Bal	Chemically Fueled Dissipative Self-Assembly that Exploits Cooperative Catalysis
P30	Tapan Ghosh	Kinetic and Thermodynamic Control over Crystallization to Yield H and J Type
F 30	Tapan Onosh	Dimers in Single Crystal: Excitonic Coupling and Resulting Optical Outputs in the
		Solid State
P31	Abhijeet R.	Radical Cascade Avenue for Direct Access to 3,4 Fused Thiophenes with 2,5-
151	Agrawal	Positions Free for Substitution
P32	Dhirendra K.	Polymer Nanorod Grafting by Halide Perovskite Nanocrystals for Hybrid Organic
_	Chaudhary	Solar Cells with ~10% Efficiency
P33	Sk. Atiur	Formation of Disulphide Linkages Restricts Intramolecular Motions of
	Rahaman	Fluorophore: Detection of Molecular Oxygen in Food Package
P34	Saswati Ghosh	Polymer-based Chemosensors for Selective Detection of Pyrophosphate in
	Roy	Semiaqueous Media ($P_2O_7^{4-}$)
P35	Krishna Gopal	Organo visible Light Photocatalyzed Synthesis of Phosphoramide Derivative by
	Ghosh	Direct C–H bond Activation
P36	Dipika Pan	Protein based Hydrogel Preparation for Detection of Nitroaromatics in Aqueous
		medium
P37	Biswajit Jana	Fabrication of ZnO nanocomposite Hydrogel for removal of Toxic Dyes
P38	Soumyadip	Photoinduced Electron Transfer with Ultrasmall Copper Nanoclusters towards
D2 0	Bhunia	Finding Characteristics of Protein Pockets
P39	Sanjib Ghosh	Light gated Modulation of Electrical Conductance of a Photochromic
D 40	D'	Coordination Polymer
P40	Biswajit Roy	Removal of Hg ²⁺ Ions from Water through the Formation of a One-Dimensional
P41	Palash Banerjee	Metal–Organometallic Polymer Dual Thermoresponsive Poly(ionic liquid) Random Copolymers
P41 P42	Susobhan Das	Introduction to Nanoindentation: Its importance, from Single Crystals to Polymers
P42	Sayan Dutta	Donor-Acceptor Interactions in Early Transition Metal Halides and Group-14
F43	Sayali Dulla	Compounds: A Theoretical Insight
P44	Dr.	Functionalization of Carbon Nano-onions for Targeted Anticancer Drug Delivery
	Rabindranath	
	Majumder	
P45	Bappaditya	Polymerization of Styrene using Pincer Type Redox active Nitrogen Donor Cobalt
	Goswami	Complexes as Catalysts
P46	Prof. Balaram	Carbohydrate Derived Multifunctional Gels
	Mukhopadhyay	
P47	Samaresh	Flexible Bichromophoric System: From Rapid and Efficient Redox-Actuation to
	Samanta	Competing Self-Assembly Pathways
P48	Sipra Ghosh	Removal of Cationic Dyes from Aqueous Medium Using Glutamic Acid-Derived
		Organogels
P49	Basudeb	Amphiphilic Mannose-6-Phosphate Glycopolypeptide and Lipid Nanocarriers for
D.C.A	Mondal	Lysosomal Storage Disorder (LSDs)Disease
P50	Cheluri	Synthesis and Performance of Proton Conducting Novel Sulfonated Poly(Oxybenzimidazole)-Graphene Oxide Intercalated Composite Membranes for
	Nagendra Prasad	Poly(Oxybenzimidazole)-Graphene Oxide Intercatated Composite Membranes for PEM-Fuel Cells
P51	Tanumoy	Photoredox Mediated Arylation of ArenesandHeteroarenes by Magnetically
131	Mandal	Active Recyclable Iron-Nanocatalyst
P52	Bibhas Hazra	pH Responsive P(LYS-HEMA) Polymer Degradation via Intramolecular
104	Biolius Huziu	Cyclization
P53	Monochura	A Reversible Photoresponsive Activity of a Carbonic anhydrase Mimic
	Saha	1 5 · · · · · · · · · · · · · · · · · ·
P54	Soumik Mitra	The Free Energy Profile of Complexation of two oppositely charged
		Polyelectrolyte Chains
P55	Mrinal Mandal	Meta-Fluorophores: Inception of a New Generation of Single Benzenic Ultra
		Small Fluorophores Exhibiting Red-NIR Fluorescence



PLENARY LECTURES

Aliphatic Polyesters: A Platform for Design of Sustainable Materials

Prof. S. Sivaram

Indian Institute of Science Education and Research, Pune- 411 008, INDIA s.sivaram@iiserpune.ac.in

Abstract: Aliphatic polyesters, a quintessential embodiment of a synthetic macromolecule, were first reported by Wallace Carothers in 1930s. However, wholly aliphatic polyesters were relegated to the background since it lacked the physical properties desired for every day applications. During the past decade there has been a resurgence of interest in this class of materials [1]. Aliphatic polyesters are biocompatible as well as biodegradable under composting conditions; In addition, many of the building blocks for aliphatic polyesters can be derived from renewable feed stocks.

However, synthesis of aliphatic polyesters from a diverse range of building blocks require a better under standing of what limits the original chemistry of Carothers and strategies to get around these limitations. In spite of many solutions, challenges still remain in the synthesis of a broad class of aliphatic polyester susing a wide range of monomers and chemistries.

This lecture will highlight current challenges in the synthesis of aliphatic polyesters using a wide variety of monomers. Our objectives are twofold. One, two explore structural diversity and its effect on polymer properties, and second, to explore methods to enhance the useful properties of aliphatic polyesters using physico-chemical approaches [2]. We will demonstrate, there is still scope for new monomers and improved chemistry to tailor the structure and properties of aliphatic polyesters.

- Schneiderman D.K.; Hillmyer, M.A. Macromolecules, 2017, 50, 3733; Tong R. Ind. Eng. Chem. Res., 2017, 56, 4207; Zhu, Y.: Romain, C.; Williams, C.K. Nature, 2016, 354, 540.
- Wilson, R.; Divakaran, A.V.; Kiran, S.; Varyambath,S.A.; Kumaran, A.;Sivaram, S.; Lakshminarayanan, R. ACS Omega, 2018, 3, 18714; Deokar, M.;Idage, B.B.;Idage, S.B.; Sivaram, S. J. Appl. Polym. Sci., 2016,133, 43267; Kulkarni, A.; Lele, A.;Sivaram, S.;Rajamohanan,P.R..; Velankar, S.;Chatterji, A. Macromolecules, 2015, 48, 6580.

Hypervalent Iodine Compounds in the Synthesis of Functional and Dynamic Polymers

Nicolay V. Tsarevsky*, Hongzhang Han, Rajesh Kumar, Kapil Dev Sayala, and AvichalVaish

Department of Chemistry, Southern Methodist University, Dallas, TX 75275, USA *Presenting Author, Email: nvt@smu.edu

Abstract: Hypervalent iodine(III) compounds with the generic structure $ArIL_2$ (Ar = aryl, L = ligand such as (pseudo)halide or carboxylate) can participate in both radical and ionic reactions, which makes them very attractive reagents for the synthesis of functional, responsive, and/or dynamic polymers. For instance, ligand exchange reactions with nucleophiles (Nu^-), afford hypervalent iodine compounds of the type ArI(Nu)L and eventually $ArINu_2$. The homolysis of the weak hypervalent I-L (or, after ligand exchange, I-Nu) bonds under thermal or photochemical conditions leads to the formation of iodoarenes ArI and radicals L^{\bullet} (or Nu^{\bullet}), which can be used to initiate polymerization¹⁻³ or to functionalize a number of substrates,⁴ including pre-made polymers. The synthesis and properties of functional linear, star-shaped, graft, branched, and crosslinked polymers via ligand exchange reactions involving hypervalent iodine(III) compounds, in some cases followed by decomposition of the products of the exchange, in addition to dynamic and self-healing polymers containing the -I(Ar)- structural motif, will be described.⁵

- 1. Han, H.; Tsarevsky, N. V. Polym. Chem. 2012, 3, 1910.
- 2. Han, H.; Tsarevsky, N. V. Chem. Sci. 2014, 5, 4599.
- 3. Kumar, R.; Cao, Y.; Tsarevsky, N. V. J. Org. Chem. 2017, 82, 11806.
- 4. Tsarevsky, N. V. J. Polym. Sci.: Part A: Polym. Chem. 2010, 48, 966.
- 5. Vaish, A.; Tsarevsky, N. V. In *Main Group Strategies towards Functional Organic Materials*; Baumgartner, T., Jaekle, F., Eds.; Wiley: 2018, p 483.

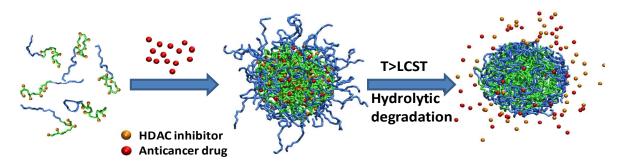
Functional Polycaprolactones for Drug Delivery Applications

Mihaela C. Stefan*, Erika Calubaquib, Pooneh Soltantabar, Hanghang Wang, Abhi Bhadran

Department of Chemistry and Biochemistry, University of Texas at Dallas, Richardson, TX, 75080, USA *Presenting Author, Email: mihaela@utdallas.edu

Abstract: Libraries of biocompatible and biodegradable thermoresponsive polycaprolactones for drug delivery of anticancer drugs and histone deacetylase (HDAC) inhibitors were synthesized by the ring-opening polymerization of various γ -substituted- ϵ -caprolactone The combination of biocompatibility, biodegradability, monomers. and tunable thermoresponsive behavior is ideal for drug delivery of anticancer drugs and HDAC inhibitors. Amphiphilic thermoresponsive polycaprolactone block copolymers with tunable thermoresponsive behavior were synthesized. The amphiphilic block copolymers selfassembled in water to form micelles with a hydrophobic core that was employed to load and deliver hydrophobic anticancer drugs. The fine tuning of the ratio between hydrophobic and hydrophilic blocks provided polymers with tunable lower critical solution temperatures (LCST) in the range of 37-55 °C. The functional groups of the hydrophobic block were varied to adjust the size of micelles which allowed the tunability of drug loading capacity. Thermoresponsive amphiphilic polycaprolactone block copolymers containing conjugated histone deacetylase inhibitors (HDACi) were also synthesized and tested for drug delivery. The HDAC inhibitor moieties were attached to the hydrophobic block through ester groups which allowed their release upon hydrolysis. Valproic acid and phenylbutyric acid were attached through ester bonds to the hydrophobic block.

The drug loading capacity of micelles was significantly improved upon co-loading of doxorubicin (DOX) with resveratrol (RES) polypehenol.



- 1. Kularatne, R. N.; Washington, K. E.; Bulumulla, C.; Calubaquib, E. L.; Biewer, M. C.; Oupicky, D.; Stefan, M. C. *Biomacromolecules* **2018**, *19*, 1082-1089.
- 2. Washington, K. E.; Kularatne, R. N.; Biewer, M. C.; Stefan, M. C. ACS Biomaterials Science & Engineering 2018, 4, 997-1004.
- 3. Washington, K. E.; Kularatne, R. N.; Du, J.; Ren, Y.; Gillings, M. J.; Geng, C. X.; Biewer, M. C.; Stefan, M. C. *Journal of Materials Chemistry B* **2017**, *5*, 5632-5640.
- 4. Senevirathne, S. A.; Washington, K. E.; Miller, J. B.; Biewer, M. C.; Oupicky, D.; Siegwart, D. J.; Stefan, M. C. *Journal of Materials Chemistry B* **2017**, *5*, 2106-2114.



INVITED LECTURES

Ionotropic Crosslinking of Chitosan towards the Synthesis of Biocompatible Hydrogels

R. Dhamodharan* and R. Kartik

¹ Department of Chemistry, IIT Madras, Chennai, Tamil Nadu 600 036, India *Presenting Author, Email: damo@iitm.ac.in

Abstract: Chitosan is crosslinked using novel negatively charged ionotropic crosslinkers such as colloidal metal salts, carbon nanodots, maleated chitosan, alkali and lignin. Among the various crosslinkers, gels based on colloidal metal salts exhibited a wide range of mechanical properties and environmental stability, while showing self-healing nature. The antimicrobial nature and low cytotoxicity of some of these gels could be suitable for application as injectable or preformed scaffolds in tissue engineering. In additions, these "metallogels" could be used as recoverable catalysts for various organic transformations. Carbon nanodots, maleated chitosan polyanionsas well as alkali lignin were also used to crosslink chitosan to produce biocompatible hydrogels. The "all-chitosan" hydrogel, prepared from chitosan and maleated chitosan, exhibited very low cytotoxicity and a conducive surface for cell attachment and proliferation. Likewise, hydrogels of chitosan-alkali lignin were nontoxic to mesenchymal stem cells, in vitro, and to zebrafish up to 100 µg/ml, in vivo. In addition, these gels provided a conducive surface for cell attachment and proliferation, making it suitable for application as scaffolds in tissue engineering. In presence of the hydrogel, NIH 3T3 mouse fibroblast cells showed good cell migration characteristics suggesting that the gel might be suitable for wound healing application.

- 1. Ravishankar, K.; Kanniyappan, H.; Shelly, K. M.; Muthuvijayan, V.; Dhamodharan, R. *Chem. Commun.*, **2018**, 54, 11582–11585.
- 2. Ravishankar, K.; Shelly, K. M.; Desingh, R. P.; Subramaniyam, R.; Narayanan, A.; Dhamodharan, R. ACS Sustain. Chem. Eng., 2018, 6, 15191–15200.
- 3. Ravishankar, K.; Venkatesan, M.; Desingh, R. P.; Mahalingam, A.; Sadhasivam, B.; Subramaniyam, R.; Dhamodharan, R. *Mater. Sci. Eng. C*, **2019**, 102, 447–457.

Click Chemistry in Polymer Science; Opportunities & Challenges

Nikhil K. Singha

Rubber Technology Centre, IIT Kharagpur, West Bengal- 721302

Abstract: Since the pioneering work of Barry Sharpless, late 1990s, 'Click Chemistry' has been an important synthetic tool to prepare varieties of functional materials for different important applications. In Polymer Science, Click Chemistry has been widely used to prepare smart functional polymer materials having application in advanced materials.

In this case, different functional polymers, hydrogels were prepared via the combination of controlled radical polymerization and click chemistry. In this case, different click reactions like Diel-Alder reaction, Alder-ene reaction, and disulfide metathesis reactions were used to prepare self-healing, hydrophobic materials based on acrylates, polyurethane as well as glycopolymers. This talk will delineate the preparation of different functional polymer materials as well as their applications.

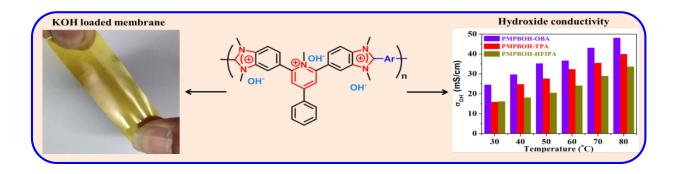
- 1. Mondal, et al (2017):Self-healable thermo-reversible functional polymer via RAFT polymerization and ultrafast 'click' chemistry using triazolinedione derivative, *Chemical Communications*, 53(62) 8715
- Behera, et al (2018):Self-Healable and Ultrahydrophobic Polyurethane-POSS Hybrids by Diels-Alder "Click" Reaction: A New Class of Coating Material, *Macromolecules*, 51(13), 4770-4781.
- 3. Banerjee, et al (2018): Self-healable Antifouling Zwitterionic Hydrogel Based on Synergistic Photo-triggered Dynamic Disulfide Metathesis Reaction and Ionic Interaction, *ACS Applied Materials & Interfaces*, 10, 27391-27406.
- 4. Bhattacharya, et al (2019): REDOX Responsive Fluorescence Active Glycopolymer Based Nanogel: A Potential Material for Targeted Anticancer Drug Delivery, *ACS Applied Bio Materials*, DOI:10.1021/acsabm.9b00267.

Polybenzimidazoles as Ion Exchange Membranes

Tushar Jana*

School of Chemistry, University of Hyderabad, Hyderabad, Telangana-500046, India *Email: tusharjana@uohyd.ac.in

Abstract: The development of polybenzimidazoles (PBIs) asion exchange membraneswith higher ionic conductivity, desirable mechanical strength, low acid leaching and high alkaline stability are the prime challenges to be solved for the successful use of these membrane in various types of fuel cell. Our group has developed and been working on several strategies: (1) synthesis of tailor made PBI structures, (2) development of a novel fabrication process called 'Gel Process', (3) blending of PBI with suitable polymers, and (4) formation of PBI hybrid nanostructures/nanocomposites with inorganic fillersto address these key challenges. In this presentation, I wish to discuss few examples arising from these approaches towards the development of PBI based proton exchange membrane. In addition, I will also highlight an important recent result on the development of PBI based alkaline anion exchange membranes (AAEMs).Two important concerns namely low hydroxide ion (OH-) conductivity and weak alkaline stability of the polymeric membrane in regard AAEMs have been resolved recently by synthesizing a series of pyridine bridged polybenzimidazole (Py-PBI) polymers consisting of dual anion conducting sites.



- 1. Sana, B.; Das, A.; Jana. T. Polymer 2019, 172, 213.
- 2. Maity, S.; Jana, T. Macroolecules 2013, 46, 6814.
- 3. Sana, K.; Jana, T. Polymer 2018, 137, 312.

Role of Synthetic Polymers in Multicellular Tumor Spheroids (MCTS) Formation

R.A. Vignesh¹; Arpita Gosh¹, Saikat Maiti,² Dibakar Dhara², Souvik Maiti¹*

¹Chemical and Systems Biology, CSIR-Institute of Genomics and Integrative Biology, Delhi, India ²Department of Chemistry, Indian Institute of Technology, Kharagpur, West Bengal, India. Email: souvik@igib.res.in

Abstract: Multi cellular tumor spheroid (MCTS) are three-dimensional (3D) cell culture system which provides more physiologically relevant information and more predictive data for in-vivo tests in contrast to the two-dimensional (2D) culture systems. MCTS model gives an idea about the cell-cell contact, cell-matrix interactions and it also mimics the micro-environment for tumor formation that is generally seen *in-vivo* and most widely studied in preclinical trials. MCTS acts as an initial platform for drug screening, toxicity testing and metastatic activity studies. MCTS can be generated either by scaffold based systems (gel matrix based methods by using natural or synthetic polymers) or by scaffold free methods such as hanging drop, forced floatation (Ultralow attachment plate), spinner flask culture (Bioreactors) and force driven methods (magnetic, acoustic or electrical force). Hanging drop method a traditional and cost effective method for the production of MCTS. However, the drawback of this method is its time consumption of more than a week for the development of spheroids. In this presentation, we will describe the effect of synthetic polymers on the MCTS formation, when the polymers are used as media additives. We have observed that the polymers play a positive role in spheroid formation. Homogeneous spheroids of more compact and robust nature were generated. Small sized spheroids were formed in two days. Further, drug uptake studies has been done to demonstrate the utility of cultured spheroids in drug screening. Hence, this method of spheroid development is cost effective to produce uniform size in a very short amount of time compared to other standard methods.

- 1. Zanoni M, Pignatta S, Arienti C, Bonafè M, Tesei A. Anticancer drug discovery using multicellular tumor spheroid models. *Expert Opin Drug Discov.* **2019**, 14(3):289-301.
- 2. Huang B.W.; Gao, J. Q. Application of 3D cultured multicellular spheroid tumor models in tumor-targeted drug delivery system research. *J Control Release*. **2018**, 270, 246-259.

Insertion Copolymerization of 1,1-disubstituted Difunctional olefins with ethylene

Samir H. Chikkali*¹, Shahaji R. Gaikwad1, Satej S. Deshmukh¹, Nilesh R. Mote¹

¹Polymer Science and Engineering Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune, Maharashtra-411008, India *Presenting Author, Email: s.chikkali@ncl.res.in

Abstract: Polymers have become indispensible in 21st century and today we produce about 300 million tons of polymers every year. Among these, polyolefins contribute more than half of the total volume of polymers produced. Most of these polyolefins are produced by a reaction called "Insertion Polymerization" or more popularly "Ziegler-Natta Polymerization".¹ Despite the seeming maturity, the insertion polymerization reaction continues to surprise us with growing complexity and is young as ever.

My talk shall take a stock of the remaining challenges in Ziegler-Natta polymerization; briefly discuss current solutions, and reiterate the enormous potential of this seventy year old reaction to meet contemporary demand. I will showcase our endeavor in insertion copolymerization of 1,1-disubstituted difunctional olefins with ethylene to prepare functional polyethylene.²⁻⁴ Synthesis of acetonitrile ligated phosphine-sulfonate palladium complex, its application in the first insertion copolymerization of 1,1-disubstituted difunctional (such as super glue) olefin with ethylene, mechanism and structure-property-performance correlation will be revealed.⁵

- Chikkali, S. H. (Eds.) in *Metal Catalyzed Polymerization: Fundamentals to Applications* (ISBN: 9781498767576). CRC Press, Taylor and Francis Group, Boca Raton, FL 33487, USA.
- 2. Gaikwad, S. R.; Deshmukh, S. S.; Koshti, V. S.; Poddar, S.; Gonnade, R. G.; Rajamohanan, P. R.; Chikkali, S. H.* *Macromolecules*, **2017**, *50*, 5748-5758.
- 3. Gaikwad, S. R.; Deshmukh, S. S.; Gonnade, R. G.; Rajamohnan, P. R.; Chikkali, S. H.*, *ACS Macro. Lett.* **2015**, *4*, 933-937.
- 4. Pandey, S.; Raj, V. K. Shinde, D. R.; Vanka, K.; Kashyap, V.; Kurungot, S.; Vinod, C. P.; Chikkali, S. H.* J. Am. Chem. Soc. 2018, 140, 4430-4439
- 5. Gaikwad, S. R.; Deshmukh, S. S.; Chikkali, S. H.* J. Polym. Sci. Part A: Polym. Chem. 2014, 52, 1-6.

Cellular uptake of mannose-6-phosphate modified glycopolypeptides and their self-assembled nanostructures

Basudeb Mondal,¹ Bhawana Pandey,² Nimisha Parekh² and Sayam Sen Gupta¹*

¹Depratment of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 721426; ²Polymer Science and Engineering, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune 411008, India, sayam.sengupta@iiserkol.ac.in

Abstract: The ubiquitous expression of mannose-6-phosphate receptor on majority of human cells makes it a valid target in the quest to deliver therapeutics selectively to the lysosome. These receptors, which include the ~300 kDa insulin-like growth factor-II (IGF-II)/cation-independent (CI) multifunctional transmembrane glycoprotein mannose 6phosphate (M6P) receptor (CI-MPR), bind lysosomal enzymes containing phosphomannosyl residues in the trans-golgi network (TGN) and transport them to an acidified compartment of lysosomes. Synthesis of high molecular weight M6P-glycopolypeptide having pendant M6P moieties in side chain as a natural mimic of proteins bearing M6P moieties can help us understand the complexity and individuality of CI-MPR trafficking for lysosomal targeting. In addition, amphiphilic glycopolypeptides bearing mannose-6-phosphate can be selfassembled into vesicles, micelles and nanorods. This lecture will discuss the cellular uptake of mannose-6-phosphate gly-copolypeptides and soft nanostructures made from these glycopolypeptides. An end functionalized polyvalent (M6P-GPs) with high molecular weights (Up to 22 KDa) have been synthesized via NCA polymerization. These synthetic M6P-GPs were found to display minimal toxicity to cells in vitro and show exceptional selectivity for trafficking into lysosomes in various cell lines. Comparison of cellular uptake behavior of M6P-GP and the corresponding Mannose-GP polymer reveals that incorporation of phosphate moiety at the 6-position of mannose completely alters its trafficking behavior and becomes exclusively lysosome specific. We also demonstrate that trafficking of M6P-GPs in mammalian cells is likely associated with the CI-MPR receptor pathway.

Chemical Strategies for Rational Design of Dynamic Supramolecular Protein Assemblies

Britto S Sandanaraj, M. Mohan Reddy, Pavankumar Bhandari

Department of Chemistry, Indian Institute of Science Education and Research, Pune *Presenting Author, Email: sandanaraj.britto@iiserpune.ac.in

Abstract: Self-assembly of proteins in to higher order super-structures is ubiquitous in biological systems. Genetic methods comprising both computational and rational design strategies are emerging as powerful methods for design of synthetic protein complexes with high accuracy and fidelity. Although useful, most of the reported protein complexes lackad vanced functions that may limit their potential applications. On the contrary, protein engineering using chemical strategies offers excellent possibilities for the design of protein complexes with stimuli-responsive functions and adaptive behavior. However, designs based on chemical strategies are not accurate and there for eyield polydisperse samples that are difficult to characterize. Here, we describe simple design principles for the construction of protein complexes through supramolecular chemical strategy. The proposed methodology is amenable for the synthesis of protein complex libraries with molecular weights and dimensions comparable to naturally occurring protein cages. The designed protein complexes display very rich structural diversity, oligomeric states, size sand surface charges that can be engineered through macromolecular design. The broad utility of his method is demonstrated by design of most sophisticated stimuli-responsive systems that can be programmed to assemble/disassemble in a reversible/irreversible fashion using pH or light as a trigger.

- 1. Sandanaraj, B. S.*; Reddy, M.; Bhandari, P.; Sugam, K.; Aswal, V. K. Chem. Eur. J. 2018, 24, 16085-16096.
- 2. Sandanaraj, B. S.; Reddy, M. M.; Bhandari, P. J.; Rao, K. US Patent, 2017 (Granted)

Polysaccharide-based graft copolymeric hydrogels/nanogels: development and applications

Sagar Pal¹*, Priyapratim Patra¹, Dipankar Das¹, Puja Das Karmakar¹, Santanu Dhara²

¹Deaprtment of Chemistry, Indian Institute of Technology (ISM), Dhanbad, Jharkhand-826004, India ²School of Medical Science & Technology, Indian Institute of Technology, Kharagpur, West Bengal-721302, India

*Presenting Author, Email: sagarpal@iitism.ac.in

Abstract: Recently, in authors' laboratory, various polysaccharide-based graft copolymeric hydrogels/nanogels have been prepared via free radical, ROP and RAFT polymerizations.¹⁻⁷ The developed copolymeric hydrogels/nanogels are biocompatible and non-toxic. They are visco-elastic in nature, demonstrate excellent reversible swelling behavior and are found to be stimuli-responsive. The copolymers can efficiently load various model drugs. Detailed investigations reveal the physical interactions between the copolymer and the therapeutics. The copolymers are able to release the entrapped drugs in controlled way in the targeted area.

- 1. 1. Patra, P.; Seesala, V. S.; Soni, S. R.; Roy, R. K.; Dhara, S.; Ghosh, A.; Patra, N.; Pal, S.Eur. Polvm. J.2019, 114, 225, 2019.
- 2. Patra, P.; Seesala, V. S.; Das, D.; Panda, A. B.; Dhara, S.; Pal, S. Polymer, 2018, 140, 122-130.
- 3. Karmakar, P. D.; Seesala, V. S.; Pal, A.; Dhara, S.; Chatterjee, S.; Pal, S. J. Polym. Sci. A, 2018, 56, 2354.
- 4. Mandal, B.; Rameshbabu, A. P.; Soni, S. R.; Ghosh, A.; Dhara, S.; Pal, S.ACS Appl. Mater. Interfaces, 2017, 9, 36583.
- 5. Patra, P; Rameshbabu, A. P.; Das, D.; Dhara, S.; Panda, A. B.; Pal, S. Polym. Chem., 2016, 7, 5426.
- 6. Das, D.; Rameshbabu, A. P.; Patra, P.; Ghosh, P.; Dhara, S.; Pal, S. Polymer, 2016, 107, 282.
- 7. Das, D.; Patra, P.; Ghosh, P.; Rameshbabu, A. P.; Dhara, S.; Pal, S. Polym. Chem., 2016, 7, 2965.

Polymer based nanocomposites for Strategic Applications

Debmalya Roy^{1*}, Kingsuk Mukhopadhyay², N. Eswara Prasad²

¹Directorate of Nanomaterials and Technologies, DMSRDE (DRDO), Kanpur, Uttar Pradesh-208013, India ²DMSRDE (DRDO), Kanpur, Uttar Pradesh-208013, India * Email: droy@dmsrde.drdo.in

Abstract: The polymer based composite products have been witnessed a radical advancement by the advent of new technological avenues. The traditional fabrication technologies and manufacturing processes are now looking forward to advance high performance spin-off under harsh environment and extreme weather conditions. The industry-academia consortiumare are actively pursuing research on visco-elastic materials and technologies to replicate the uniformity in tailor-make products with durability and excellent performance thresholds. The use of nanomaterials provides an unprecedented opportunity to improve and reconcile the material system for multiple performance objectives.

Our directorate has been working on in house development the nanocomposite materials with intended properties for various divergent tactical applications. The important products in the areas of fuel, healthcare and structural systems have been developed to cater for specific strategic needs of Indian defence. We have worked on several projects of national importance and helped to mature a few important polymer nanocomposite based products to self reliance in the domain which will be highlighted in the presentation.

- Janghela, S.; Neeraj, N. S.; Agarwal, N.; Agarwal, K.; Roy, D.; Mukhopadhyay, K.; Prasad, N. Eswara. Phys. Chem. Chem. Phys. 2018, 20, 29847-55 2. Bhattacharyya, R.; Janghela, S.; Saraiya, A.; Roy, D.; Mukhopadhyay, K.; Prasad, N. Eswara. J. Phys. Chem. B. 2018, *122*, 2683-93
- Roy, D.; Tiwari, N.; Kanojia, S.; Mukhopadhyay, K.; Saxena, A. K. J. Phys. Chem. C. 2015, 119, 16678-87
- Roy, D.; Shastri, B.; Mukhopadhyay, K.; Saxena, A. K. United States Patent US20150151971A1

Macromolecular Assembly by Orthogonal Non-covalent Interactions

Anindita Das*

¹School of Applied and Interdisciplinary Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700032, India *Presenting Author, Email: (psuad2@iacs.res.in)

Abstract: Precise organization of synthetic macromolecules into well-defined nanostructures is relevant in various applications including biomedicine, organic electronics or catalysis. Nature displays examples of biopolymers such as proteins that utilize directional interactions such as H-bonding as the primary tool for adopting well-defined conformation, which is essential for their incredible complex functions. To emulate the structural elegance and functional diversity of biological system, self-assembly of foldamers, amphiphilic block copolymers and various other exciting hybrid materials such as polymer-peptide conjugates have been studied with great interest. However, introduction of specific directional supramolecular interactions into polymeric scaffolds and thereby investigating their impact in programming macromolecular assembly is still at its infancy.

In the recent past, halogen (X)-bonding interactions have gained renewed interest particularly in the field of crystal engineering, while little is known about their influence in solution states. It is envisaged that orthogonal self-assembly (systems where more than one type of molecular interaction operates independently) of H- and X-bonding motifs can be an interesting combination for introducing structural complexity in simple polymeric systems.

With this idea, we have studied the co-assembly of a polymeric halogen bond (XB) donor with an XB accepting aromatic discotic molecule, which can grow into a 1D supramolecular polymer (SP) on its own by 3-fold H-bonding and pi-stacking. Concomitantly, orthogonal X-bonding plays a decorative role by organizing the macromolecules or other functional molecules into the periphery of the SP. Such unique hybridization of a covalent polymer with its supramolecular analogue by orthogonal non-covalent interactions creates higher order structures in solution phase with unprecedented stability and multi-stimuli responsive properties. This concept of orthogonal self-assembly and its generalized implications in macromolecular organization will be the topic of the oral presentation.

References

- 1. Hofmeier, H.; Schubert, U. S. Chem. Commun. 2005, 2423-2432.
- 2. Wei, P.; Yan, X.; Huang, F. Chem. Soc. Rev. 2015, 44, 815-832.
- 3. Priimagi A.; Cavallo, G.; Metrangolo, P.; Resnati, G. Acc. Chem. Res. 2013, 46, 2686-2695.
- 4. Vanderkooy, A.; Taylor, M. S. J. Am. Chem. Soc. 2015, 137, 5080-5086.

Smart Polymer Materials: Design, Synthesis and Applications

Sk. Arif Mohammad, Shashikant Shingdilwar, and Sanjib Banerjee*

Department of Chemistry, Indian Institute of Technology Bhilai, Raipur 492015, Chhattisgarh, India *Presenting Author, Email: Sanjib.banerjee@iitbhilai.ac.in

Abstract: Stimuli-responsive materials undergo changes in response to external stimuli such as change of temperature, pH, light, etc. Multi-stimuli responsive polymer materials exhibit improved diversity compared to single- or dual-stimuli responsive polymers.¹ However, the ability of the current multi-stimuli responsive polymers to provide the required specificity and tunability is still in its infancy. This is due to the complexity in balancing the material parameters of functionality, reaction feasibility, degradability, hydrophilicity etc. Furthermore, challenging synthesis protocols for these multi-responsive polymers has resulted in lack of fundamental understanding of the detailed structure-activity relationship.

3D-printed anatomical models for surgical planning and clinical training have wide applications in the hospital inpatient setting.^{2,3} This leads to better outcomes, both clinically and economically, for patients, care-providers/doctors and payers.We have developed multistimuli responsive multi-arm-star polymers as a tunable platform to fabricate nanoengineered 3D-printed anatomical models for surgical planning and clinical training. ⁵Novel functional polymers with multiple tunable responses exhibiting large changes in swelling and wettability properties in response to external stimuli (e.g. pH, temperature and light) has been designed, synthesized and characterized. The utility and impact of these multi-stimuli responsive polymer-based materials are demonstrated by the construction of adaptive and intelligent models.

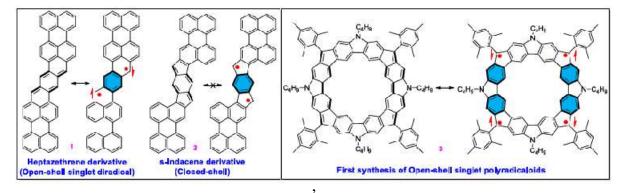
- 1. Schattling, P.; Jochuma, F. D.; Theato, P.Polym. Chem. 2014, 5, 25.
- Bücking, T. M.; Hill, E. R.; Robertson, J. L.; Maneas, E.; Plumb, A. A.; Nikitichev, D. I. PLOS One 2017, 12, e0178540.
- 3. Perica, E.; Sun, Z. Quant Imaging Med Surg. 2017, 7, 668.
- 4. Mohammad, S. A.; Shingdilwar, S.; Banerjee, S. 2019, manuscript under preparation.

Open-shell Singlet Diradicaloid to Polyradicaloid Polycyclic Hydrocarbons

Soumyajit Das

Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar, Punjab-140001, India Email: chmsdas@iitrpr.ac.in

Abstract: π -Conjugated polycyclic hydrocarbons (PHs) can either accommodate π -electrons in the bonding orbitals to form a closed-shell ground state or show open-shell ground state due to the existence of one or more unpaired electrons.¹ Organic electronics area is mainly dominated by the closed-shell molecules, but a resurgence of interest in the open-shell molecules due to their unusual electronic structure revealed that open-shell diradicaloids can be excellent alternatives in the area of organic electronics, photonics, as well as spintronics.² In this presentation, the fundamentals of open-shell diradicaloid PHs will be discussed citing the examples of pro-aromatic zethrene derivative **1**, and related anti-aromatic *s*-Indacene derivative **2**.³ The discussion will include their challenging synthesis, characterization of the ground states, and stabilization approaches. Such fundamental studies enabled design and isolation of the first macrocyclic singlet polyradicaloids (**3**) with tunable physical propoerties.⁴



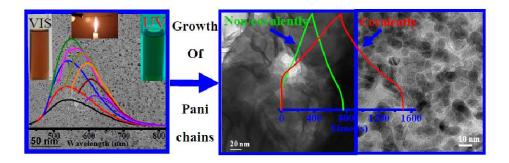
- (a) Das, S.; Wu, J. Polycyclic Hydrocarbons with an open-shell ground state. In *Chemistry of Carbon Nanostructures*; ed. Müllen, K.; Feng, X. Walter de Gruyter GmbH: Berlin, 2017, 253.
- (a) Hu, X.; Wang, W.; Wang, D.; Zheng, Y. J. Mater. Chem. C 2018, 6, 11232. (b) Datta, S.; Cai, Y.; Yudhistira, I.; Zeng, Z.; Zhang, Y. W.; Zhang, H.; Adam, S.; Wu, J.; Loh K. P. Nat. Commun. 2017, 8, 677.
- (a) Das, S.; Lee, S.; Son, M.; Zhu, X.; Zhang, W.; Zheng, B.; Hu, P.; Zeng, Z.; Sun, Z.; Zeng, Z.; Li, R. -W.; Huang, K.; Ding, J.; Kim, D.; Wu, J. *Chem. -Eur. J.* 2014, 20, 11410. (b) Sun, Z.; Zeng, Z.; Wu, J. *Acc. Chem. Res.* 2014 47, 2582.
- Das, S.; Herng, T. S.; Zafra, J. L.; Burrezo, P. M.; Kitano, M.; Ishida, M.; Gopalakrishna, T. Y.; Hu, P.; Osuka, A.; Casado, J.; Ding, J.; Casanova, D.; Wu, J. J. Am. Chem. Soc. 2016, 138, 7782.

Synthesis of Nano Structured Carbon Nano Dot Grafted Polyaniline Using Controlled Polymerization of Aniline

Dhruba P. Chatterjee

Assistant Professor, Department of Chemistry, Presidency University, Kolkata

Abstract: A general approach for controlled grafting of polyaniline (PANI) chains from the surface of nano-structured carbon materials following a 'grafting from' strategy through oxidative polymerization of aniline is developed. Fluorescent spherical carbon nano-dots (CNDs) are obtained through HNO₃ oxidation followed by size separation from an easily available and cheap source like candle soot. Oxidative polymerization of aniline under dilute acid conditions is conducted in the presence of CNDs tethered to the mono-amine group of N,N'-bis(4'-aminophenyl)-1,4-quinonediimine (APQD, in the emeraldine state) (CNDT), as the initiator. The appreciably lower oxidation potential of APQD compared to aniline directs the growth of PANI chains preferentially from these moieties acting as 'seeds'. Furthermore, the conditions are optimized to complete the entire polymerization within the duration of the induction period (IP) for the oxidative polymerization of aniline under similar conditions to ensure the grafting of PANI chains from the CND surface only. The covalently attached carbon nano-dot/ polyaniline shows a remarkably higher specific capacitance of 972 F/g with 90% retention after 2000 cycles, in comparison to only 482 F/g for the non-covalently attached composite. The excellent electrochemical performance is attributed to the formation of the nano-structured composite material.



- 1. T. Ghosh, R. Ghosh, U. Basak, S. Majumdar, R. Ball, D. Mandal, A. K. Nandi, D. P. Chatterjee. J. Mater. Chem. A, 2018, 6, 6476-6492.
- 2. N. Gospodinova and L. Terlemezyan, Prog. Polym. Sci., 1998, 23, 1443-1484.

Silicone Elastomer: A Typical Elastomer for Speciality Applications Sandip Mitra¹

¹Wacker Metroark Chemicals Pvt.Ltd. D.H. Road Chnadi, 24 Parganas (S) West Bengal 743 503, India. *Email: sandip.mitra@wacker.com

Abstract: Basic Chemistry of Silicone & Silicone Elastomer. Various Type (HCR, LSR, RTV-2 &1) & brief applications in various Industrial use.

Reference:

Wacker Chemie GmbH

Silicones, also known as polysiloxanes, are polymers that include any synthetic compound made up of repeating units of siloxane, which is a chain of alternating silicon atoms and oxygen atoms, combined with carbon, hydrogen, and sometimes other elements.

Silicone rubbers are often one- or two-part polymers and may contain fillers to improve properties or reduce cost. Silicone rubber is generally non-reactive, stable, and resistant to extreme environments and temperatures from -67 °F to 572 °F (-55 °C to 300 °C) while still maintaining its useful properties. Due to these properties and its ease of manufacturing and shaping, silicone rubber can be found in a wide variety of products, including: voltage line insulators, automotive applications; cooking, baking, and food storage products; apparel such as undergarments, sportswear, and footwear; electronics; medical devices and implants; and in-home repair and hardware with products such as silicone sealants.

Silicone rubber may be cured by a platinum-catalyzed cure system, a condensation cure system, a peroxide cure system, or an oxime cure system.

Applications of Silicone Elastomer in various Industries:

- HCR : Automotive, Power Trasmission & Distribution,
- LSR : Health Care, Baby Care, Textile Coating
- RTV-2 : Mold making, Pad Printing, Gel & Thermal Interface Material in Automotive, Electronics, LED etc
- RTV-1 : Sealing, Bonding, Adhesive

Silicone rubber can withstand Ozone, UV, heat and other aging factors. This makes silicone rubber one of the elastomers of choice in many extreme environments. Silicone rubber is highly inert and does not react with most chemicals. Due to its inertness, it is used in many medical applications including medical implants.

Trends and Challenges in Petrochemical Industry

Raj Datta

Haldia Petrochemicals Ltd.



Trends & Challenges in Petrochemical Industry

Mr. Raj Datta

Chief General Manager - Product Development & Technical Support Haldia Petrochemicals Limited Kolkata, India



Coating Technology in Recent Times

Tapan Kumar Dhar

Vice President(R&D), Berger Paints India Ltd., 14 & 15 Swarnamoyee Road, Howrah Email: tapandhar@bergerindia.com

Abstract: Paints and coating is as old as human civilization. Still per capita consumption of paint in India is much lower than that of developed countries. This gives an opportunity to the coating industry for faster growth. Current Growth rate of the Industry is about 1.5 times of GDP and the industry is expected to be of 70,000 Cr size in the year 2020-2021.

With the passage of time multi-functional attribute of paint has become more important than mere aesthetics. Nowadays paints with stain resistance, dirt and dust repellence with long lasting colour, water proofing, paints for cool roof are made available. Convenience and customer satisfaction is playing a major role in all the sectors of coating industry. In case of decorative convenience is reflected as colour visualization tool, mechanized application for faster painting, paint for easy maintenance against dirt and stain etc. People look for experience of the product through online demonstration. This has an impact in paint industry as well. While the product needs to be developed for convenience, the supplier also needs to be extremely careful on quality perception of the customer as well. The quality perception of a customer is not just the product specification. It is based on product positioning, the brand image as well as the communication through advertisement. The need for multi surface application with demanding functional requirement, easy to apply has led to the need for newer technology in the area of polymer chemistry, materials science and dispersion science and technology.

Increased awareness on environment and health has led to work with VOC reduction, use of environmental friendly & sustainable materials. Concept of green and low carbon foot print is getting popular in paints as well. This has also brought focus on water based technology for industrial application. Apart from environment water based systems are more convenient for application also. However the technology challenges of water based industrial coating are much more complex & demanding in view of the stringent performance requirement.

The presentation deals with some of the examples of recent work done at Berger Paints in the area of polymer colloid, surfactant, nanotechnology, polymer morphology, cross linking, inorganic organic hybrid polymerto meet the customer needs of recent times.

Nanostructured metallo-supramolecular polymer based electrochromic devices: The sub-second switching time with high colouration

Chanchal Chakraborty^{1,*}

¹Department of Chemistry, Birla Institute of Technology and Science (BITS) Pilani, Hyderabad Campus, Jawahar Nagar, KapraMandal, Hyderabad-500078, India *Presenting Author, Email: chanchal@hyderabad.bits-pilani.ac.in

Abstract: Electrochromism is a unique non-emissive chromic effect which can reversibly alter their optical properties controlled by electrical signals.¹ The electrical bias can effectively change the electrochemical redox state of the electrochromic (EC) materials as well as the optical colour change. This commercially demanding display technology is mostly used in smart window, information display etc.² Metallo-supramolecular polymers (MSPs) are the newly added 4th generation EC materials in this regards.²⁻³ MSPs are the quite fast switching EC materials than the commercially available products as their switching times are usually~3-5s. However, the modern dynamic EC smart windows requires ultrafast subsecond color witching along with very high coloration efficiencies.

Herein, we have synthesized a purple colored Fe(II)-containing metallo-supramolecular polymer (polyFe) as a potential EC material and subsequently fabricated nanostructured of polyFe by controlled counter anion exchange with another polymer like sodium polystyrenesulfonate (PSS)⁴ or modified nanoclays (HNT) to provide polymer nanocomposites. The nanostructure formation considerably enhances the counter-ion diffusion and ionic conductivity inside the EC polymer films and effectively improves the switching times. The solid state gel-type electrochromic devices (ECDs) exhibit the colour change from pristine purple to transparent pale greenish under a controlled potential switching from -2 V to +3 V along with bleaching and coloration time in sub-second range along with improved coloration efficiencies. We have also introduced interface complexation to provide MSPs with improved colour fastness.

- 1. Mortimer, R. J.Chem. Soc. Rev., 1997, 26, 147-156.
- 2. Higuchi, M.J. Mater. Chem. C, 2014, 2, 9331-9341.
- 3. Chakraborty, C.; Pandey, R. K.; Rana, U.; Kanao, M.; Moriyama, S.; Higuchi, M.J. Mater. Chem. C, 2016, 4, 9428-9437.
- 4. Roy, S.; Chakraborty, C. J. Mater. Chem. C 2019, 7, 2871-2879.

Click Inspired Chemistry for Biomedical Applications

Shivshankar R. Mane*

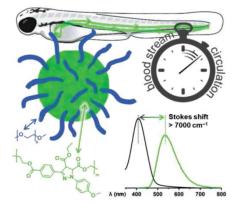
Polymer Science and Engineering Division, CSIR-National Chemical Laboratory Pune, Dr. Homi Bhabha Road, Pashan, Pune-411008, India * Email:shivshankar.mane@gmail.com; s.mane@ncl.res.in

Abstract: Click chemistry-a facile, fast and ambient-temperature avenue for providing a platform for technology; orsynthesize a polymer with common reagents and subsequently employ this polymer with no further functionalization and efficiently carry out conjugation without catalyst in biologically relevant media via click reaction.^{1,2}

Recent advances in super-resolution microscopy and fluorescence bioimaging allow exploring previously in accessible biological processes. To this end, there is a need for novel fluorescent probes with specific features in size, photophysical properties, colloidal and optical stabilities, as well as biocompatibility and ability to evade the reticuloendothelial system. Herein, we report chemically synthesized highly fluorescent polymeric nanoparticles from non-fluorescence precursors. A novel fluorescent nanoparticles are introduced based on an inherently fluorescent polypyrazoline (PPy) core and a polyethyleneglycol (PEG) shell via nitrile imine tetrazole-enecyclo addition (NITEC) polymerization method., which address all aforementioned challenges.

The corresponding nanoparticles are characterized for their luminescent properties and

hydrodynamic size in various aqueous environments cellculture media). PPv nanoparticles (e.g., particularly exhibit a large Stokes shift ($\Delta \lambda = 160$ nmor $\Delta v > 7000 \text{ cm} - 1$) with visible light excitation and strong colloidal stability. While clearance by macrophages and endothelial cells is minimal, PPy displays good biocompatibility. Finally, PPynanoparticles prove to belong circulating when injected in zebrafish embryos, as observedby in vivo



time-lapse fluorescence microscopy. In summary, PPynanoparticles are highly promising to be further developed as fluorescent nanodelivery systems with low toxicity and exquisite retention in the blood stream.³

- 1. Mane, S. R.; Sarkar, S.; Rao, V.; Sathyan, A.; Shunmugam, R. RSC Adv., 2015, 5, 74159.
- 2. Mane, S. R.; Beloqui, A.; Langer, M.; Delaittre, G.; Barner- Kowollik, C. Angew. Chem., Int. Ed., 2019 (submitted)
- 3. Mane, S. R.; Hsiao, I. L.; Le, D.; Straehle, U.; Wiess, C.; Barner- Kowollik, C.; Delaittre, G. *Small*, **2018**, *14*, 1801571.

Stimuli-Responsive Unorthodox Macromolecular Luminogens and Its Sensing Applications

Kamal Bauri,^{1*} Biswajit Saha,² Priyadarsi De²

¹Department of Chemistry, Raghunathpur College, Purulia, West Bengal-723133, India ²Polymer Research Centre and Centre for Advanced Functional Materials, Department of Chemical Sciences, India Institute of Science Education and Research Kolkata, Nadia, West Bengal-742146, India *Presenting Author, Email: kamalsom98@gmail.com

Abstract: Recently, fluorescent polymers lacking traditional conjugated chromophores have drawn increasing interests owing to their fundamental importance and promising applications. Also, stimuli-responsive polymers have been developed for various interesting applications. Amalgamation of the fluorescence property of unorthodox macromolecular luminogens with "smart" stimuli-responsiveness in a single polymer system will give a new class of polymeric material with diversified functions. We have designed a straightforward approach for the synthesis of stimuli-responsive nonconventional macromolecular luminogens based on poly(styrene-*alt*-maleimide) skeleton *via* reversible-addition fragmentation chain transfer (RAFT) polymerization. The synthesized polymers have been characterized by various techniques including ¹H NMR, ¹³C NMR, SEC and MALDI-TOF-MS. We have employed those polymers for nitroexplosive and small volatile organic compound detection in 1005 aqueous environment.

- 1. Saha, B.; Bauri, K; Bag, A.; Ghorai, P. K.; De, P. Polym. Chem. 2016, 7, 6895.
- 2. Bauri, K; Saha, B.; Mahanti, J.; De, P. Polym. Chem. 2017, 8, 7180.
- 3. Saha, B.; Choudhury, N.; Bhadran, A.; Bauri, K.; De, P. Polym. Chem. 2019, DOI: 10.1039/C9PY00462A

Gamut of prospective and challenges of polymeric Scaffold for Facilitating Cellular Repairment and Regeneration by employing Tenet of Tissue Engineering

Beauty Das*, Dipankar Chattopadhyay

Department of Polymer Science and Technology, University of Calcutta, 92 A.P.C Road, Kolkata-700009, India *Presenting Author, Email: dasbeauty01@gmail.com

Abstract: Polymeric biomaterials are significantly very competent to design advanced biomaterials owing to the innovations in nanotechnology, and deeper understanding of biointerfacial interactions. Recently, a paradigm shift towards the development of injectable scaffolds from pre-formed scaffold is sensed. The chief benefit of injectable scaffold over the preformed one is easy administration into a patient. But, it is practically difficult to exactly presume its stability in *in-vivo* conditions owing to delayed crosslinking or fast dissolution. Though the implantation of preformed scaffold is a difficult task, but it ensures stability within the host, and it could be predicted that it would not disintegrate immediately and thereby supporting the cellular growth from the initial hours. Therefore, an inevitable debate persists in the scientific community to choose an appropriate approach. In this context, preformed and injectable scaffolds were synthesized, by exploring in-situ forming hydrogel, polyurethane and its nanocomposites. The physico-chemical and bio-interfacial performance were performed. Mechanically strong hyperbranched polyurethane based scaffold was prepared and the properties of the optimized composition were improvised by the incorporation of CNT/iron oxide nanomaterials. The in-situ hydrogel were prepared exploring thermosensitive methylcellusose and the effect of the size/ concentration of additives or biocompatible glycosaminoglycan was comprehensively studied.

- 1. Das B.; Chattopadhyay P.; Maji S.; Upadhyay A.; Purkayastha M.D.; Mohanta C.L.; Maity T.K.; Karak N. *Biomed. Mater.* **2015**, *2*, 025011.
- Das B.; Chattopadhyay P.; Upadhyay A.; Gupta K.; Mandal M.; Karak N. New J. Chem. 2014, 38, 4300-4311
- Shu X. Z.; Liu Y.; Palumbo F.S.; Luo Y.; Prestwich G. D.; *Biomaterials*, 2014, 25, 1339-1348
- Liu M.; Zeng X.; Ma C.; Yi H.; Ali Z.; Mou X.; Li S.; Deng Y.; He N. Bone Res. 2017, 5, 17014
- 5. Gogoi S.; Kumar M.; Mandal B. B.; Karak N. RSC Adv. 2016, 6, 26066-26076



POSTERS

Ρ1

Development of a Neoteric Melt-Processable Thermoresponsive Self-Healable Elastomer, its Characterization, and its Quantification by a Novel 'Software Imaging' Technique

Poulomi Dasgupta¹, Sayan Basak¹*, Abhijit Bandyopadhyay¹**

¹Department of Polymer Science & Technology, University of Calcutta, 92, A.P.C. Road, Kolkata- 700009, India

¹* Presenting Author Email: sayancupst@gmail.com

¹**Corresponding Author's Email: abpoly@caluniv.ac.in

Abstract

In this study, we had tried to synthesize a propitious Thermoresponsive Self Healable Elastomer using the blends of Thermoplastic Polyurethane (TPU) and Ethyl Vinyl Acetate (EVA). Keeping the industrial and economical friendliness at the backdrop, we used the melt blending technique over the conventional solution mixing. By the same token, since there has been a rising demand for various environmental friendlier processes to fabricate synthetic materials; we strived to be a step ahead in developing our material through an unhackneyed technology of masterbatch.

In addition to the above, we did contrive an original futuristic model in which we had tried to analyze and quantify the healing efficacy of the system by using software imaging. Interestingly, we perceived a relation between the data obtained from the software and the data obtained by the traditional testing methods, which makes our pioneering software technology to investigate the healing phenomenon more viable and operable on an industrial scale.

We tuned the TPU/EVA blend ratio to an optimal one to augment the existing properties, thus bolstering the fact that the subsumption of EVA in the TPU matrix resulted in more controlled and effective healing than the sole TPU matrix. We further anticipate that the embodiment of our methodology in synthesizing our material does have the potential of being scaled up to the industry in terms of sustainability, especially in insulation, electronics, and soft touch application.

Keywords

Thermoplastic Elastomer, Software Imaging, Melt Blend Processing, MasterBatch Technology, Self-Healing, Smart Materials, Stimuli-Responsive Polymers.

P2

Synthesis of PVDF based Graft Copolymers for the Fabrication of Affinity Membrane

Udayan Basak¹*, Radhakanta Ghosh², Tapas Ghosh¹, Mahuya Pakhira², Dhruba P. Chatterjee¹

¹Department of Chemistry, Presidency University, Kolkata, West Bengal – 700073, India ²School of Applied & Interdisciplinary Sciences, IACS, Kolkata, West Bengal – 700072, India *Presenting Author, Email: udayanbasak6@gmail.com

Abstract: A new "grafting from" strategy for grafting of different monomers on commercially available poly(vinylidene fluoride) (PVDF) backbone is designed using Atom Transfer Radical Polymerization (ATRP). Random copolymers of Furfuryl Methacrylate (FMA), Oligoethyleneglycol Methacrylate (OEGMA), Di(ethyleneglycol)methylether Methacrylate (DEGMEM) and n-Butyl Methacrylate (BMA) on PVDF backbone is synthesized by ATRP. The reactive furan rings present in the substitution of grafted PFMA chains are subsequently used as 'dienes' for Diels-Alder cycloaddition reaction with maleimides. This allowed installation of specific H-bonding capable moieties showing complementarity with different nucleobases (like adenine, melamine and uracil etc.). Analysis of polymerization kinetics, molecular weight evolution with monomer conversion and Size Exclusion Chromatography (SEC) has shown a nicely controlled graft copolymerization initiated by PVDF backbone as macroinitiator. ¹H-NMR spectroscopy has been used for structure elucidation and calculation of absolute molecular weight of the graft copolymers. The FTIR analysis indicates shift of PVDF crystallites from α -polymorph to β polymorph with grafting of polymethacrylate chains. A spherulitic morphology of the PVDF which gets shifted to self aggregated spherical morphology in the graft copolymers as observed from FESEM and AFM analysis of the DMF casted solvents. Membrane fabrication by the synthesized graft copolymers are conducted following 'breath figure' followed by 'immersion precipitation' techniques. This results in development of membranes having temperature dependent porosity.

- 1. Samanta, S.; Chatterjee, D.P.; Manna, S.; Mandal, A.; Garai, A.; Nandi, A.K. *Macromolecules* **2009**, *42*, 3112.
- 2. Singh, N.; Husson, S.M.; Zdyrko, B.; Luzinov, I. Journal of membrane science 2005, 262, 81.
- 3. Braga, F. J. C.; Rogero, S. O.; Couto, A. A. Mater. Res. 2007, 10, 247.
- 4. Chen, Y.; Ying, L.; Yu, W.; Kang, E. T.; Neoh, K. G. Macromolecules 2003, 36, 9451.

P3

Cyclic Hypervalent Iodine(III) Reagents as Inimers for the Synthesis of Branched Polymers

Kapil Dev Sayala^{*1}, Rajesh Kumar¹, Nicolay. V. Tsarevsky¹

¹Department of Chemistry, Southern Methodist University, Dallas, Texas-75275, United States of America *Presenting Author, Email: ksayala@smu.edu

Abstract: Novel cyclic hypervalent (HV) iodine(III) compounds containing methacrylic and acrylic moieties, have been synthesized, isolated, characterized by ¹H, ¹³C nuclear magnetic resonance (NMR) spectroscopy and the crystal structures were determined by single crystal X-ray diffraction. Owing to the presence of a polymerizable moiety and an initiating site (I–O bond), they can generate radicals upon ultraviolet (UV) light-induced homolysis, thereby serving as inimers1. These inimers were employed in the synthesis of branched polymers through the popular self-condensing vinyl polymerization approach. The thermal stability of inimers was investigated by thermogravimetry analysis (TGA) and their hydrolytic stability was studied and compared to that of alkoxy analogues. (Co)polymerization was performed under different wavelength UV source with various monomers and also by varying ratio of monomer with respect to inimer. The corresponding polymers were characterized using size exclusion chromatography (SEC). Ongoing research includes determining the degree of branching through Multi-Angle Light Scattering (MALS) analysis and it's correlation with concentration of inimer, UV source wavelength.

Reference:

1. Han, H.; Tsarevsky, N. V. Polym. Chem. 2012, 3, 1910.

Chemical Modification of Polyisoprene using Tetrazole containing Hypervalent Iodine(III) Reagents

Rajesh Kumar¹, Kapil Dev Sayala^{*1}, Nicolay. V. Tsarevsky¹

¹Department of Chemistry, Southern Methodist University, Dallas, Texas-75275, United States of America *Presenting Author, Email: ksayala@smu.edu

Abstract: The modification of cis-1,4-polyisoprene (polyIP), using hypervalent (HV) iodine(III) reagents with various tetrazole ligands (PhI(N4CR)2) (R = CH3, C6H5, 4-CH3-C6H4) in the presence of iodine was found to be a very efficient way to iodotetrazolylate polyIP. The pendant alkyl iodide functionalities were converted to azides by nucleophilic substitution reaction with NaN3 in DMF. The presence of azide groups in the polymers was confirmed by infrared spectroscopy. For the proof of concept, the azido-tetrazolylated polymers were reacted with alkyne-terminated poly(ethylene glycol), PEG, in the presence of CuBr and pentamethyldiethylenetriamine (PMDETA) to yield PEG grafted polymers (products of click coupling). Furthermore, the alkyl iodide functionalities were employed as macro-chain transfer agents for iodine-transfer polymerization (ITP) of methyl methacrylate to synthesize graft copolymers. All the polymers were characterized by 1H and 13C and infrared spectroscopy, size exclusion chromatography, differential scanning calorimetry, and thermo-gravimetric analysis. The results indicated successful modification of polyIP in 10 minutes, opening a new avenue to previously inaccessible functional and reactive (including energetic) materials.

Controlled Synthesis of Nano Structured Polyaniline on Graphene Oxide Sheets for Efficient Energy Storage Application

Tapas Ghosh¹*, Radhakanta Ghosh², Udayan Basak¹, Dhruba P. Chatterjee¹

¹Department of Chemistry, Presidency University, Kolkata, West Bengal – 700073, India ²School of Applied & Interdisciplinary Sciences, IACS, Kolkata, West Bengal – 700072, India *Presenting Author, Email: tapasghosh.orgchem@gmail.com

Abstract: A significant research efforts are devoted for the development of graphene/polyaniline (PANI) hybrid supercapacitor electrode fabrication where integration of capacitive performance of graphene/graphene oxide nano sheet (GNS) and pseudo capacitance of PANI is accomplished. Covalent attachment of PANI chains on GNS surface is acceptably the best way for extracting their maximum synergy.¹ In this respect, it is more desirable strategy to grow PANI chains from GNS surface following a 'grafting from' strategy, as it allows retention of the structural sophistication of the GNS support. However, it requires the growth of PANI chains in a controlled fashion. The literature reports show attempts for growth of PANI chains initiated from monomeric aniline moieties anchored on GNS surface.² However, given the mechanism of PANI, this strategy should result in the formation of significant amount of non-grafted chains from the aniline molecules present in the bulk during oxidative polymerization of aniline. Here we report a new strategy for growth of PANI chains initiated from N,N'-bis(4'-aminophenyl)-1,4-quinonediimine (APQD, a trimer of aniline in emaraldine state) moieties attached on graphene oxide nano sheets. Formation of very interesting 'marigold' flower like structures or 'agave' plant like structure is frequently observed in cases of covalently attached nano composite (GOTP) which gives capacitance value 1303 F/g with 86% cyclic stability compared to noncovalently attached GOP giving capacitance value 610 F/g with 62% cyclic stability.

- 1. Ghosh, T.; Ghosh, R.; Basak, U.; Majumdar, S.; Ball, R.; Mandal, D.; Nandy, A.K.; Chatterjee, D.P. *J.Mater. Chem. A*, **2018**, *6*, 6476.
- 2. Kumar, N. A.; Choi, H.-J.; Shin, Y.R.; Chang, D. W.; Dai, L.; Baek, J.-B. ACS Nano 2012, 6, 1715.

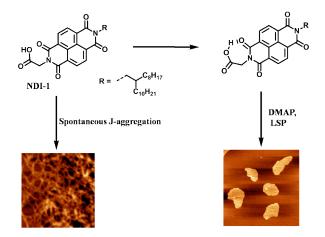
Organobase Triggered Controlled Supramolecular Ring Opening Polymerization and 2D Assembly

Anwesha Chakraborty^{*}, Goutam Ghosh, Suhrit Ghosh

School of Applied and Interdisciplinary Sciences, Indian Association for the Cultivation of Sciences, Kolkata, West Bengal-700032, India *Email: psuac2@iacs.res.in

Abstract: Supramolecular polymers albeit having an internal order are far behind to their covalent counterpart in terms of macroscopic structural precision and also the existing methodologies lack the ability to synthesize block copolymer or end-functionalized

Such possibilities have been chains. recently explored in the emerging synthetic technique known controlled as supramolecular polymerization (CSP)¹. In almost all cases, CSP has been demonstrated using a seed as the initiating site which unfortunately is not a molecular entity, rather a small fragment of a preformed aggregate. We have recently explored molecule (not seed) triggered CSP of NDI-1 which spontaneously forms fibrillar network in decane. On the other



hand, by fine-tuning the sample preparation condition, the carboxylic acid groups can be arrested by intra-molecular H-bond with the adjacent imide carbonyl (in the same solvent and concentration) which the which retards the spontaneous aggregation. In presence of catalytic amount of DBU or DMAP, the meta-stable monomer exhibits supramolecular polymerization through a thermodynamically controlled pathway involving simultaneous H-bonding and π -stacking and generates ultra-thin 2D nano-sheet. in sharp contrast to the spontaneously assembled fibers. Mechanistic investigation suggested, DMAP/DBU helps in ring-opening of the intra-molecularly H-bonded monomer and *in situ* breeds the free acid, which, beyond a critical concentration, initiates controlled supramolecular ring opening polymerization (SROP) via chain-growth mechanism. It appears in this case, the stacking involves monomeric uni-directional orientation allowing simultaneous H-bonding and π -stacking. The average size of the sheets could be systematically varied by changing concentration of organo-base. The pre-formed nano-sheet, when used as a macro-initiator to polymerize a fresh batch of monomer, produced larger sheets confirming livingness of this polymerization.

Reference:

1. Zwaag D. van der, de Greef T. F. A., Meijer E. W. Angew. Chem. Int. Ed. 2015, 54, 8334-8336.

Synthesis of Covalently Connected Graphene Oxide-g-Chiral Polyaniline Nanocomposite with Improved Energy Storage

Ranjit Das¹*, Tapas Ghosh², Subhadip Roy³, Dhruba P. Chatterjee⁴

¹Department of Chemistry, Presidency University, Kolkata, West Bengal-700073, India *Presenting Author, Email: ranjitdas23051995@gmail.com

Abstract: The present work reports enantioselective synthesis of chiral PANI chains covalently attached on GO sheets. This is a first time report for the synthesis of carbon PANI based chiral nano composite with predetermined chirality and halicity at the PANI chains. GO nano sheet attached with oligomer aniline moieties are used for initiation of PANI chains in an oxidative polymerization at aniline, in presence of optically pure dopants like L-CSA or D-CSA. Interestingly it is observed that growth at chiral PANI chains does not occur when aniline oligomer attached carbon nano dots are used inhibitors. Therefore a significant effect at the architecture at the carbon nano materials is there. Furthermore lie degree of chiral induction has been found to increase manifold when PANI is synthesized in presence of oligomers. Measurements of electrochemical properties of GO-g-PANI nano composite have shown much improvement compared to the achiral or non-covalently attached composite material. This has been attributed to the better synergy between GO and PANI components when covalently attached and possible greater exposed surface area at helical PANI chains compare to the agglomerates fibrous PANI chains.

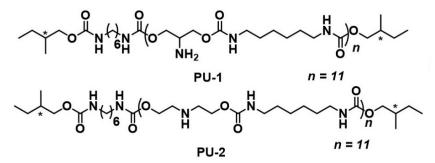
- 1. Ghosh, T.; Ghosh, R.; .Basak, U.; Masumder, S.; Ball, R.; Mondal, D.; Nandi, A.K.; Chatterjee, D.P. *J.Mater.Chem.A.* **2018**, *6*, 6476.
- 2. Moutet, J. C.; Saintaman, E.; Tranvan, F.; Angibeaud, P. Utille, J. P. AdV. Mater. 1992, 4, 7.
- 3. Bross, P. A.; Schoberl, U.; Daub, J. AdV. Mater. 1991, 3, 198.

Antimicrobial Polyurethane with Selective Activity against E. coli

Ranajit Barman*, Tathagata Mondal, Jayita Sarkar, Amrita sikder and Suhrit Ghosh

School of Applied and Interdisciplinary Sciences, Indian Association for the Cultivation of Science, Kolkata, West Bengal-700032, India *Presenting Author, Email: ranajitbarman1993@gmail.com

Abstract: Antibacterial polymers have been extensively studied in the recent past.¹ Herein we report antimicrobial activity of two segmented amphiphilic polyurethanes PU-1 and PU-2, containing a primary or secondary amine group, respectively. In acidic water, intra-chain H-bonding among the urethanes followed by hierarchical assembly resulted in formation of capsules ($D_{\rm h} = 100-120$ nm) with highly positive surface charge.



Antimicrobial studies with *E. coli*. revealed very low MIC values of 7.8 µg/ mL and 15.6 µg/ mL for PU-1 and PU-2, respectively, indicating their ability to efficiently kill Gram negative bacteria. Killing of Gram positive *S. aureus* was noticed only at $C = 500 \mu$ g/ mL, indicating unprecedented selectivity for *E. coli* which was further confirmed by SEM studies. Hemolysis assay revealed HC₅₀ values of 453 and 847 µg/ mL, for PU-1 and PU-2 respectively, which are > 50 times higher than their respective MIC values and thus make them attractive antimicrobial material. ONPG assay and live-dead fluorescence assay confirmed that for both of the polymers, the membrane disruption pathway was operative for wrapping of the bacterial membrane, similar to what has been proposed for the antimicrobial peptides. SEM images of polymer treated *E. coli* bacteria helped in visualization of the pore formation and disrupted membrane structure.

Reference:

1. Konai, M. M.; Bhattacharjee, B.; Ghosh. S.; Haldar, J. Biomacromolecules 2018, 19, 1888.

Tryptophan-Based Polymeric chemosensor for sensing and removal of Cu(II) and Hg(II) from aqueous media

Neha Choudhury, Priyadarsi De*

Polymer Research Centre and Centre for Advanced Functional Materials, Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur - 741246, Nadia, West Bengal, India. *CorrespondingAuthor, Email: p_de@iiserkol.ac.in

Abstract: A tryptophan-based fluorescent polymeric sensor has been synthesized, targeting selective sensing and removal of toxic metal ions from aqueous media. The sensor is highly responsive to both Cu(II) and Hg(II) in neutral aqueous solution and displays excellent selectivity in the presence of various competing metal ions. Further addition of Cu(II) ion causes a colorimetric change from yellow to green, providing a simple and effective method for distinguishing solutions containingCu(II) and Hg(II). Both Cu(II) and Hg(II) are trapped when they are passed through a column containing polymeric sensor.

- 1. Choudhury, N.; Mete, S.; Kambalapalli, S.; De, P. J. Polym. Sci., Part A: Polym. Chem. 2018, 56,914.
- 2. Choudhury, N.; Saha, B.; Ruidas, B.; De, P.ACS Appl. Polym. Mater. 2019, 1, 461.

A Simple Strategy for the gram-scale Synthesis of Graphene Quantum Dot with Unique Optical Property

Subhadip Roy¹ *, Tapas Ghosh¹, Dhruba P. Chatterjee¹

¹ Department of Chemistry, Presidency University, Kolkata, West Bengal – 700073, India, *Presenting Author, Email: roysubhadip1234@gmail.com

Abstract: The present work reports an oxidative cutting route to synthesize Graphene Quantum Dots (GQD) from Graphene oxide (GO) prepared from graphitic flakes using a modified Hummer's method. Oxidation carried out with 70% HNO3 at 80°C for 12 hr and then GQD particles are collected from the supernatant solution after size separation. The method allows gram-scale synthesis of GQD which are highly soluble (>40gm/L) with tremendous solubility (more than ~ 6 months). The aqueous GQD solution shows a green fluorescent with quantum yield (\emptyset %) of ~ 4% which increase to ~ 11% upon reduction with NaBH₄. A tremendous effect of medium pH on the optical properties of the aqueous GQD solution is observed .Under acidic condition (pH=2-4) green light emission is observed with maximum intensity when exited at 460 nm. However, as the alkali solution is added medium pH sharply increases from 4 to 13 showing a blue shift in the absorption from 350 nm to 275 nm along with a similar blue shift of PL maximum to 438 nm under excitation at 348 nm. In addition to it a new signal is developed at 625 nm with maximum intensity when excited at \sim 540 nm. All the GQD solution irrespective of the medium pH has shown excitation dependent PL emission, which is a signature of carbon quantum dots. The change in optical properties at the aqueous GQD solution with pH variation is very much reversible and is visually observed by of the solution colour from light orange to dark orange. The variation in colour very much resembles the changes as observed with acid-base indicators (i.e. like phenolphthalein). An explanation for the probable reason behind the change in optical properties with medium pH has been forward.

- 1. Konstantatos, G.; Badioli, M.; Gaudreau, L.; Osmond, J.; Bernechea, M.; De Arquer, F. P. G.; Gatti, F. and F. H. L. Koppens, F. H. L. *Nat. Nanotech.*, **2012**, *7*, 363-368.
- Song, S. H.; Jang, M. H.; Jeong, J.M.; Yoon, H.; Cho, Y. H.; Jeong, W. I.; Kim, B. H and Jeon, S.; *Chem. Commun.* 2015, *51*, 8041-8043.

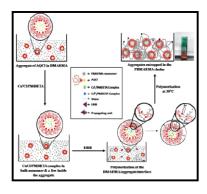
Synthesis of Living poly (2-Dimethylaminoethyl Methacrylate) by Solvent Free ATRP in Ambient Temperature

Tuhin Ghosh^{3*}, Udayan Basak¹, Radhakanta Ghosh², Dhruba Prosad Chatterjee¹

Department of Chemistry, Presidency University, Kolkata, West Bengal, 700073, India ² School of Material Science, IACS, Jadavpur, Kolkata, West Bengal, 700032, India ³ Departmentof Chemistry, Durgapur Government College, Durgapur, West Bengal, 713214, India

*Presenting author's e-mail: tuhinghoshbuchem@gmail.com

Abstract: Living poly(2-dimethylaminoethyl methacrylate) (PDMA) has been synthesized by Atom Transfer Radical Polymerization (ATRP) of 2-dimethylaminoethyl methacrylate (DMA) in bulk at 30°C using CuCl/*N*,*N*,*N'*,*N''*-pentamethyldiethylenetriamine (PMDETA) catalyst.^{[1],[2]} Addition of catalytic amount of tricaprylylmethylammonium chloride (Aliquat[®]336)(AQCl) keeps the deactivator cupric complex soluble throughout the polymerization. The solubility of the charged cuprous/cupric complexes in bulk DMA is proposed through their entrapment within the ionic core of the reverse micelle like aggregates formed by AQCl in DMA medium, as observed from dynamic light scattering analysis.^[3] Synthesized PDMA molecules have been successfully chain extended with different methacrylate monomers in one pot for the synthesis of various stimuli responsive, multifunctional di- or triblock copolymers.^[4] An adventitious role of water molecules in respect of kinetics and control over polymerization is noted when moist monomer or AQCl is taken for reaction.



- 1. Matyjaszewski, K.; Xia, J. Atom Transfer Radical Polymerization. Chem. Rev.2001, 101, 2921.
- 2. Coessens, V.; Pintauer, T.; Matyjaszewski, K. Functional polymers by atom transfer radical polymerization. *Prog. Polym. Sci.*2001, *26*, 337.
- 3. Starks, C. M.; Liotta, C. L.; Halpern, M. *Phase-Transfer Catalyst, Fundamentals, Applications and Industrial Perspectives,* 2nd ed.; Chapman & Hall: New York, 1994.
- 4. Pantoustier, N.; Moins, S.; Wautier, M.; Deqee, P.; Dubois, P. Solvent-free synthesis and purification of poly [2-(dimethylamino)ethyl methacrylate] by atom transfer radical polymerization. *Chem. Comm.* **2003**, 340.

Multitasking single-crystal-to-single-crystal /solid state photopolymerization

Ranita Samanta¹*, Subhrokoli Ghosh², Dachi Kitagawa³, Rajadurai Chandrasekar⁴, C Malla Reddy¹

¹Department of Chemical Sciences, India Institute of Science Education and Research Kolkata, Mohanpur, West Bengal-741246, India
 ²Department of Physical Sciences, India Institute of Science Education and Research Kolkata, Mohanpur, West Bengal-741246, India
 ³Department of Applied Chemistry, Graduate School of Engineering, Osaka City University, 3-3-138 Sugimoto, Sumiyoshi-ku, Osaka558-8585, Japan
 ⁴School of Chemistry, University of Hyderabad, Gachibowli, Hyderabad, Telangana-500046, India
 * Email: samantaranita@gmail.com

Abstract: In the recent years, mechanical work converted from energy like light, heat by stimuli responsive materials has attracted attention due to their potential application in optoelectronics, sensors, actuators etc. Furthermore, in this connection, if those materials are of photochromic in nature, they might be used in multitusking forms like single crystal heterostructure formation, inkless printing mataerial, sequrity code genaration as well. This work presents one such multitasking material as discussed below.

We have prepared1,1'-dioxo-1H-2,2'-biindene-3,3'-diyl didodecanoate (BIT-dodeca₂), which is a photochromatic molecule. This molecule undergoes single-crystal-to-single-crystal polymerization reaction under sun light/visible as well as UV light. This study exhibits the possibility of utilization of topochemical polymerization reactions for photomechanical actuation. The results presented here demonstrate how a chemical reaction with high yield can be used to prepare a mechanically responsive crystal. It paves the way for the development of other bending crystals using other photochemical reactions associated with high yield and crystal integrity. Here we have demonstrated how the single crystal of above photochromic compound, BIT-dodeca₂ can be converted to single crystal monomer-polymer microrods as well. This switching property can be used in one time readable digital binary memory devices. Moreover, this can also be used as an inkless printing material and for developing QR code.

- 1. Samanta, R.; Ghosh, S.; Devarapalli, R.; Reddy, C. M. Chem. Matter. 2018, 30, 577-581.
- 2. Garai, B.; Mallick, A.; Banerjee, R. Chem. Sci.2016, 7, 2195-2200.
- 3. Dou, L.; Zheng, Y.; Shen, X.; Wu, G.; Fields, K.; Hsu, W.; Zhou, H.; Yang, Y.; Wudl, F. Science 2014, 343, 272-277.

Modified starch-based graft copolymeric flocculant for treatment of blast furnace effluent

Priyapratim Patra¹, Suprotim Das² and Sagar Pal¹*

¹Deaprtment of Chemistry, Indian Institute of Technology (ISM), Dhanbad, Jharkhand-826004, India ²Environmental Research Group (R&D), Tata Steel India Ltd., Jamshedpur, India *Presenting Author, Email: patrapriyapratim@gmail.com

Abstract: Recently, a high-performancefunctionalized starch-based flocculant has been developed at authors' laboratory.¹ The starch has been grafted with polyacrylamide (PAAm) and poly (2-methacryloyloxy ethyl trimethyl ammonium chloride) (PMETAC) through free radical polymerization. The developed flocculant has been characterized using several sophisticated materials characterization techniques. Finally, the developed copolymer demonstrates an excellent efficiency as a flocculant for the treatment of industrial blast furnace effluent (of Tata Steel, Jamshedpur).

Reference:

1. Das, S; Patra, P.; Singha, K; Biswas, P; Sarkar, S;Pal, S.Int. J. Biol. Macromol. 2019, 125, 35-40.

Supramolecular Assembly by Orthogonal Hydrogen and Halogen Bonding

A. Jamadar* and A. Das

School of Applied and Interdisciplinary Sciences, Indian Association for the Cultivation of Science, Kolkata- 700 032, India

Abstract: Supramolecular polymers, which are polymers based on monomeric units held together with directional and reversible secondary interactions. Due to their reversible nature, supramolecular polymers can adopt unique properties, such as adaptability, recyclability, and self-healing characteristics, which makes them interesting for various applications. Multi-component self-assembly, in which several distinct molecular motifs are associated together by specific non-covalent interactions offers a superior strategy for creating functional supramolecular polymers with higher degree of complexity and advanced properties. Such complex systems can be achieved by rationally employing multiple non-covalent interactions operating simultaneously and orthogonally i.e. without interfering with each other. Such strategies have been used with orthogonal hydrogen-bonding and pi-stacking, metal-ligand coordination and host-guest complexation etc. It is known to be superior to extensively investigate hydrogen-bonding in terms of directionality. Halogen-bonding has recently emerged as a powerful tool for specific molecular interactions. Orthogonal self-assembly of hydrogen- and halogen-bonding motifs is a unique and interesting combination for constructing functional supramolecular polymeric materials.

In the present work we demonstrate a novel design principle for creating stimuli-responsive supramolecular graft copolymers where the macromolecular backbone is constructed by hydrogen bonding and pi-stacking while orthogonal halogen bonding play a structural supporting role for grafting polymeric side chains to the backbone. Our preliminary results reveal that such orthogonal assembly not only contributes to the fabrication of the 2D architectures but also enhances the inherent stability of the copolymer in aqueous phase. Synthesis, self-assembly studies, stimuli-responsive behavior and future implications of this system will be the topic of this poster presentation.

- Mes, T.; Smulders, M. M. J.; Palmans, A. R. A.; Meijer, E. W. Macromolecules, 2010, 43, 1981-1991.
- 2. Wei, P.; Yan, X.; Huang, F. Chem. Soc. Rev. 2015, 44, 815-832.
- 3. Priimagi A.; Cavallo, G.; Metrangolo, P.; Resnati, G. Acc. Chem. Res. 2013, 46, 2686-2695.
- 4. Vanderkooy, A.; Taylor, M. S. J. Am. Chem. Soc., 2015, 137, 5080-5086.
- 5. Hofmeier, H.; Schubert, U. S. Chem. Commun., 2005, 2423-2432.

Modulation of Side Chain Crystallinity in Fatty Acid and MethoxyPoly(ethylene glycol) Containing Alternating Copolymers

Krishna Gopal Goswami,[‡]Sourav Mete,[‡] and Priyadarsi De*

Polymer Research Centre and Centre for Advanced Functional Materials, Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur - 741246, Nadia, West Bengal, India *Corresponding author: email: p_de@iiserkol.ac.in

‡ These authors contributed equally to this work.

Abstract: Several crystalline alternatingcopolymers are synthesized through reversible addition-fragmentation chain transfer (RAFT) polymerization fatty acid-based maleimide (**MF**) and methoxypoly(ethylene glycol) (mPEG) attachedstyrenic (**VBP**) monomers. The alternating placement of the two monomers throughout the polymer main chain is systematically established through both ¹H and ¹³C NMR spectroscopic analysis.¹ The copolymers form a well-ordered lamellar morphologywith alternate layer of mPEG and fatty acid alkyl segment.² Small-angle X-ray scattering (SAXS) analysis denotes a gradual increase of inter-lamellar spacing (*d*) as a result of enhancing the mPEG chain lengths. The existences of a lamellar pattern as well as a higher order periodicity were evidenced from atomic force microscopy (AFM) and transmission electron microscopy (TEM) micrographs. Remarkably, differential scanning calorimetry (DSC) thermogramsshow a regularvariation of crystalline melting temperature (T_m) corresponding to a fixed length of fatty acid segments with increasing the mPEG chain lengths. The current approach has significant usefulness towards the regulation of side chain crystallinity in synthesized polymeric materials.

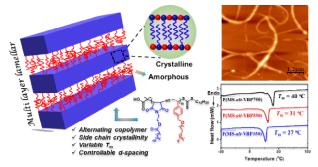


Figure 1. Formation of multilayer structure and the variation of T_m values in the crystalline copolymers.

- 1. Ha, N. T. H. Polymer 1999, 40, 1081-1086.
- Hattori, G.; Takenaka, M.; Sawamoto, M.; Terashima, T. J. Am. Chem. Soc. 2018, 140, 8376-8379

Dendron Conjugated Carbon Quantum Dot for Selective detection of Breast Cancer and Gene Therapy

Krishanu Ghosal¹*, Shantanu Ghosh¹, Kishor Sarkar¹

¹Gene Therapy and Tissue Engineering Lab, Department of Polymer Science and Technology, University of Calcutta, 92, A.P.C. Road, Kolkata- 700009 *Presenting Author, Email: krishanughosal01@gmail.com

Abstract: Breast cancer is the second leading cause of death in women worldwide. Among the different types of breast cancers diagnosed, triple negative breast cancer (TNBC) is the most fatal subtype among all other types of breast cancer due to lack of estrogen receptor (ER), progesterone receptor (PR) and human epidermal growth factor receptor-2 (HER-2). It is observed that Memo is an essential enzyme for the breast cancer cell motility in association of various receptor tyrosine kinases. It is further noticed that Memo increases the local reactive oxygen species (ROS) production only in the presence of Cu(II) ion among the eight different cations and results cell migration and finally metastasis [1]. Therefore, Cu(II) ion has an important role on tumor growth and angiogenesis. Over the last few years, carbon quantum dots (CQDs) have gained marvelous attention due to its exceptional water solubility, low toxicity, ease of synthesis and functionalization, exceptional photoluminescence (PL) and optical properties and large scale of production with low cost [2,3]. Herein, we developed a targeted non-viral vector which could efficiently deliver the gene of interest and could also diagnose of TNBC. We have synthesized CQD from sweet lemon peel followed by conjugation with different generation of polyamidoamine (PAMAM) dendrimers to get CD-PAMAM conjugates (CDPs). RGDS peptide was further conjugated to CDP to target $\alpha_{\nu}\beta_{\beta}$ integrin which is over expressed in TNBC. DNA complexation assay, cellular cytotoxicity, hemolysis assay, DNase I assay, cellular uptake and *in vitro* transfection showed CDP3 as a promising gene carrier system TNBC gene therapy. Besides, CDP3 shows selective quenching of fluorescence in presences of Cu(II) with a quenching efficiency of about 93%. As the Cu(II) ion concentration remains up-regulated in TNBC. Therefore, CDP3 could be a promising theranostic tool for TNBC treatment.

- 1. MacDonald, G.; Nalvarte, I. et al. (2014) Sci. Signal. 7, ra56-ra56.
- Ghosh, S.; Ghosal, K.; Mohammad, A. Sk.; Sarkar, K. (2019). Chemical Engineering Journal, 373, 468-484.
- 3. Ghosal, K.; Sarkar, K. (2018), ACS Biomaterials Science & Engineering. 4, 2653-2703.

RAFT Polymerized Amino Acid Based Cationic Polymer for Excellent Gene Transfection Efficiency in Triple Negative Breast Cancer

Rima Saha^{*}, Kishor Sarkar[†]

Gene Therapy and Tissue Engineering Lab, Department of Polymer Science and Technology University of Calcutta, 92, A.P.C. Road, Kolkata-7 00 009, India * Email: saharima188@gmail.com †Corresponding author, Email: kishorpst@gmail.com

Abstract: Over the last few decade, gene therapy has become promising modern therapeutic tool to treat incurable genetic diseases from Alzheimer to cardiovascular problems to cancer. Despite the remarkable transfection efficiency of viral vectors, severe toxicity, immunogenicity and high production cost limit its clinical application. Polymeric nonviral vectors have shown extensive interest due to its comparatively low toxicity, ease of production and nonimmunogenicity [1-4]. However poor transfection efficiency limits its clinical application. Reversible addition–fragmentation chain-transfer (RAFT) polymerization has gained tremendous attention due to its wide range of functional monomers, reaction media, narrow molecular weight distribution and lack of toxic metals as used in ATRP.

In this work, we synthesized brush polymers using glycine, leucine and phenyalanine amino acids conjugated with hydroxyethylmethacrylate (HEMA) monomer. Polymer/pDNA complex (polyplex) formation was determined by agarose gel electrophoresis assay, DLS and TEM. *In vitro* toxicity assay and transfection efficiency were performed on MDA-MB-231 triple negative breast cancer cell. Blood compatibility of the polymers was confirmed by hemolytic assay.

In vitro toxicity and hemolytic assay showed that the polymers are totally nontoxic and blood compatible even at very high concentration. The polymers also showed extensively high pDNAcomplexation capability at very low N/P ratio although it was dependent on types of amino acids. Apart from these, the polymers showed excellent gene transfection efficiency against triple negative breast cancer.

Therefore, the amino acid based polymers may be attractive candidate for cancer gene therapy application.

- 1. Ghosh, S.; Ghosal, K.; Mohammad, A. Sk.; Sarkar, K.* Chem. Eng. J. 2019, 373, 468.
- 2. Sarkar, K.; Meka, S. R. K.; Madras, G; Chatterjee, K. RSC Adv. 2015, 111, 91619.
- 3. Sarkar, K.; Madras, G., Chatterjee, K. RSC Adv. 2015, 5, 50196.
- 4. Sarkar, K.; Banerjee, S. L.; Kundu, P.P.; Madras, G., Chatterjee, K. J. Mater. Chem. B. 2015, 3, 5266.

Carbon Dot Functionalized Nanoengineered Template for Targeted Doxorubicin Delivery to Triple Negative Breast Cancer

Priyatosh Sarkar, Shantanu Ghosh, Kishor Sarkar*

Gene Therapy and Tissue Engineering Lab, Department of Polymer Science and Technology University of Calcutta, 92, A.P.C. Road, Kolkata-7 00 009, India *Email: kishorpst@gmail.com/kspoly@caluniv.ac.in *Presenting Author, Email: pspst rs@caluniv.ac.in

Abstract: Triple negative breast cancer (TNBC) is the most fatal subtype among all other types of breast cancer due to lack of estrogen receptor (ER), progesterone receptor (PR) and human epidermal growth factor receptor-2 (HER-2). Despite the advancement of clinical research, chemotherapy still remain most popular therapeutic approach for cancer treatment. Among the various chemotherapeutic drugs, doxorubicin (DOX) still holds its popularity over decades. But, drug-related toxicity and multi drug resistance (MDR) of DOX based cancer therapy are the major concern to the clinicians. Targeted DOX delivery may reduce unwanted toxicity to normal cell. Recently image guided drug delivery system has received tremendous attention due to tracking capability of the drug to the target site of disease [1,2]. The inherent fluorescence property, nontoxicity and water solubility of carbon dot (CD) show widespread application in biomedical field [3]. Due to the over expression of folate receptor on cancer cell surface, folic acid derived CD may be an attractive cancer targeted and imaging probe for DOX delivery system.

Here, we have synthesized lipid conjugated polyethyleneimine (PEI) amphiphilic polymer with various mole ratio followed by conjugation of folic acid derived CD. The synthesis was confirmed by NMR, IR, XRD, SEM, TEM, fluorescence spectrophotometer, DLS etc. DOX loaded amphiphilic polymeric nanomicelle was characterized by UV spectroscopy and TEM. The amphiphilic nanomicelle showed the size of 50-100 nm with spherical morphology. Uptake study of the CD conjugated micelles were performed using MDA-MB231 cell lines under CLSM. Then the carbon dot tagged micelles were loaded with dox and subjected to MTT assay. As the loading value suggested the 1 μ g/ml of the formulation should contain 0.04 microgram of DOX and this amount could produce a similar result as free Dox could do it at 10 μ g/ml. So it clearly signify the capability of the formulation which results in 250 fold more activity than the free Dox.

- 1. Sarkar, K.; Meka, S. R. K. et al. (2015). RSC Advances, 5(111), 91619-91632.
- 2. Sarkar, K.; Banerjee, S. L. et al. (2015) Journal of Materials Chemistry B, 3(26), 5266-5276.
- 3. Ghosh, S.; Ghosal, K.; Mohammad, A. Sk.; Sarkar, K.* (2019). Chemical Engineering Journal, 373, 468-484.

P19 Targeted Gene Therapy for Hepatocellular Carcinoma by Gelatin Based Silver Nanoparticle

Shuvam Ghosh^{1*}, Pratik Das^{1,2}and KishorSarkar^{1†}

¹Gene Therapy and Tissue Engineering Lab, Department of Polymer Science and Technology University of Calcutta, 92, A.P.C. Road, Kolkata-700009, India ²Department of Biomedical Engineering, Jadavpur University, Kolkata 700032, India, *Email:shuvamg.ghosh@gmail.com [†]Email: kishorpst@gmail.com/kspoly@caluniv.ac.in

Abstract: Hepatocellular carcinoma (HCC) is the 3rd leading cause of cancer related death worldwide. Among various therapies, chemotherapy is still endured most attractive therapies for HCC patients, although it possesses severe side-effects and dose limitation. Recently silver nanoparticles (AgNPs) have received superior attention owing to its unique inherent antibacterial activities. Recent study of AgNPs showed anticancer effect though apoptotic cell death. Gene therapy has been emerged as a potential approach for treatment of cancer. Therefore, the hypothesis of the present work was to targeted therapeutic gene delivery with the aid of AgNPs for bimodal therapy of HCC patients using the inherent anticancer effect of AgNPs. Due to over expression of the tri-peptide, Arg-Gly-Asp (RGD) receptor integrin receptors, especially $\alpha_{\nu}\beta_{3}$ and $\alpha_{\nu}\beta_{5}$ on the angiogenic endothelium cells of HCC, RGD peptide decorated gene carrier may be a promising for HCC therapy [1, 2, 3].

Gelatin based AgNPs (GT-AgNP) were synthesized in one-pot green synthesis method without using any toxic reducing agents or solvents and the AgNP synthesis was confirmed by UV spectrophotometer, DLS, FTIR and transmission electron microscopy (TEM). The toxicity of AgNPs was observed on HepG2 and HeLa cell lines. The pDNA complexation was carried out low molecular weight polyethyleneimine functionalized GT-AgNPs and was confirmed by agarose gel electrophoresis.

Interestingly, GT-AgNPs showed severe toxicity on different cell lines. The one-pot facile green synthesis of gelatin based AgNPs might be an efficient nanomedicine for the treatment of HCC patients.

- 1. Ghosh, S.; Ghosal, K.; Mohammad, A. Sk.; Sarkar, K. *Chemical Engineering Journal.* **2019**, 373,468-484.
- 2. Sarkar, K.; Meka, S. R. K. et al. *RSCAdvances*. 2015, 5(111), 91619-91632.
- 3. Sarkar, K.; Banerjee, S. L. et al. Journal of Materials Chemistry B. 2015, 3(26), 5266-5276.

P20 Design of Malonic Acid Based Linker and ConjugatedAmphiphilic Theranostic System for Effective Cancer Therapy

Tapan K. Dash^{1*}, Diptendu Patra¹ and Raja Shunmugam¹

¹Polymer Research Centre, Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur, Nadia, West Bengal. *Presenting Author, Email:polyraja@gmail.com

Abstract: Progressive research led to development of different branches of polymeric drug delivery out of which theranostic system which combine therapeutic and diagnostic is gaining significant attention over the past decade. Here we developed novel malonic acid based linker to enrich a polymeric system with cobalt based MRI contrast agent and targeting moiety along with chemotherapeutic agent.¹ Amphiphilicity of the system was a feature by design that contains hydrophobic undecanoic chain and PEG-folate as hydrophilic targeting moiety. Amphiphilicity was optimized by altering different PEG chain length between (0.6-6.0 kD). All the synthetic intermediates were confirmed by standard analytical technique. From pyrene aggregation studies, the system with PEG 4K was found to be much stable with CMC of 63 μ g/mL. Relaxation of water molecule in presence of developed system was analyzed to ensure MRI capability of synthesized macromolecule.²In vitro uptake was dependent of folate mediated endocytosis phenomenon. cell viability assay showed dose dependent cytotoxicity of the macromolecule comparable to that of small molecule. The newly developed system is expected to have much significant contribution in development of targeted theranostic system.

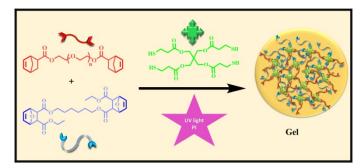
- 1. Kuznik, N.; Wyskocka, M. Eur J Inorg Chem. 2016, 2016, 445-458.
- 2. Patra, D.; Mukherjee, S.; Chakraborty, I.; Dash, T. K.; Senapati, S.; Bhattacharyya, R.; Shunmugam, R. *ACS BiomaterSciEngg*.**2018**, 4, 1738-1749.

P21 A Study on the Effect of PEG in the Thiol-norbornene Crosslinked Network for the Removal of Toxic Cationic Dye

Sayantani Bhattacharya and Raja Shunmugam*

Centre for Advanced Functional Materials, Polymer Research Centre, Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur, West Bengal, 741246, India, *Email: sraja@iiserkol.ac.in

Abstract: With the aim to develop a chemical adsorbent that is inherently non-toxic to living things and the environment, we have synthesised gel systems based on thiolnorbornene photo click reactions. Norbornene is functionalised with different PEG chains to produce PEG funtionalised cross-linkers. The effect of having PEG in the cross-linked network is evaluated on the basis of their toxicant removing efficiency. Characterisation of all the cross-linkers are carried out by standard spectroscopic and analytical techniques. The gels show excellent swelling in organic solvents which increased with increase in PEG chain length. The rheological measurements of the as synthesised materials also exhibit the presence of elasticity in the network. The materials possess excellent thermal stability as revealed from TGA analysis. The kinetics of the dye removal is studied. The results indicate that the dye removal proceeds via pseudo-second-order kinetics. The study of adsorption isotherm of the removal process indicate that the adsorption follows Langmuir isotherm model. To the best of our knowledge, this is the first report unfolding the effect of having PEG in the norbornene backbone which show excellent efficiency towards removal of toxic cationic dye from wastewater.



Cartoon representation of synthesis scheme of the gel

- 1. Bhattacharya, S.; Nair, A.; Bag, A.; Ghorai, P. K.; Shunmugam, R. *MOJ Research Review*. **2019**, *2*, 69.
- 2. Kumar, R.; Shunmugam, R. ACS Omega 2017, 2, 4100.

P22 The Role of Aliphatic chains on Crystallinity of Fatty Acid Containing Styrenic Polyperoxides

Sourav Mete and Priyadarsi De*

Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur -741246, Nadia, West Bengal, India *Corresponding author E-mail: p de@iiserkol.ac.in

Abstract: Vinyl polyperoxides belong to an important class of degradable polymers, which is alternating copolymers of vinyl monomers and molecular oxygen. Polyperoxide contains flexible peroxy (-O-O-) bonds in the back bone due to that they are commonly viscous amorphous material. In the present study, crystalline polyperoxides have been synthesized by radical oxidative polymerization from styrenic monomers having fatty acid moieties attached to the phenyl ring at 100 psi of molecular oxygen pressure. The ¹³CNMR spectroscopy and electron impact mass spectroscopy (EI-MS) have been employed to confirm the alternating placement of -O-O- bonds in the copolymer main chain. From differential scanning calorimetry (DSC), it was observed that polyperoxide degrades highly exothermically and resulting degradations products have been identified from EI-MS study. Strikingly, DSC thermograms reveal a gradual enhancement of crystalline melting temperature (T_m) with the increase of fatty acid chain lengths. The crystalline behaviour of the polymer was investigated from powder X-ray diffraction (PXRD) studies. The crystalline morphology and thelattice thickness of the polymer was obtained from polarized optical microscopy (POM) and transmission electron microscope (TEM), respectivelywhich exemplify a lamellar morphology in the resulting polymers. Theoretical studies have been performed by density functional theory (DFT) to support the experimental interlamellar distance from PXRD studies.

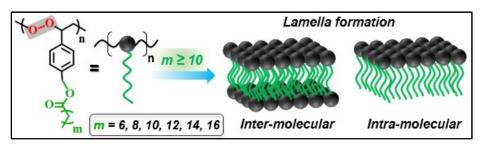


Figure 1. Crystalline domain formation in the polyperoxides.

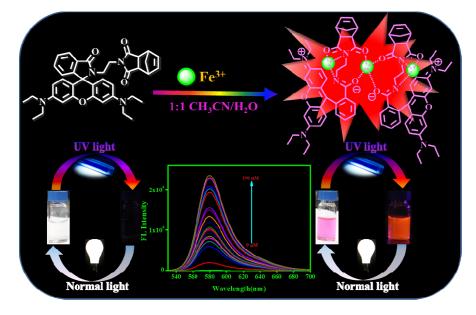
- 1. Matsumoto, A.; Higashi, H. Macromolecules 2000, 33, 1651.
- Mandal, J.; Krishna Prasad, S.; Shankar Rao, D. S.; Ramakrishnan, S. J. Am. Chem. Soc. 2014, 136, 2538.

P23 Poly-Norbornene coupled Rhodamine-B Derivative as an Excellent Fe(III) ion Chemodosimeter in Semi-aqueous medium: A Colorimetric and Fuorimetric Approach

Tapendu Samanta and Raja Shunmugam^{*}

Polymer Research Centre, Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, West Bengal, Mohanpur-741246, India *Tapendusamanta, Email: totapendu@gmail.com

Abstract: Norbornene based rhodamine derivative (**NR**) was observed as an "off-on" probe for Fe³⁺ion both colorimetrically and fluorimetrically in aqueous environment. **NR** and it'shomopolymer(**PNR**) were capable of detecting Fe³⁺ion with high selectivity and sensitivity in aqueousenvironment. For **NR** and **PNR** the limit of detection (LOD) towards Fe³⁺ionwas found to be 49 nM and 19 nM respectively, which made these materials very efficient. Most interestingly **PNR**had more efficacies for the detection of Fe³⁺ ions than **NR** which is expected due to the favourable side chain interaction due to the presence of multiple sensing motifs between the polymer chains. Sensing behaviour was thoroughly studied using spectroscopic techniques. Fe³⁺-**NR** ratios as well as binding sites were supported by theoreitical studies. We hypothesized that Fe³⁺ion was expected to induce the spirolactam ring opening of rhodamine unit due to it's Lewis acid nature and preferable interacting with the N and O atoms presenst in **NR** as well as **PNR**. Figure 1 depicts the overall sensing proccess of NR towards Fe³⁺ ion.



Cartoon representation of overall sensing phenomeone.

P24 Schellman Loop from small α-Peptides: Hydrogen bond Arrangements

Sujay Kumar Nandi and DebasishHaldar*

Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur, West Bengal – 741252, India. E-mail: deba_h76@iiserkol.ac.in

Background: Helical structures are ubiquitous in nature. In proteins, two types of helices are common, the Pauling α -helix and the 3₁₀-helix.¹ A stable helical structure for polypeptides depends on hydrogen bonding between backbone amide donor and acceptor units. Schellman has identified the frequent termination of α -helical structures in proteins by an achiral glycine residue with α_L conformation ($\phi = 50^\circ$, $\psi = 60^\circ$).²This reversal of helical sense at the C-terminus leads to the formation of a hybrid helix with i+5 \rightarrow i (C₁₆) and i+3 \rightarrow i (C₁₀) hydrogen bonds. There are four types of intramolecular hydrogen bonds possible in Schellman motif (Figure1).²Most of the Schellman motif formed at the C-terminus of an α -helix where residues i, i+1, i+2 and i+3 have major role.

Result: We have synthesized pentapeptidesBoc-Phe-Aib-Leu-Aib-Val-OMe1 and Boc-Phe-Ala-Leu-Aib-Val-OMe2. The peptide has same type of 3D conformation in solution state, which was confirmed by CD spectroscopy, NMR titration and 2D NMR study. Similar hydrogen bonding nature of peptides 1 and 2 in solid state was confirmed by FT-IR. The pentapeptide1 with -Aib-L-Val-OMe C-terminal segment forms a Schellman loop with both $i+3 \rightarrow i$ and $i+5 \rightarrow i$ hydrogen bonding interactions in a crystal. A second $i+5 \rightarrow i$ hydrogen bonding helps to stabilize the Schellman loop.

Conclusion: From solution and solid state studies, the pentapeptides form Schellman loop stabilized by multiple intramolecular hydrogen bonds. To the best of our knowledge, these are the shortest peptide showingShellman loop. The results presented here may foster new studies for foldamer engineering.

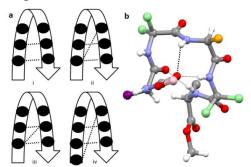


Figure 1. a)Intramolecular Hydrogen bond arrangementsof Schellman loops; b) X-ray structure of Boc-Phe-Aib-Leu-Aib-Val-OMe.

- 1. J. Donohue, Proc. Natl. Acad. Sci. U.S.A. 1953, 39, 470-478.
- 2. C. Schellman, *Protein Folding;* Jaenicke, R., Ed.; Elsevier/North Holland Biochemical Press: Amsterdam, **1980**; pp 53-61.

P25 Arm First Approach towards Synthesis of Core Cross-Linked Star Polymer with Hydrophobic Corona Via Click Chemistry

Pousali Samanta*, Saikat Maiti, Dibakar Dhara^a

Department of Chemistry, Indian Institute of Technology Kharagpur, West Bengal 721302 India Email: *samantapousali.19@gmail.com, ^adibakar@chem.iitkgp.ernet.in

Abstract: Cross-linked star polymers are very useful because of their applications in drug delivery, tissue engineering, chemical sensing, cosmetics, etc. Instead of the conventional copper-based reagents for the development of star-branched polymers, we have established a novel and environmentally benign method, whereby a 1,3-dipolar cyclo-addition reaction using a non-toxic reagent, iodosobenzenediacetate [PhI(OAc)₂]. A well-defined block copolymer with acrylate functionalized middle-block was synthesized by controlled radical polymerization technique in the initial step. Then, core cross-linked star (CCS) polymers were synthesized by reacting the above block copolymer and oxime-functionalized crosslinkers (two and four armed) via the formation of isoxazoline ring using 'click reaction' between acrylate functionalities in the polymer chain and in situ generated nitrile oxide groups from oxime functionalized cross-linker. In another system, two well-defined block copolymer chains having acrylate-functionalized middle-block and oxime-functionalized middle-block was synthesized by RAFT polymerization technique. CCS polymers were synthesized by reacting the above two block copolymer chains via the formation of isoxazoline ring using 'click reaction' between acrylate functionalities in one polymer chain and nitrile oxide groups from another polymer chain. Formation of cross-linked polymers and isoxazoline ring was confirmed by fourier transform infrared spectroscopy, gel permeation chromatography, NMR spectroscopy, and dynamic light scattering studies. In aqueous medium, these CCS polymers produce polymeric nanoparticles, which could potentially serve as a carrier of hydrophobic drug molecules. Their drug loading capacity was investigated using coumarin dyes through steady state and time resolved fluorescence spectroscopy studies. The polymeric NPs were also shown to successfully encapsulate a hydrophobic drug doxorubicin. This new green synthetic strategy for ccs formation may thus be employed effectively for the development of new polymeric architectures with potential applications in the field of advanced material science and smart drug delivery.

- 1. Maiti, S; Samanta, P; Biswas, G; Dhara, D. ACS Omega 2018,3, 562.
- 2. Banerjee, R; Maiti, S; Dhara, D. Green Chemistry 2014,16, 1365.

Synthesis of Temperature, Redox, pH Triple Responsive Amphiphilic Block Copolymers for Potential Drug Delivery Applications

Puja Poddar, Saikat Maiti, Dibakar Dhara^{*}

Departmentof chemistry Indian Institute of Technology Kharagpur West Bengal 721302,India *e-mail: dibakar@chem.iitkgp.ac.in

P26

Abstract: Triple responsive polymeric nanoparticle for disbursing anticancer drugs with little water solubility both at the tumor site and intracellular compartments are made for challenging improvement in cancer treatment.Internal as well as external stimuli, such as temperature¹, pH², enzymes³ and reductive⁴ were applied to disassemble the responsive polymer carriers in drug delivery.Recent studies showed that different kind of stimuliof the cancer tissues are slightly different (pH < 6.0 and T= 40–43 °C, glutathione conc.>10 mM) compared to that of the normal tissues (pH 7.4 and T= 37 °C, glutathione conc.< 10mM). Drugs can be selectively delivered in the cancer tissues by taking advantage of the above mentioned differential parameters. For accomplishing this goal, a new copolymer havingthermoresponsiveness as well as redox and pHresponsiveness was conceived. ApH responsive monomer 2-(2-((3,4 bis(hexyloxy)benzyloxy)carbonyl)ethylthio)ethyl methacrylate (HBCEEM)was synthesized andpolymerised byRAFT polymerisation using a redox sensitive group containing chain transfer agent (CTA)havingan alkyne endgroup. Separately, another CTA with azide end was used for synthesizing thermoresponsive poly(NIPA-*r*-PEGMA) following our previous method⁵. Finally, by CuBr click chemistry 1,3dipolar cycloaddition was performed between azideand alkyne terminals of polymers to form a thermo, pH, and redox triple responsive block copolymer. The block copolymer was characterized by gel permeation chromatography, NMR spectroscopy, dynamic light scattering and scanning electron microscopy. The copolymer formed self-assembled nanostructure in aqueous medium which was loaded with an anticancer drug, doxorubicin. The release of drug was influenced by these three stimuli (pH, temperature, redox). Thus, this copolymer can be potentially useful in delivery of anticancer drugs.

- 1. Li, Y.; Li, J.; Chen, B.; Chen, Q.; Zhang, G.; Liu, S.; Ge, Z. *Biomacromolecules***2014**, *15*, 2914–2923.
- 2. Du, J.-Z.; Du, X.-J.; Mao, C.-Q.; Wang, J. J. Am. Chem. Soc. 2011, 133, 17560–17563.
- 3. Ding, Y.; Kang, Y.; Zhang, X. Chem. Commun.2015, 51, 996-1003.
- 4. Maiti, C.; Parida, S.; Kayal, S.; Maiti, S.; Mandal, M.; Dhara, D. *ACS Appl. Mater. Interfaces***2018**, *10*, 5318–5330.
- 5. Banerjee, R.; Dhara, D. Langmuir2014, 30, 4137–4146.

P27 Cationic Block Copolymers with Different Architectures and their Capability towards DNA Condensation and De-condensation

Satyagopal Sahoo*, Dibakar Dhara

Department of Chemistry, Indian Institute of Technology Kharagpur, West Bengal 721302 India *Email: sahoosatyagopal@gmail.com

Abstract: Characterization of spontaneous formation of polplexes coupling between DNA and water soluble cationic polymer as well as release of DNA from polyplexes have recently attracted significant attention across the world, particularly owing to their potential applications in the field of non-viral gene delivery and gene transfection. One of the potential routes by which this DNA-binding modulation or switching may be achieved is via the use of responsive or 'smart' polymers that are capable of conformational or phase changes under different regimes of pH and temperature. We have studied the interaction behavior of the thermo-responsive polymers synthesized using reversible addition fragmentation transfer (RAFT) with DNA at different temperatures varying from room temperature to above LCST using differen techniques. We have also presently developed a cationic fluorescent amphiphilic copolymerhaving pendent cholate moiety linked through a redox responsive disulfide bond. These micellar nanoparticles through self-assembly were subsequently utilized in encapsulating hydrophobic anticancer drug in the core of the micelles, whereas the cationic shell of the micelles were used for complexation with oppositely charged DNA to form micelleplexes. The study implies that this redox responsive cationic micelle might have the potential towards co-delivery of DNA and anti-cancer drugs.

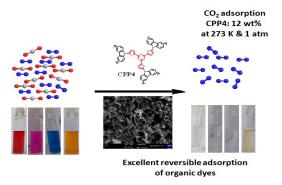
- 1. Sahoo, S.; Bera, S.; Maiti, S.; Dhara, D. ACS Omega2017, 2, 7946-7958.
- 2. Dey, D.; Kumar, S.; Banerjee, R.; Maiti, S.; Dhara, D. J. Phys. Chem. B.2014, 118, 7012–7025.
- 3. Sahoo, S.; Dey, D.; Dhara, D. Colloid. Polym. Sci.2018, 296, 183–193.

P28 2,4,6-Tri(thiophen-2-yl)-1,3,5-triazine based Conjugated Porous Polymers for Reversible Dye Adsorption and CO₂ Capture

Neha Rani Kumar* and Sanjio S. Zade

Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur 741246, Nadia, West Bengal, India nrk14rs020@iiserkol.ac.in

Abstract: A series of conjugated porous polymers (CPPs) were synthesized using 2,4,6tri(thiophen-2-yl)-1,3,5-triazine as the main building block and other nitrogen rich moieties. CPP1, CPP2 and CPP3 were obtained by Sonogashira-Hagihara coupling of 2,4,6-tris(5ethynylthiophen-2-yl)-1,3,5-triazine with 3,6-dibromo-9H-carbazole, 3,3',6,6'-tetrabromo-9,9'-bicarbazole and tris(4-bromophenyl)amine respectively. Carbazole substituted 2,4,6tri(thiophen-2-yl)-1,3,5-triazine was polymerised using FeCl₃ under different reaction conditions viz. oxidative polymerisation, Friedel-Crafts polymerization, competitive oxidative/Friedal-Crafts polymerization, by variation of solvent and use of additive to give polymers CPP4(a-g). The porosities and morphologies of all CPPs were studied and compared. Amongst all these **CPPs**, **CPP4a** displayed highest BET surface area of 1059 m²g⁻ ¹ and Langmuir surface area of about 1980 m^2g^{-1} and an average pore width of 4 nm. With high surface area, excellent thermal stability and porous structure, CPP4 exhibited excellent size dependant adsorption of organic dyes, congo red, methylene blue, rhodamine B and methyl orange from their aqueous solution with an initial concentration of 25 mg L⁻¹ All the polymers of CPP4 series were tested for CO₂ adsorption and a maximum uptake of approximately 12 wt% was obtained for CPP4a. CPP4a with its excellent adsorption properties is a potential candidate for water purification, gas separation and heterogeneous catalysis.



- Wang, H.; Cheng, Z.; Liao, Y.; Li, J.; Weber, J.; Thomas, A.; Faul, C. F. J. Chem. Mater. 2017, 29, 4885–4893.
- 2. Zhang, X.; Lu, J.; Zhang, J. Chem. Mater. 2014, 26, 4023–4029.
- 3. Chen, Q.; Luo, M.; Hammershoj, P.; Zhou, D.; Han, Y.; Laursen, B. W.; Yan, C-G.; Han, B-H. J. Am. Chem. Soc. 2012, 134, 6084–6087.

P29 Chemically Fueled Dissipative Self-Assembly that Exploits Cooperative Catalysis

Subhajit Bal *, Krishnendu Das, Sahnawaz Ahmed, and Dibyendu Das

Department of Chemical Sciences and Centre for Advanced Functional Materials, Indian Institute of Science Education and Research (IISER), Kolkata, Mohanpur 741246, India E-mail: sb17rs060@iiserkol.ac.in

Abstract: In living systems, dissipative processes are driven by the endergonic hydrolysis of chemical fuels such as nucleoside triphosphates. Now, through a simple model system, a transient self-assembled state is realized by utilizing the catalytic effect of histidine on the formation and breaking of ester bonds. First, histidine facilitates the ester bond formation, which then rapidly co assembles to form a self-supporting gel. An out of equilibrium state is realized owing to the cooperative catalysis by the proximal histidines in the assembled state, driving the second pathway and resulting in disassembly to sol. Cooperative effects that use the dual role of imidazoles as nucleophile and as proton donor is utilized to achieve transient assemblies. This simple system mimics the structural journey seen in microtubule formation where the substrate GTP facilitates the non-covalent assembly and triggers a cooperative catalytic process, leading to substrate hydrolysis and subsequent disassembly.

References:

1. Bal, S.; Das, K.; Ahmed, S.; Das, D.; Angew. Chem. Int. Ed. 2019, 58, 244-247

P30 Kinetic and Thermodynamic Control over Crystallization to Yield H and J Type Dimers in Single Crystal: Excitonic Coupling and Resulting Optical Outputs in the Solid State

Tapan Ghosh, Kalyan Jyoti Kalita, Srikanth Birudula, Ratheesh K Vijayaraghavan*

Department of chemical science, Indian Institute of Science Education and Research Kolkata, Mohanpur-741246, WB., India.

Email: ratheesh@iiserkol.ac.in

Abstract: Optical properties of molecular semiconductors are exceedingly dependent on intermolecular electronic coupling and are very much illustrious in their solid state and thin film devices.¹ The photophysical behaviour in such films and devices are known to be governed by the mode of aggregate which is dominated by columbic intermolecular interaction and is classified in two most authoritative forms of *J* and *H* aggregates, described by Devydov and Kasha in their molecular exciton theory.² In molecular aggregates, the columbic coupling between two neighbour chromophores results in the band energy change of excitons in *J* and *H* aggregates states leading to the change of their optical properties.³

Here we present a donor-acceptor small molecular semiconductor (25TR) in which the thiophene and rhodanine groups were defined as donor and acceptor units respectively. Interestingly, 25TR crystallizes in two different forms which were distinctly different in their colour and shape of the crystals. One was yellow in colour which crystallize in monoclinic form whereas the other form appeared to be crimson red in colour which crystallizes in triclinic phase. The most fascinating observations about these two polymorphs is as follows: their single crystal molecular packing revealed that the yellow form subsist as perfect cofacially arranged molecular stack whereas the crimson form in a slipped stack configuration. It was a unique example of a single molecular semiconductor crystallized in two forms of their molecular aggregates viz, H (Yellow) and J (Crimson) states with the characteristic optical outputs of the respective aggregated state. Interestingly the yellow form was non fluorescent, while the crimson form of the same compound afforded bright orange fluorescence upon exposure to UV light. Upon mechanical grinding or shearing of the yellow crystalline form of the 25TR, we observed the transformation of the non-fluorescent form to the fluorescent form. A detailed spectroscopic and X-ray diffraction data analysis and computational analysis will be presented in the poster to divulge the mechanism of these phenomenon.

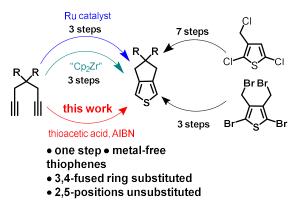
- Liess, A. Lv, A. Arjona-Esteban, D. Bialas, A. Krause, V. Stepanenko, M. Stolte, F. Würthner, *Nano Lett.* 2017, 17, 1719–1726.
- 2. N. J. Hestand, F. C. Spano, Chem. Rev. 2018, 118, 7069-7163.
- 3. K. Isayama, N. Aizawa, J. Y. Kim, T. Yasuda, Angew. Chem. Int. Ed. 2018, 57, 11982 11986.

P31 Radical Cascade Avenue for Direct Access to 3,4 Fused Thiophenes with 2,5-Positions Free for Substitution

Abhijeet R. Agrawal*, Neha Rani Kumar, Sashi debnath, Sanjio S. Zade.

Department of Chemical Sciences, Indian Institute of Science Education and Research, Kolkata, Email: ara14rs015@iiserkol.ac.in

Abstract: A single step intramolecular radical cascade reaction of divnes and thioacetic acid in presence of catalytic amount of azobisisobutyronitrile (AIBN) has been developed to synthesize thiophenes. This method allows easy and effective construction of thiophene scaffold having 3,4-fused ring substitution and unsubstituted 2,5-positions for further functionalization and polymerization. Using this method, derivatives of (CPT), 3,4-ethylenedioxythiophene (EDOT) cyclopenta[*c*]thiophene and thiophene containing spiro compound have been synthesized. For an example of functionalization, 2,5dibromo compounds of few cyclopenta[c]thiophene derivatives have been successfully synthesized for further prospects of synthesizing oligomers and polymers. The time consuming protection and deprotection strategies have been avoided to synthesize thiophenes having 3,4-fused ring substitution and unsubstituted 2,5-positions. In this synthetic strategy the use of hazardous and toxic regent and metal catalysts have been avoided.



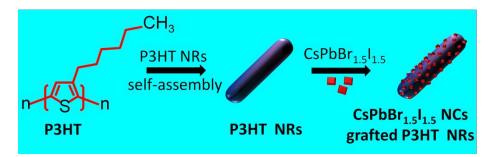
- 1. D. W. H. MacDowell, T. B. Patrick, B. K. Frame, D. L. Ellison, J. Org. Chem. 1967, 32, 1227
- 2. K. Matsui, M. Shibuya, Y. Yamamoto, Angew. Chem. Int. Ed. 2016, 55, 15397 –15400
- 3. B. Jiang, T. D. Tilley, J. Am. Chem. Soc. 1999, 121, 9744-9745

P32 Polymer Nanorod Grafting by Halide Perovskite Nanocrystals for Hybrid Organic Solar Cells with ~10% Efficiency

Dhirendra K. Chaudhary, Anima Ghosh* and Sayan Bhattacharyya

Department of Chemical Sciences, and Centre for Advanced Functional Materials, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur - 741246, India *Presenting Author, Email: animaghosh10@gmail.com

Abstract: The tremendous interest of organic-inorganic hybrid solar cell in recent times are due to wide range of tunability in absorption, band alignment for better charge collection/separation and prevalent optoelectronic properties of hybrid organic-inorganic photoactive layer using suitable nano/quantum structures. Here we propose a hybrid device architecture consisting of Poly(3-hexylthiophene) (P3HT) and all-inorganic perovskite CsPbBr_{1.5}I_{1.5} nanocrystals (NCs) for highly enhanced device performance. The optimised device structure with CsPbBr_{1.5}I_{1.5} NCs grafted on P3HT nanorods (NRs) shows a photoconversion efficiency (PCE) of $9.72 \pm 0.4\%$. The improvement is twice more than the P3HT:PCBM reference devices (4.09 ± 0.2 %). The life time of NC grafted photoactive layer is ~380 h in comparison to only ~120 h for P3HT:PCBM based devices. Uniform NC grafting is propitious over inhomogeneous blending since structurally stable CsPbBr_{1.5}I_{1.5} NCs not only act as additional light absorbing material, but their chemical grafting onto the P3HT NRs improves charge transport with decent charge mobility and better charge percolation pathway. The higher crystallinity of the P3HT NRs than bulk P3HT also helps in reducing the trap states. Furthermore, the better crystal stability and decent charge mobility of CsPbBr_{1.5}I_{1.5} NCs has been validated by Density Functional Theory (DFT) calculations.



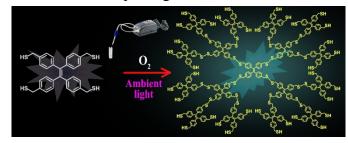
Schematic representation of NC grafting on P3HT NRs

P33 Formation of Disulphide Linkages Restricts Intramolecular Motions of Fluorophore: Detection of Molecular Oxygen in Food Package

Sk. Atiur Rahaman, Subhajit Bandyopadhyay*

Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur, India, West Bengal – 741246, India. Email: rsk.atiur1990@gmail.com

Abstract: Reliable and easy detection of oxygen in food packaging without the aid of sophisticated instruments is highly coveted. A tetraphenylethene (TPE) probe based on the oxygen mediated polymerization via the formation of disulfides causes restricted intramolecular rotation of the TPE phenyls resulting in a >100 fold enhancement of emission and thus detects O_2 in food package.



Graphical abstract of detection of molecular oxygen using a tetraphenylethene fluorophore through a non-AIE mechanism.

The probe exploits the simple chemistry where the thiol units readily form disulfide linkages and results in a restricted intramolecular rotation of the phenyl rings of the molecule. Moreover, the scanning electron microscopy (SEM), the advanced Polymer Chromatography (APC) and the dynamic light scattering (DLS) measurements were performed to confirm the formation of a polymer upon introducing of oxygen in the THF solvent. This is different from the classical mechanism of aggregation-induced emission (AIE) effect, where the enhancement is due to the polymerization and not on the stacking of the TPE units.

- 1. Zach, P. W.; Hofmann, O. T.; Klimant, I.; Borisov, S. M. Anal. Chem., 2018, 90, 2741-2748.
- Sun, Z.; Cai, C.; Guo, F.; Ye, C.; Luo, Y.; Ye, S.; Luo, J.; Zhu, F.; Jiang, C. Nanotechnology, 2018, 29, 145704.
- 3. An, J.; Shade, C. M.; Chengelis-Czegan, D. A.; Petoud, S.; Rosi, N. L. J. Am. Chem. Soc., **2011**, 133, 1220–1223.
- 4. Eltermann, M.; Kiisk, V.; Berholts, A.; Dolgov, L.; Lange, S.; Utt, K.; Jaaniso, R. Sensors and Actuators B, 2018, 265, 556–564.
- 5. Zhaoa, Q.; Liu, Y. Chem. Commun., 2018, 54, 6068-6071.
- 6. Mei, J.; Leung, N. L. C.; Kwok, R. T. K.; Lam, J. W. Y.; Tang, B. Z. Chem. Rev., 2015, 115, 11718–11940.

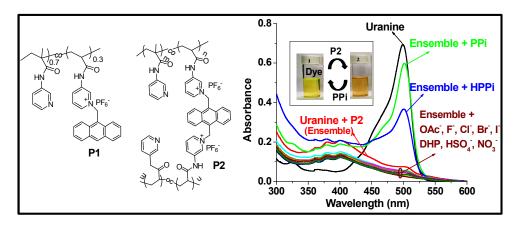
P34 Polymer-Based Chemosensors for Selective Detection of Pyrophosphate in Semiaqueous Media (P₂O₇⁴⁻)

Saswati Ghosh Roy* and Kumaresh Ghosh

Department of Chemistry, University of Kalyan, W.B.-741235, India. *Presenting Author, Email: saswati.ghoshroy9@gmail.com

Abstract: The detection of phosphate–based anions such as pyrophosphate ($P_2O_7^{4^-}$, PPi) and nucleotide phosphates is an important research topic in supramolecular chemistry as PPi is involved in many cellular processes such as ATP hydrolysis, DNA and RNA replication, enzymatic reactions, etc. Abnormal level of PPi causes severe medical condition due to vascular calcification. However, selective and reliable sensing of these anions in pure aqueous or semi aqueous media is difficult to accomplish due to their significant solvations. Various small molecular architectures are reported in this regards^{1,2} and in relation to this, polymer-based optical chemosensors which show several advantages such as signal amplification, increaseed binding efficiency and recognition selectivity, fabrication of polymer film-based chemosensors into devices, etc are less in number.³

Herein, we wish to report our endeavour on the design and synthesis of pyridinium motif appended copolymer (P1) and cross-linked polymer (P2) chemosensors containing anthracene as flurophore moiety. While copolymer P1 shows selective detection of hydrogen pyrophosphate (HP₂O₇³⁻, HPPi) in DMSO/H₂O (3:1, v/v), cross-linked polymer P2 exhibits selective detection of PPi in DMSO/H₂O (1:1, v/v, pH = 6.8) at very low cocentration. Further, P2 efficiently senses PPi *via* indicatior displacement assay technique.



- 1. Ghosh, K.; Sarkar, A. R.; Samadder, A.; Khuda-Bukhsh, A. R.Org. Lett., 2012, 14, 4314-4317.
- 2. Ghosh, K.; Kar, D.; Chowdhury, P. R. Tetrahedron letters, 2011, 52, 5098-5103.
- 3. Kim, H. N.; Guo, Z.; Zhu, W.; Yoon, J.; Tian, H. Chem. Soc. Rev., 2011, 40, 79-93.

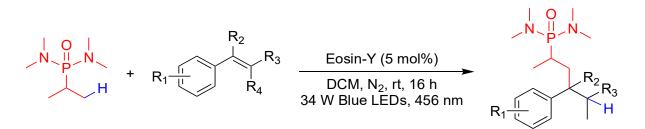
P35 Organo visible Light Photocatalyzed Synthesis of Phosphoramide Derivative by Direct C–H bond activation

Krishna Gopal Ghosh, Devarajulu Sureshkumar*

Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur, West Bengal – 741 246, India Email: kgg15rs014@iiserkol.ac.in & suresh@iiserkol.ac.in

Abstract: Organo phosphorus compounds and their derivative are of great interest for modern organic chemist because of its broad applicability in pharmaceutical, agrochemical and industrial area.¹ Among the organo phosphorous moiety, phosphoramidates are widely found in natural products and have tremendous application in biological systems such as insecticides, fungicides, antibacterial and antitumor agents.² Phosphoramide derivatives can also be used as catalysts for various organic transformation³ and in coordination chemistry.⁴ Considering the fact of immense applicability of phosphoramide derivatives, we developed a simple and straightforward strategy using visible light photocatalysis.⁵ Our method has advantages like broad substrate scope, highly chemoselective, external additive free, and high chemical yield. Further, we demonstrate the synthetic utility of our method by performing the reaction in a gram scale.

In this poster, we present the metal free visible light photocatalyzed synthesis of phosphoramides scaffolds under very mild reaction conditions by direct C–H bond activation. We use economically beneficial and commercially available EOSIN-Y as a hydrogen atom transfer photocatalyst for the C–H bond activation of phosphoramide derivatives followed by its subsequent reaction with a diverse set of electron deficient olefins with excellent chemical yield. Furthermore, there is no necessity of any external additive for this transformation.



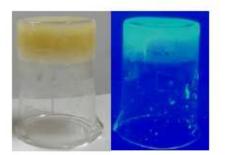
- 1. Hudson H. R., Wardle N. J., Bligh S. W., Greiner I., Grun A., Keglevich G. *Mini-Rev. Med. Chem.* 2012, *12*, 313.
- 2. Eto M. Organophosphorus Pesticides: Organic and Biological Chemistry, CRC Press Inc. USA, 1974.
- 3. Leca D., Fensterbank L., Locate E., Malacria M. Chem. Soc. Rev. 2005, 34, 858.
- 4. Zubiri M.R.I., Woollins J.D. Comments Inorg. Chem. 2003, 24, 189.
- 5. Romero N. A., Nicewicz D. A. Chem. Rev. 2016, 17 10075.

P36 Protein based Hydrogel Preparation for Detection of Nitroaromatics in Aqueous medium

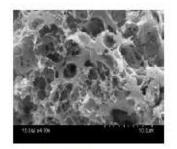
Dipika Pan*, Nira Parshi, Dr. Jhuma Ganguly

Department of Chemistry, Indian Institute of Engineering Science and Technology, Howrah, West-Bengal, 711103, India. * Email: pandipika15@gmail.com

Abstract: Hydrogels are the macromolecular randomly crossslinked polymeric arrangements, with multifunctionalility and it can stored large amount of water or biological fluids. Herein, we report, the preparation of a crosslinked, auto-fluorescent hydrogel (BG) by simple modification of free amine groups present in Bovine Serum Albumine (BSA) protein. The structural elucidation has been analysed by FTIR, Rheology and pH dependent swelling study. Storage modulus (G') and Loss modulus (G'') data from rheology clearly proves the high mechanical stability as strong gel. SEM analysis provides the existence of porous network within the architect of BG. It shows a sharp emmision peak at 354nm which is mainly attributed by the fluorophore present in BSA moities. Nitroaromatic entities have a remarkable quenching effect on fluorescence of hydrogel in aqueous medium. Recently, rapid sensing for Nitroaromatic compounds is a sensitive demand from researcher for security in many civilian and defence environments. The developed protein based hydrogel could significantly expand the scope of detection of hazardous materials in water.



Visible light UV light



SEM image

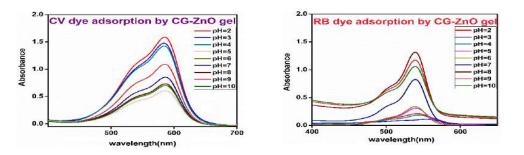
- 1. Maity, S.; Parshi, N.; Prodhan, C.; Chaudhuri, K.; Ganguly, J. *Carbohydr Poly.*, **2018**, 193, 119.
- 2. Sun, X.; Ma, X.; Kumar, C. V; Lei, Y. Anal. Methods. 2014, 6, 8464.
- Guo, X.; Li, X.; Jiang, Y.; Yi, L.; Wu, Q.; Chang, H.; Diao, X.; Sun, Y.; Pan, X.; Zhou, N. J Lumin. 2014, 149, 353.

P37 Fabrication of ZnO Nanocomposite Hydrogel for removal of Toxic Dyes

Biswajit Jana*, Narendra Jaiswal and Jhuma Ganguly

Indian Institute of Engineering Science and Technology, Shibpur Howrah-711103, West Bengal, India Heritage Institute of Technology, Kolkata-700107, West Bengal, India *Biswajit Jana, Email: biswajitchem06@gmail.com

Abstract: Polysaccharides are currently very effective bioresources with vast societal and industrial importance, being biodegradable, recyclable and renewable. Bio-based products from polysaccharides impart several benefits: lightweight, sustainability and biodegradability. Chitosan based Hydrogels are effective and efficient bio-based materials for their low cost, recyclable, and easy degradable without any harmful wastage. Here, we focus on the preparation of ZnO nanocomposite hydrogel from glutaraldehyde crosslinked chitosan and ZnO nanoparticles. The structural investigation are performed by FTIR, rheology and pH depended swelling study. SEM and TEM analysis establish the nanoparticles encapsulated three dimensional networks. Composite hydrogel has a prominent fluorescence efficiency due to the presence of ZnO nanoparticles. The quantification for the incorporated ZnO in Hydrogel is studied using fluorescence technique. The porous nature from hydrogel for adsorption and the degraded efficiency of ZnO nanoparticles are combined together in composite. The composite shows excellent performance for the removal of toxic dyes, Rose Bengal, Crystal Violet, from water medium. The performance for the adsorption, removal and degradation of the dyes using Composite hydrogel, have been carried out with change in doses, pH and temperature. Composite hydrogel has a great potential in removing toxic dyes from aqueous system without any further formation of wastage materials. The composite can be reusable and recylable.



- 1. Maity, S.; Datta, A.; Lahiri, S.; Ganguly, J. RSC Advances. 2016, 84, 81060.
- 2. Maity, S.; Naskar, N.; Lahiri, S.; Ganguly, J. Environ. Sci.: Water Res. Technol. 2019
- 3. Maity, S.; Ray, S, S.; Chatterjee, A.; Chakraborty, N.; Ganguly, J.ChemistrySelect.2018, 23, 6575

P38 Photoinduced Electron Transfer with Ultrasmall Copper Nanoclusters towards Finding Characteristics of Protein Pockets

Soumyadip Bhunia^{1*}, Pradipta Purkayastha²

¹Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, West Bengal-741246, India ²Department of Chemical Sciences and Center for Advanced Functional Materials (CAFM), Indian Institute of

²Department of Chemical Sciences and Center for Advanced Functional Materials (CAFM), Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, West Bengal-741246, India *Presenting Author, Email: bitu.chem93@gmail.com

Abstract: Proteins possess various domains and subdomain pockets with varying hydrophobicity/hydrophilicity.^{1,2} The local polarities of these domains play a major role in oxidation–reduction-based biological processes. Herein, we have synthesized ultrasmall fluorescent copper nanoclusters (Cu NCs) that are directed to bind to the different domain specific pockets of the model protein bovine serum albumins (BSA).³ Potential electron acceptors, methyl viologen (MV) derivatives, were chosen such that they specifically reach the various domains following their hydrophobicity/hydrophilicity.⁴ Here, we have used MV²⁺, HMV⁺, and DHMV²⁺, possessing hydrophilic, intermediate, and hydrophobic specificities. Being electron acceptors, these derivatives draw electrons from the Cu NCs through photoinduced electron transfer (PET). The rate of PET varies at the different domains of BSA based on the local environment which has been analyzed. Here, PET is confirmed by steady state as well as time-resolved fluorescence spectroscopy. This study would provide a measurable way to identify the location of the different domains of a protein which is scalable by changing the superficial conditions without unfolding the protein.

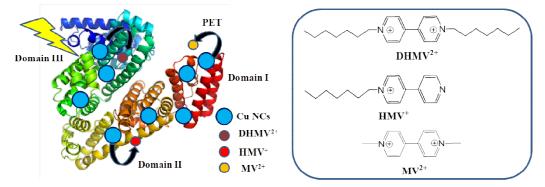


Figure 1.Graphical representation of domain specific binding and electron transfer from CuNCs to various MV derivatives.

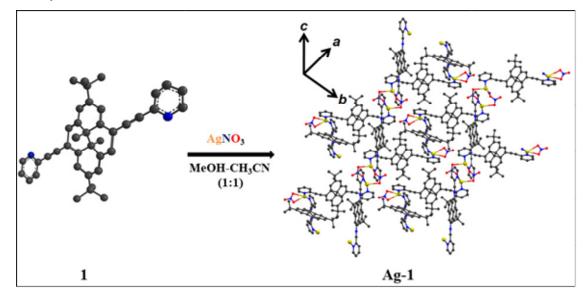
- 1. Jisha, V. S.; Arun, K. T.; Hariharan, M.; Ramaiah, D. J. Am. Chem. Soc. 2006, 128, 6024-6025.
- 2. Stank, A.; Kokh, D. B.; Fuller, J. C.; Wade, R. C. Acc. Chem. Res. 2016, 49, 809-815.
- 3. Bhunia, S.; Kumar, S.; Purkayastha, P. ACS Omega2019, 4, 2523-2532.
- 4. Chen, W. T.; Hsu, Y. J.; Kamat, P. V. J. Phys. Chem. Lett. 2012, 3, 2493–2499.

P39 Light gated Modulation of Electrical Conductance of a Photochromic Coordination Polymer

Sanjib Ghosh* and Subhajit Bandyopadhyay

Department of Chemical Sciences, Indian Institute of Science Education and Research, Mohanpur, West Bengal-741246, India Email: sg14rs042@iiserkol.ac.in

Abstract: Coordination polymers are composed of metal nodes connected by multidentate organic linkers.¹ Our group has earlier reported a one-dimensional Hg²⁺-based MOF that was effective in removal of the mercury ions from contaminated water samples.² We have also reported a light-driven coordination polymer where an Al³⁺ ion was used as the metal node to connect to an azobenzene-based photochromic linker where the binding to the metal ion was reversibly controlled by light.³ In the present work, a photoresponsive π -switch (1) decorated with pyridine donor centres were connected by Ag⁺ nodes to create a coordination polymer (Ag-1) that can be switched ON and OFF resulting in an effective modulation of the length of the π -conjugation. This coordination polymer was structurally characterized by single crystal X-ray diffraction studies. Using visible and ultraviolet light, we have successfully modulated the electrical conductance of the polymer reversibly. The less conducting form can be switched on to the conducting form thermally as well.



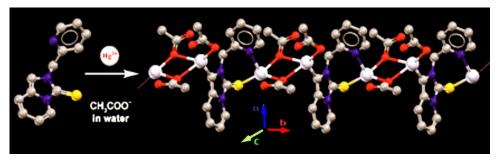
- 1. Férey, GChem. Soc. Rev. 2008, 37, 191.
- 2. Rahaman, S. A.; Roy, B.; Mandal, S.; Bandyopadhyay, S.Inorg. Chem.2016, 55, 1069.
- 3. Hatai, J.; Bandyopadhyay, S. Chem. Eur. J.2014, 20, 10020.

Removal of Hg²⁺ Ions from Water through the Formation of a One-Dimensional Metal–Organometallic Polymer

Sk. Atiur Rahaman, Biswajit Roy*, Soumik Mandal, and Subhajit Bandyopadhyay

Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER), Kolkata Mohanpur, West Bengal 741246, India *Email: biswajit1108@iiserkol.ac.in

Abstract: Certain bacterial species are resistant to inorganic and organomercury compounds because of the presence of a series of proteins that protects them from these toxic compounds by effciently uptaking, transporting, converting the mercury compounds to less toxic species and eliminating them. The Walsh,¹ Omichinski,² Parkin³ groups have contributed immensely to the understanding the mechanism of the organomercury degrading proteins and the chemistry of the toxicity of mercury compounds in general. The toxicity of mercury containing compounds results owing to their binding to the thiols of the cysteine residues of the proteins. These proteins have multiple cysteines⁴ in their mercury-binding sites. In this work, a pyridine appended 2-mercaptoimidazolyl scaffold was used as a mimic for the effcient binding of mercury(II) ions. In the presence of Hg²⁺ ions an aryl C-H bond of the ligand is activated. The sulphur and nitrogen donors on the other end of the ligand coordinates with another Hg²⁺ ion. This motif in the presence of acetate ion froms a one dimensional crystalline network with high affnity and removes Hg²⁺ ions from the mixture. The binding of mercury is indicated by quenching of the fluorescence of the ligand in the coordination network.



- 1. Moore, M. J.; Distefano, M. D.; Zydowsky, L. D.; Cummings, R. T.; Walsh, C. T. Acc. Chem. Res. 1990, 23, 301.
- 2. Omichinski J. G. Science 2007, 317, 205–206.
- 3. Melnick, J. G.; Parkin, G. Science 2007, 317, 225.
- 4. Lafrance-Vanasse, J.; Lefebvre, M.; Di Lello, P.; Sygusch, J.; Omichinski, J. G. J. Biol. Chem. 2009, 284, 938.

P41 Dual Thermoresponsive Poly(ionic liquid) Random Copolymers

Palash Banerjee,^{*} Yajnaseni Biswas, Priyanka Dinda, Tarun Mandal

School of Chemical Sciences, Indian Association for the Cultivation of Sciences, Kolkata, West Bengal-700032, India

*Email: psupb2@iacs.res.in

Abstract: The interest in thermoresponsive polymers has steadily grown in the last few decades and a great deal of work has been devoted for developing new smart materials which offer great perspectives in the fields of targeted and triggered drug delivery as well as for industrial applications such as smart polymeric coatings, or membranes etc. Here, we report the synthesis of a series of dual ion- and thermo-responsive random copolymers comprising of segments of either hydrophobic polymers [poly(methyl methacrylate) (PMMA) and polystyrene (PS)] or hydrophilic polymers [poly(2-hydroxyethyl methacrylate) (PHEMA) and poyl(N-isopropyl acrylamide) (PNIPAM)] with a poly(ionic liquid)(PIL), poly(triphenyl-4-vinylbenzylphosphonium chloride) (P[VBTP][Cl]) segment previously respoted from our laboratory,¹ using either conventional free radical polymerization or controlled RAFT polymerization techniques. The obtained P[VBTP][C1]-ran-PMMA, P[VBTP][C1]-ran-PS and P[VBTP][C1]-ran-PHEMA copolymers exhibit upper critical solution temperature (UCST)-type turbid-to-transparent phase transition whereas P[VBTP][C1]-ran-PNIPAM copolymers show lower critical solution temperature (LCST)-type transparent-to-turbid phase transition in water/methanol in the presence of externally added halide anions. Furthermore, the UCST-type/ LCST-type cloud points ($T_{cp}s$) of these copolymers can be fine-tuned with respect to the copolymer compositions and concentrations of anions. More interestingly, P[VBTP][C1]-ran-PNIPAM copolymer containing higher amount of ionic P[PVBTP][C1] segment initially show LCST-type soluble-to-insoluble followed by an UCST-type insolubleto-soluble phase transitions in the presence of halide ions at lower and higher temperature respectively.

Reference:

1. Biswas, Y.; Maji, T.; Dule, M.; Mandal, T. K., Tunable doubly responsive UCST-type phosphonium poly(ionic liquid): a thermosensitive dispersant for carbon nanotubes. *Polymer Chemistry* **2016**,*7* (4), 867-877.

P42 Introduction to Nanoindentation: Its importance, from Single Crystals to Polymers

Susobhan Das*, SurojitBhunia, Amit Mondal, SaikatMondal, RanitaSamantaand C Malla Reddy*

Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur Campus, Mohanpur – 741246, West Bengal, India Email: dassusobhan.chem@gmail.com & cmallareddy@gmail.com

Abstract: Instrumented nanoindentation technique has enabled great advances in nanomechanical studies of various materials, including organic crystals and polymers. Nanoindentation can be used to measure the mechanical properties (most importantly Young's modulus and nanohardness) of materials with high precision, even when the samples are available only in small quantities ($>0.5 - 100 \text{ m}^3$). Thus, it has gained the tremendous attention of the crystal engineering community, who are not only interested in measuring the properties of single crystals of organic, inorganic and hybrid structures, but also wish to correlate the measured responses with the underlying structural features and intermolecular interactions. At the same time, the mechanical characterization of polymers on nanometer scale is highly useful in polymer science for several reasons, like mapping local mechanical properties is possible on samples characterized by variation of composition as well as heterogeneity induced by solidification during processing or complex morphologies as arising in biological samples. However, for ploymer samples, the issue with pile-up and its viscoelesnatic nature should be considered. So, the preliminary nanoindentation has been used to determine the mechanical properties of isoanisotropic crystalsandisotropic polymers. Parallely there is also great opportunity to explore several stress-induced phenomena that largely unexplored: are mechanoluminescence, mechanochromism, and triboluminescence, both in single crystals and polymers.

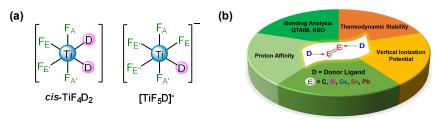
- 1. Varughese, S.; Kiran, M. S. R. N.; Ramamurty, U.; Desiraju, G. R. Angew. Chem. Int. Ed. 2013, 52, 2701.
- 2. Samanta, R.; Ghosh, S.; Devarapalli, R.; Reddy, C. M. Chem. Mater. 2018, 30, 577.
- 3. Devarapalli,R.;Kadambi, S.B.; Chen, C-T.; Krishna, G.R.; Kammari, B. R.; Buehler, M. J.; Ramamurty, U.; Reddy, C.M. *Chem. Mater*.2019, *31*, 1391.
- 4. Oliver, W.C.; Pharr, G.M.J. Mater. Res., 2004, 19, 3.
- 5. Tranchida, D.; Piccarolo, S.; Loos, J.; Alexeev, A.Macromolecules2007, 40, 1259.

P43 Donor–Acceptor Interactions in Early Transition Metal Halides and Group-14 Compounds: A Theoretical Insight

Sayan Dutta*, Debasis Koley

Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur - 741 246 *Presenting Author, Email:sd14rs069@iiserkol.ac.in

Abstract: During the past two decades, Lewis acid-base chemistry has undergone a profound revolution. Though, till date, Lewis acid-base adducts of electron-deficient group 13 halides $(ECl_3, E = B-In)$ are widely explored, ¹very few similar benchmark studies exploiting Lewis acidic early transition metal compounds e.g. titanium tetrahalides (TiF₄, TiCl₄) have been reported.²In this context, we have investigated the electronic structure and bonding scenarios in different *cis*-TiF₄D₂ and $[TiF_5D]^-$ complexes (D = neutral donor ligand), employing DFT calculations (Scheme 1a).³Additionally, we have computed the formation energies of these complexes for various reaction routes both in the gas phase and solution medium. Significant effort has been paid to obtain intrinsic Lewis base strengths of the ligands with respect to TiF₄ as reference Lewis acid. Furthermore, the isomerism of mixed chloro and fluoro titanium complexes supported by neutral ligands is studied. The unique electronic feature of the neutral ligands specially carbene results the ongoing "renaissance" in the stabilization of various unstable chemical species, radicals and elements in their different unusual oxidation states. In this regard, we have made an attempt to explore theoretically the electronic structure and bonding perspectives in different bis-donor stabilized E₂ (E=C-Pb) compounds (D-E₂-D; Scheme 1b).⁴The thermodynamic stabilities of these compounds are computed toidentify the viable targets for synthesis.



Scheme 1. (a) Schematic representation of the cis-TiF₄D₂ and [TiF₅D]⁻ complexes. (b) Schematic representation of the D–E₂–D compounds.

- 1. Jonas, V.; Frenking, G.; Reetz, M. T. J. Am. Chem. Soc., 1994, 116, 8741.
- 2. Beste, A.; Krämer, O.; Gerhard, A.; Frenking, G. Eur. J. Inorg. Chem., 1999, 2037.
- 3. Dutta, S.; Mondal, T.; De, S.; Rudra, K.; Koley, D. Inorg. Chim. Acta, 2019, 485, 162.
- 4. Mondal, T.; Dutta, S.; De, S.; Thirumalai, D.; Koley, D. J. Phys. Chem. A, 2019, 123, 565.

Functionalization of Carbon Nano-onions for Targeted Anticancer Drug Delivery

Rabindranath Majumder¹, Bhuban Ruidas¹, Sutapa Som Chaudhury ¹, Chitrangada Das Mukhopadhyay¹*

¹Centre for Healthcare Science and Technology, Indian Institute of Engineering Science and Technology, Shibpur, Botanic Garden-711103, Howrah, India.

Correspondence to: chitrangadadas@yahoo.com

Abstract: Though many drug candidates are being tested till date for their anticancer potency, targeted drug delivery is still an unmet challenge in cancer therapeutics. The probable reason behind this phenomenon is mainly the failure of proper delivery and identifying the exact target. In this regard, we have tried to deploy carbon nano onions (CNO) as a cargo encapsulated with an anticancer drug carmustine and conjugated with folic acid as ligand to achieve effective cancer target. Drug loaded CNO with conjugated ligand were characterized by FTIR, UV-VIS, and Raman spectra followed by the investigation of their size and morphology by DLS, FESEM and TEM analyses. The non-toxicity of the drug encapsulated CNO was confirmed by 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide (MTT) reduction assay and haemocomapatibility test. An extensive fluorescence microscopic study reflected the drug internalization phenomenon in cancer cell line. Drug induced cell apoptosis was visualized under confocal microscope followed by the observation of anti-invasion and anti-migratory effects. A reactive oxygen species (ROS) mediated drug action was observed by DCFDA method. Moreover, the cancer metastasis and apoptosis related protein expression studies by enzyme linked immunosorbent assays (ELISA) in breast cancer cells gave a complete scenario of drug action. Finally, all these findings together suggested that the drug loaded and folic acid conjugated CNO may play a crucial role as the most effective cargo for accounting the exact target in new age cancer therapeutics.

Keywords: anticancer potency, carbon nano onion, haemocomapatibility, drug interlization, ROS, metastasis, apoptosis

P45 Polymerization of Styrene using Pincer Type Redox active Nitrogen Donor Cobalt Complexes as Catalysts

Bappaditya Goswami*¹, Manas Khatua¹ and Subhas Samanta^{1,2}

¹Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, India. ²Present address: Department of Chemistry, Indian Institute of Technology Jammu, Jammu 181121, India. *Presenting Author, Email: bg17rs024@iiserkol.ac.in

Abstract: Pincer type of redox active non-innocent ligands have received much attention in modern co-ordination Chemistry to understand new forms of reactivity and catalysis study.¹ Thus, a number of pincer ligand systems have been developed and their metal mediated polymerisation reactivity of olefins and other saturated monomer has been explored.² The field of early transition metal catalyzed olefin polymerization has continued to grow worldwide in both industry and academics after the discovery of Ziegler-Natta catalyst. Later on, it is tuned to late transition metal complexes when the first report came in 1995 by Brookhart and co-workers.² Then onwards there has been an intense search for new generation catalysts for the polymerization of olefin and other unsaturated monomer.³ With the aim of studying the catalytic properties of the late metal complexes for styrene polymerization, we have been exploiting the synthesis and reactivity of redox non-innocent pincer type NNN-donor cobalt complexes and used as catalyst precursors with the activation of methylaluminoxane (MAO). Herein, we present the novel examples of this type of transition metal complexes exhibited good activity for styrene polymerisation even at room temperature with high conversion, which is very much beneficial in terms of energy savings.(Figure 1).



Figure 1. Schematic representation of the work

- (a) Vlugt, J. I. v. d.; Reek, J. N. H. Angew. Chem. 2009, 121, 8990-9004; Angew. Chem. Int. Ed. 2009, 48, 8832–8846.(b)Gunanathan, C.; Milstein, D. Acc. Chem. Res. 2011, 44, 588– 602.
- 2. Johnson, L. K.; Killian, C. M.; Brookhart, M. J. Am. Chem. Soc. 1995, 117, 6414-6415.
- 3. Cho,W.; Cho, H.; Lee, C. S.; Lee, B. Y.; Moon, B.; Kang, J. Organometallics 2014, 33 (7), 1617-1622
- 4. Goswami, B.; Khatua, M.; Samanta, S. Manuscript under preparation.

Carbohydrate Derived Multifunctional Gels

Prof. Balaram Mukhopadhyay

Professor Sweet Lab, Department of Chemical Sciences Indian Institute of Science Education and Research (IISER) Kolkata Mohanpur, Nadia 741246 sugarnet73@hotmail.com, mbalaram@iiserkol.ac.in

Abstract: Owing to their versatile applications in the areas of dye-sensitized solar cells, soft optical devices, cosmetics, template materials, drug delivery agents, magneto-optical switches and crystal engineering, low molecular weight organogelators (LMOGs) have gained enormous interest in recent times. They are normally constituted of organic small molecules (Mw<1000) that can ordered self-assembly through various non-covalent interactions i.e. H-bonding, π - π interaction, van Der Walls forces and electrostatic interactions. These large self-assembled supramolecular architectures can entrap significant amount of liquids inside the internal void spaces.

The urge of designing efficient gelators with multiple applications potential attracted almost all classes of organic molecules. However, considering the applications in the interface of biology demanded more biocompatible and non-toxic materials. To address this issue, extensive use of carbohydrate gelator we found that simple carbohydrate-derived molecules show efficient gelation abilities with various oils and organic liquids. It turned out to be more interesting when we observed that these gelators possess considerable self-healing property, recharge ability, phase-selectivity in the aqueous-organic interface and the gels can efficiently block the transmission of UV light. Such properties triggered us to explore the supramolecular architecture involved in the formation of the gels. The present poster will highlight our findings with carbohydrate-derived small molecule gelators.

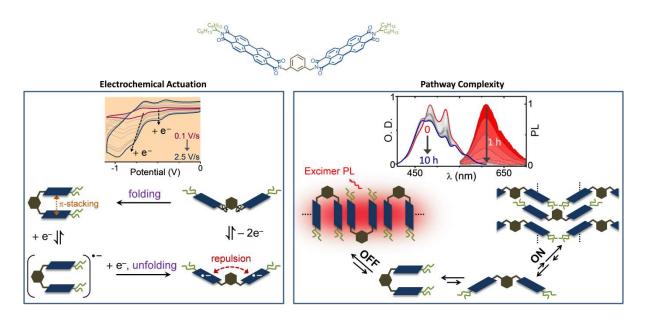
- 1. Simple Carbohydrate-Derived Multifunctional Gels: AnkitaMitra, Vikramjit Sarkar and BalaramMukhopadhyay, *ChemistrySelect***2017**, *2*, 9958-9961.
- 2. Carbohydrate-based safe fuel gel with significant self-healing property: Kumar Bhaskar Pal and BalaramMukhopadhyay, *ChemistrySelect***2017**, *2*, 967-974.
- 3. A correlation study between hydrogen bonded network and gelation ability of three galactose derivatives: Somnath Mukherjee, G. Rama Krishna, Balaram Mukhopadhyay, C. Malla Reddy, *Crystal Engineering Communications* **2015**, *17*, 3345 3353.
- 4. Phase-selective carbohydrate gelator: Somnath Mukherjee and BalaramMukhopadhyay *RSC Advances* **2012**, *2*, 2270 2273.

P47 Flexible Bichromophoric System: From Rapid and Efficient Redox-Actuation to Competing Self-Assembly Pathways

Samaresh Samanta, Narottam Mukhopadhyay, Debansu Chaudhuri

Department of Chemical Sciences, Indian Institute of Science Education and Research (IIESR) Kolkata, Mohanpur (India)

Abstract: The ability to control interchromophoric interactions in a multichromophoric system creates several exciting and often unseen possibilities. We present a flexible perylene bisimide (PBI) dimer, whose ability to exist in two distinct conformations (open vs. folded) was exploited to realize interesting properties, in both molecular and supramolecular regimes. Being electron deficient, PBI has a fairly low reduction potential. Also the barrier to conformational change in the PBI dimer depends strongly on the redox state of the PBI unit. This allowed us to achieve a rapid and very large conformational change (actuation) at a fairly low applied voltage. The same conformational flexibility also plays a key role in the dimer self-assembly. We show the existence of two competing aggregation pathways with distinctly different thermodynamics and kinetics. A crossover from one pathway to the other leads to an efficient suppression of excimer formation in the H-aggregated state.



- 1. S. Samanta, N. Mukhopadhyay, D. Chaudhuri, Chem. Mater. 31, 899. (2019).
- 2. S. Samanta, D. Chaudhuri, J. Phys. Chem. Lett. 8, 3427. (2017).

P48 Removal of Cationic Dyes from Aqueous Medium Using Glutamic Acid-Derived Organogels

Sipra Ghosh¹ and Priyadarsi De^{*2}

¹Departments of Chemistry, University of Kalyani, Kalyani 741235, India

²Polymer Research Centre, Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur-741246, India Presenting Author: (sipraghosh88@gmail.com)

Abstract: During the last few decades, many researchers have been focusing on specific methods and technologies for removing toxic dyes from different kinds of waste water streams.^[1-4] Accordingly, the purpose of this study is to develop glutamic acid derived crosslinked polymeric organogels for dye adsorption from aqueous media. The dimethyl 2-(methacrylamido)pentanedioate (Boc-Glu-MAC) was polymerized using diethylene glycol dimethacrylate (DEGDMA) as cross-linker via reversible addition-fragmentation chain transfer (RAFT) technique to synthesize cross-linked polymeric organogels with pendant glutamic acid derivative. The mechanical property of organogels was examined by rheological study. The organogels exhibited higher value of storage modulus (G') than the loss modulus (G'') within the linearity limits of deformation, and strong dependence of G'values on the extent of cross-linking in the gel matrix. Field emission scanning electron microscopy (FE-SEM) showed porous structure of the gel matrix, thus organogels showed swelling behaviours in organic solvents such as dichloromethane, N,N-dimethylformamide, tetrahydrofuran, acetone and methanol. Dye adsorption properties of these organogels were investigated using different aqueous dye solutions, such as crystal viotet, malachite green, rhodamine-B and uranine. The gels showed high dye adsorption capacities ($\geq 97\%$) towards cationic dyes like crystal viotet and malachite green. Therefore, the synthesized organogels could be used for removal of cationic pollutant dyes (crystal viotet and malachite green) from waste water.

- 1. Y. Fu, T. Viraraghavan, Bioresour. Technol. 2001, 79, 251.
- 2. T. Lazar, Color Res. Appl. 2005, 30, 313.
- 3. N. Daneshvar, M. Ayazloo, A. R. Khataee, M. Pourhassan, *Bioresour. Technol.* 2007, 98, 1176.
- 4. L. S. Oliveira, A. S. Franca, T. M. Alves, S. D. F. Rocha, J. Hazard. Mater. 2008, 155, 507.

Amphiphilic Mannose-6-Phosphate Glycopolypeptide and Lipid Nanocarriers for Lysosomal Storage Disorder (LSDs)Disease

Basudeb Mondal^{1*}, Apurba Das², RupakDutta² and Sayam Sen Gupta¹

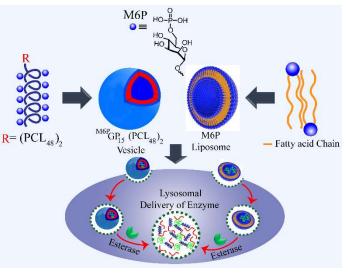
^a Department of Chemical Sciences, Indian Institute of Science Education and Research, Kolkata, West Bengal-741246, India

^bDepartment of Biological Sciences, Indian Institute of Science Education and Research, Kolkata, West Bengal-741246, India

E-mail: sayam.sengupta@iiserkol.ac.in & basude92@gmail.com

Abstract: Developing nanomaterial which can target lysosome could be used as an alternative to conventional therapies for various lysosomes related diseases and becomes a

potential medical tool.Nano-carriers with mannose-6-phosphate (M6P) on the surface represent a very interesting class of delivery vehicles since M6P receptors are presenton cell surface and overexpress on cancer cell surface.Herein, we have developed miktoarm star amphiphilic copolymers comprising M6P functionalized polypeptide and



poly(ε -caprolactone) and M6P functionalized lipids. The amphiphilic copolymers and lipids were self-assembled in water into morphologies such as vesicles and liposomes with M6P displayed on the surface. These nanostructures were characterized in detail using a variety of techniques such as electron microscopy, dye and enzyme encapsulation techniques. We have shownthe non-cytotoxicity ofM6Pliposomeson HEK-293 cell line. Finally, we will show*enzyme*delivery for Lysosomal Storage Disease (LSDs).

- 1. Pati, D.; Das, S.; Patil, N. G.; Parekh, N., Anjum, D. H.; Dhaware, V.; Ambade, A. V.; Sen Gupta, S. *Biomacromolecules* **2016**, *17*, 466–475
- 2. Das, S.; Parekh, N.; Mondal, B.; Sen Gupta, S. ACS Macro Lett. 2016, 5, 809-813.
- 3. Pandey, B.; Patil, N.; Bhosle, G.; Ambade. A. V.; Sen Gupta, S.*Bioconjugate Chem.*, **2019**, *30*, 633–646
- 4. Mondal, B.; Pandey, B.; Parekh, N.; Sen Gupta, S. Manuscript under process.

Synthesis and Performance of Proton Conducting Novel Sulfonated Poly(Oxybenzimidazole)-Graphene Oxide Intercalated Composite Membranes for PEM-Fuel Cells

Cheluri Nagendra Prasad*, Tharanikkarasu Kannan

Department of Chemistry, Pondicherry University, Pondicherry - 605014, India. *E-Mail: cnp.org.chem@gmail.com

Abstract: The most attractive Proton exchange membrane fule cells (PEMFCs) are considered as powerful green energy sources for portable, stationary and tranport applications because of clean, quiet and eco-friendly nature¹. Until now, among the PEMs Nafion is the state-of the-art PEM due to its good thermal and chemical stabilities, superior mechanical properties as well as high proton conduction ability. However, Nafion exhibits some drawbacks such as high cost, fuel crossover, low proton conductivity at elevated temparature^{2,3}. In view of this, tremendous efforts have beenexplored to the modification of Nafion or development of alternativemembrane materials including, sulfonated polyimides (SPIs), sulfonated poly (arylene ether) s (SPAEs), sulfonated polybenzimidazoles (SPBIs) and their composites are the focus of current investigations on PEMs.

Currently, GO is highly attractive for many applications as a result of outstanding thermal and mechanical properties. In the present work, thenovel SPOBI-60 was synthesized via coplycondensation and a series of correspondindg composites withdifferent contents of a graphene oxide (GO) were prepared inorder to study the effects of GO contenton the SPOBImembranes properties. Our investigation revealed a structural reorganization in the composite, showing clearly that the incorporation of the proper amount of GO in SPOBI-60 enhanced the thermal, oxidative hydrolytic stabilities, mechanical properties, and increased the proton conductivity and power density and current density values (i.e., PEM fuel cell performance) as comparable to that of Nafion-117. Finally the results obtained from our studies are indicated that the syntesized membranes were expected to be new options as promising PEM materials in fuel cell technology.



Fig. 1. Photographs of SPOBI /GO Composite- Membranes

- Wang, Y., Chen, K. S., Mishler, J., Cho, S. C. & Adroher, X. C. *Appl. Energy*88, 981–1007 (2011).
- De Bruijn, F. A., Makkus, R. C., Mallant, R. K. A. M. & Janssen, G. J. M. Adv. Fuel Cells1, 235–336 (2007).
- 3. Kraytsberg, A. & Ein-Eli, Y. Energy & Fuels28, 7303-7330 (2014).

Photoredox Mediated Arylation of ArenesandHeteroarenes by Magnetically Active Recyclable Iron-Nanocatalyst

Tanumoy Mandal, Sanju Das, Ashwin Chaturvedi, and Suman De Sarkar¹*

¹Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur-741246, West Bengal, India *E-mail: sds@iiserkol.ac.in*

Abstract: Light is an inexpensive, abundant, and endlessly renewable source of clean energy. Thus, visible light photoredox catalysis as an effective and versatile method has become a powerful and promising tool. However, the main drawback arises in this context is that most of the photocatalysts are precious and some of them are not eco-friendly.² On the otherhand, scientists have paid countless attention in this particular field of heterogeneous catalysis. In this case, a catalyst is employed to drive the reaction and after completing the catalytic cycle, the regenerated catalyst can be isolated easily from the reaction mixture for further use. There are few reports to apply the complex of MOF and costly organocatalyst for photoredox reactions to utilize this recyclable strategy.³

Herein, we have synthesized magnetically active nano-particles of Fe_3O_4 , disclosed its photophysical properties and demonstrated the application of this nano-catalyst in C-C bond forming reaction under photoredox condition. This arylation reaction of arenes or heteroarenes with *in situ* generated diazonium salts reveals the potent redox phenomenon of the nano-catalyst via an oxidative quenching pathway.



- 1. Prier, C. K.; Rankic, D. A.; MacMillan, D. W. Chem. Rev. 2013, 113, 5322.
- 2. Shaw, M. H.; Twilton, J.; MacMillan, D. W. J. Org. Chem. 2016, 81, 6898.
- (a) Chakraborty, S.;Ahmed, J.;Shaw, B. K.;Jose, A.; Mandal, S. K.*Chem. Eur. J.*2018, 24, 17651.
 (b) Luo, J.;Zhang, X.;Zhang, J. ACS Catal. 2015, 5, 2250.

P52 pH Responsive P(LYS-HEMA) Polymer Degradation via Intramolecular Cyclization

Bibhas Hazra, Neha Choudhury, Priyadarshi De, Pradip Kumar Tarafdar*

Department of Chemical Sciences, IISER Kolkata, Mohanpur, West Bengal – 741246, India Email: tarafdar@iiserkol.ac.in

Abstract: Over the past several years, stimuli responsive degradable polymeric materials have increased considerably.¹ Such materials find major applications in self-healing and reinforced composites, in tissue engineering and adhesives, drug delivery and biosensors. Intramolecular cyclization assisted fast degradation of ornithine-based poly(ester amide)s suggest that cyclization may be an important strategy for degradation of polymer and drug release.² To characterize the extent of intramolecular cyclization in monomer and in polymer backbone, we have synthesized several P(LYS-HEMA) polymers. ¹H-NMR titration experiments suggest that the intramolecular cyclization increases with pH and polymeric backbone facilitates the cyclization.

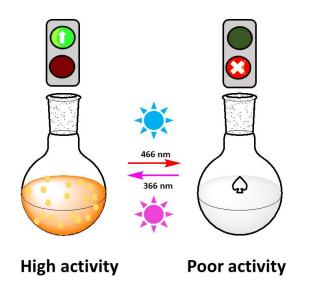
- T. P. Lodge, C. K. Ober, S. Z. D. Cheng, P. T. Hammond, M. Muthukumar, E. Reichmanis, K. L. Wooley. Macromolecules 2009, 42, 465–471.
- 2. Caroline de Gracia Lux, Jason Olejniczak, Nadezda Fomina, Mathieu L. Viger, Adah Almutairi. Journal of Polymer Science, Part A: Polymer Chemistry **2013**, *51*, 3783–3790.

P53 A Reversible Photoresponsive Activity of a Carbonic anhydrase Mimic

Monochura Saha, Subhajit Bandyopadhyay*

Department of chemical science, Indian Institute of Science Education and Research, Mohanpur, Nadia, Westbengal – 741246, India sb1@iiserkol.ac.in

Abstract: Carbonic anhydrase (CA) is an enzyme that reversibly transforms carbondioxide and water to a carbonate ion and a proton. Considering the importance of the enzyme, a number of CA-mimics have been reported previously. However, photoresponsive enzyme mimics, where the CA-activity can be turned on and off with light, has not been reported so far. Considering the active site of the enzyme, we have designed an active site mimic that can offer reversible control on the catalytic activity using light. Moreover, in the presence of a polymeric system, we demonstrate that the carbonic anhydrase activity can show a better rate enhancement in the active *cis*-form of the photoisomer. A photochromic azobenzene based Zn^{2+} -complex shows efficient carbonic anhydrase activity in the *cis*-form. In the presence of a cationic polymer that can stabilize the transition state, the activity further improves. Reversible control of the activity was achieved by the photoswitching of the complex with light.



- 1. M. Saha, S. Bandyopadhyay, Chem. Commun., 2019, 55, 3294-3297.
- 2. M. Saha, S. Ghosh, S. Bandyopadhyay, New J. Chem., 2018, 42, 10784-10790.

P54 The Free Energy Profile of Complexation of two oppositely charged Polyelectrolyte Chains

Soumik Mitra¹*, Arindam Kundagrami ^{1,2}

1Department of Physical Sciences, IISER Kolkata, Nadia, West Bengal-741246, India 2Centre for Advanced Functional Materials, IISER Kolkata, Nadia, West Bengal-741246, India *Presenting Author, Email: sm13ip032@iiserkol.ac.in

Abstract: We report a study of the complexation process of two oppositely charged polyelectrolyte (PE) chains in dilute solution interacting through an attractive screened Coulomb potential. The system is modeled using the PE chains free energy within the uniform spherical expansion approximation where the two PE chains as well as the neutral complex are considered to be hypothetical spheres whose radii quantitatively denote the sizes of the respective chains. The two chains start overlapping due to the entropy gain of free counterions, as well as the mutual attraction between the oppositely charged monomers. The complexation process ends up in the formation of a neutral coecervate through mutual adsorption of oppositely charged monomers, with associated release of all counterions of both types. The free energy profile that follows this pathway is studied by obtaining the variations of the total free energy, as well as the various individual energy and entropy contributions, as functions of the extent of overlap of the two chains. Also the behavior of the chain size and charge as functions of overlap is presented. These results elucidate the competition of the various driving forces, both enthalpic and entropic in nature, which lead to complexation.

- 1. Ou, Z.; Muthukumar, M. J. Chem. Phys. 2006, 124, 154902.
- 2. Winkler, R. G.; Steinhauser, M. O.; Reineker, P. Phys. Rev. E. 2002, 66, 021802 .
- 3. Muthukumar, M. J. Chem. Phys. 2004, 120, 9343.

Meta-Fluorophores: Inception of a New Generation of Single Benzenic Ultra Small Fluorophores Exhibiting Red-NIR Fluorescence

Mrinal Mandal^{1,*}, Prasun K. Mandal^{1,2}

¹Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) - Kolkata, Mohanpur, West- Bengal, India- 741246 ²Centre for Advanced Functional Materials, Indian Institute of Science Education and Research (IISER) -Kolkata, Mohanpur, West- Bengal, India- 741246. *Email: mm13ip017@iiserkol.ac.in (MM); prasunchem@iiserkol.ac.in (PM)

Abstract: To design smaller fluorophores exhibiting red-NIR emission has been an ominous challenge towards vast applications such as OLEDs, bioimaging, chemical sensor etc.¹ To achieve red emission, extended π -conjugation has been employed which is achieved through fusing several benzene rings together in which donor-acceptor groups are para-oriented.¹ A new general methodology for designing red-NIR emitting ultra-small fluorophores has been proposed in which donor-acceptor groups are meta-oriented (henceforth termed as metafluorophores). Based on this approach, several single benzenic meta-fluorophores, 1-8 (Fig. 1) have been synthesized. These ultra-small meta-fluorophores exhibit fascinating emission properties such as tunable emission (blue-green-red-NIR) in solution as well as in solid state, large Stokes shift and large solvatochromic shift. In literature, smallest reported red emitting fluorophores has a MW of 252.5 Da.^{2, 3} However, that particular fluorophore does not exhibit any significant Stokes shift or solvatochromic shift.^{2, 3} Employing current approach red emission have been achieved with ultra-small meta fluorophores having lowest molecular weight of 177.1 Da. Interestingly, the magnitude of the Stokes shift (260 nm) and solvatochromic shift (160 nm) are much higher in meta-fluorophores than the corresponding para derivatives. These simply synthesizable, small sized single benzenic meta fluorophores, could be employed towards cost-effective, bright white light emission.



Figure 1. Meta benzenic rainbow fluorophores (MBRFs).

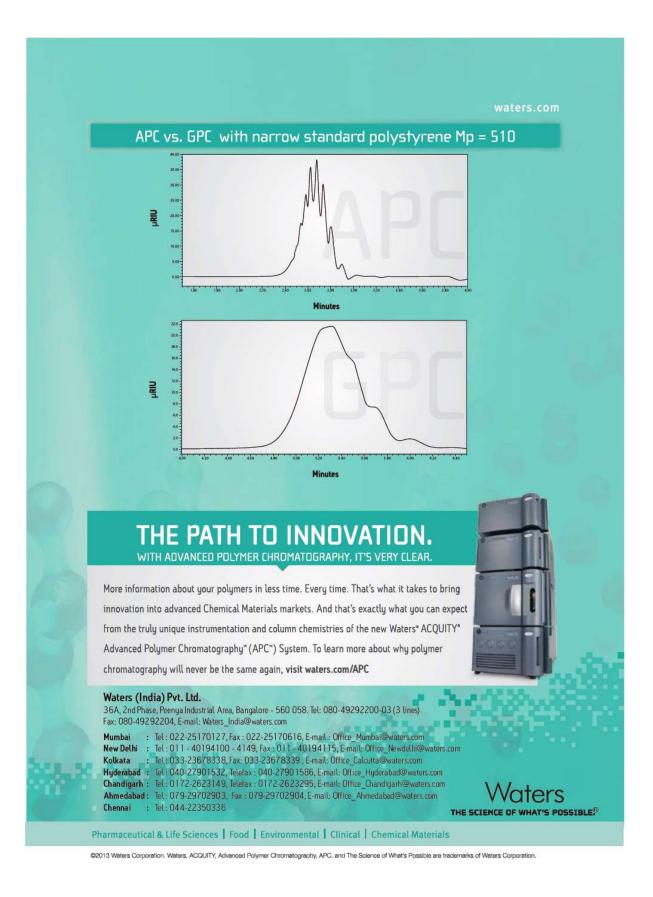
Reference:

P55

- 1. Lackowicz, J. R. Principles of Fluorescence Spectroscopy. 3rd ed.; Springer: 2006.
- 2. Tang, B.; Wang, C.; Wang, Y.; Zhang, H. Angew. Chem. Int. Ed. 2017, 56, 12543.
- Zhang, J. N.; Kang, H.; Li, N.; Zhou, S. M.; Sun, H. M.; Yin, S. W.; N. Zhao; Tang, B. Z. Chem. Sci. 2017, 8, 577.



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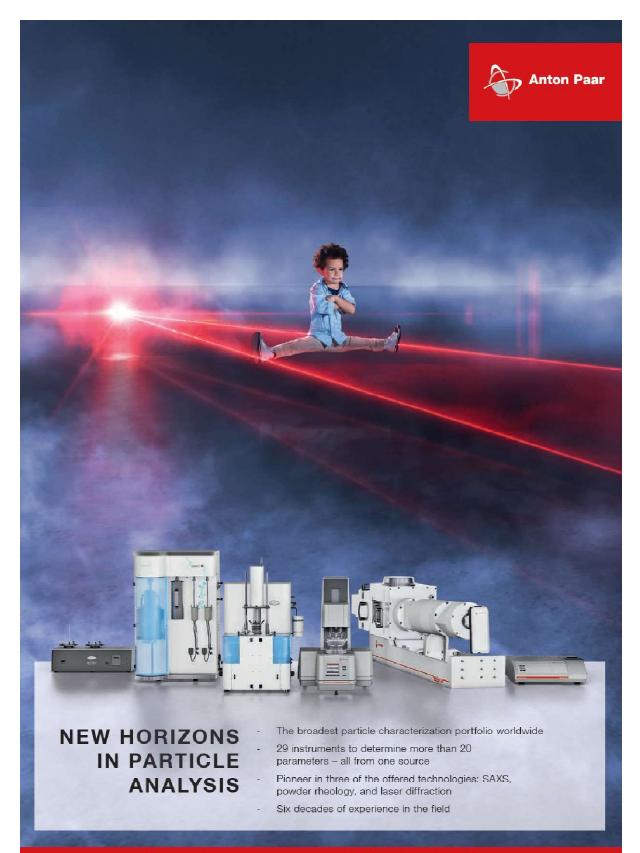
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