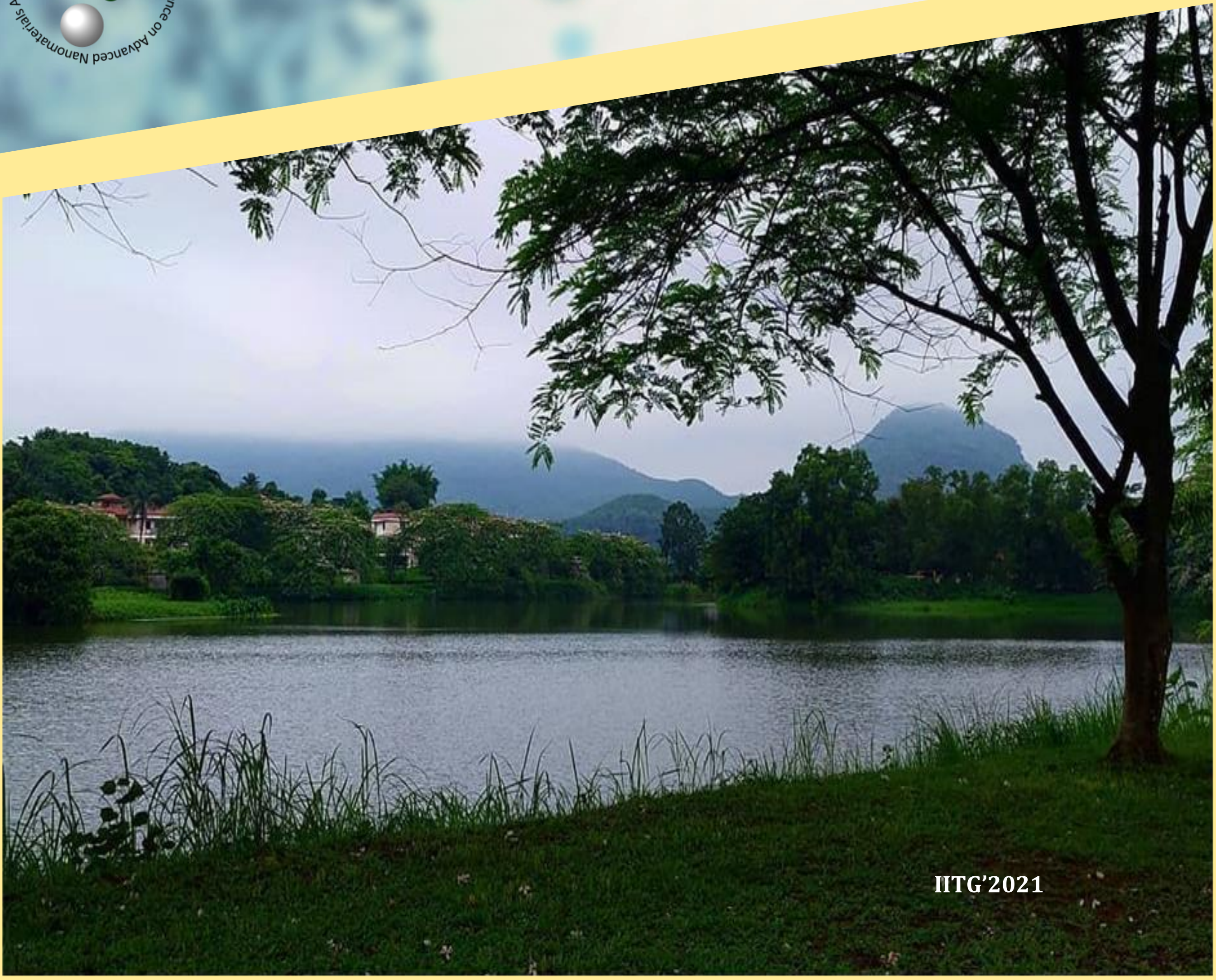
ICANN2021

7TH INTERNATIONAL CONFERENCE ON ADVANCED NANOMATERIALS AND NANOTECHNOLOGY

14-17 DECEMBER 2021
IIT GUWAHATI, ASSAM, INDIA

ABSTRACT BOOK



Welcome to

7th International Conference on Advanced Nanomaterials and Nanotechnology

ICANN2021

Organized by

Centre for Nanotechnology

INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

Guwahati–781039, Assam, INDIA

CAMPUS MAP

INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI

7th International Conference on
Advanced Nanomaterials and Nanotechnology
(ICANN-2021)
14-17 Dec, 2021

भारतीय प्रौद्योगिकी संस्थान गुवाहाटी
INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
Center for Nanotechnology
Guwahati –781039, Assam, INDIA

Dear Participants of the ICANN2021 conference,

On behalf of the faculty, staff, students and administration at Indian of Technology Guwahati, we are very happy to welcome you to the 7th International Conference on Advanced Nanotechnology (ICANN 2021). It has been our intention that ICANN2021 provides the profession, excitement and scientific vision of the International Nanomaterials and Nanotechnology community and we heartily welcome all our distinguished guests for the online conference. ICANN2021 will provide an international forum for professional networking, scientific knowledge sharing, research collaboration, interdisciplinary education of most recent scientific advances.

We also take this opportunity to write few words on the Centre for Nanotechnology at IIT Guwahati, established in the year of 2004. IITG possesses a vision to foster the development of research and education in multidisciplinary area of Nanotechnology at Centre for Nanotechnology, IIT Guwahati, to develop human resources gifted with leading-edge competitive advantages in the multi-disciplinary area of Nanotechnology. Prof. Arun Chattopadhyay the founding Head of this Centre for Nanotechnology from April 2009-June 2013, further enhanced the activities of this Centre by promoting various activities like organizing ICANN conference series in the years 2009, 2011, 2013, 2015, 2017 and 2019 with the aim to promote active interdisciplinary research and education activities for participants. Following this tradition, Prof. Siddhartha S. Ghosh and Prof. Roy P. Paily also continued the this tradition and we are organizing the ICANN2021 conference with the active support of Prof. Dipankar Bandopadhyay, the present Head, Centre for Nanotechnology. Pandemic has forced us to conduct the conference in online mode for the first time. Active physical interaction and discussion will surely be missed along with Assam Tea and North Eastern India cusine and the scenic beauty. The faculty, staff, students and local committee have worked hard to put together the ICANN2021 conference and we encourage your active participation in this conference. We strongly believe that your knowledge, contribution and sharing of scientific advances from your vast experience will help in resolving critical issues in the frontiers area of Nanoscience and Technology.

Once again, we welcome you to IIT Guwahati and best wishes for a highly successful meeting.

Sincerely

Siddhartha S. Ghosh

&

Parameswar K. Iyer

Convener-ICANN-2021

7th International Conference on Advanced Nanomaterials & Nanotechnology

14-17 December, 2021

Indian Institute of Technology Guwahati, Guwahati -781039
Assam, India

Local Organizing Committee

Prof. Akshai Kumar Alape Seetharam
Prof. Ashok Kumar Dasmahapatra
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Centre for Nanotechnology
IIT Guwahati, Guwahati

Schedule

ICANN2021 SCHEDULE

14.12.2021

December 14 15:00-15:15

Session 1 A (M1)

Inauguration

15:00-15:02	Prof. Parameswar Krishnan Iyer
15:02-15:06	Prof. Dipankar Bandopadhyay
15:06-15:13	Director IIT Guwahati
15:13-15:15	Prof. Siddhartha S Ghosh

December 14 15:15-16:45

Session 1 B (M1)

Chair: Prof. Dipankar Bandopadyay

IT1	15:15-15:45	Prof. Bin Liu (NUS, Singapore)
IT2	15:45-16:15	Prof. Rajeev Ahuja (IIT Ropar)
IT3	16:15-16:45	Prof. T Govindaraju (JNCASR)

BREAK

December 14 17:00-18:00

Session 1 C (M1)

Chair: Dr. Nageswara R Peela

A1083	FT1	17:00-17:07	Rakesh K Behera
G1079	FT2	17:08-17:15	Viresh Kumar
A1134	FT3	17:16-17:23	Pratibha Agrawal
E1149	FT4	17:24-17:31	Surendra K Saini
A1111	FT5	17:32-17:39	Rupam Roy
K1066	FT6	17:40-17:47	Nirmal Roy
A1041	FT7	17:48-17:55	Archana Kumari

M1 - Meeting 1@ICANN2021

M2 - Meeting 2@ICANN2021

IT- Invited Talk
ST- Short Talk
FT- Flash Talk

M1 -Sessions (1A, 1B, 1C, 2A, 2C, 2E, 2G, 3A, 3C, 3E, 3G, 4A, 4C)
M2- Sessions (2B, 2D, 2F, 2H, 3B, 3D, 3F, 3H, 4B)

DAY 2 -M1

December 15 09:00-11:00

Session 2A (M1)		
Chair: Dr. Selvaraju Narayanasamy		**Nano material**
IT4	09:00-9:30	Prof. Arindam Banerjee (IACS, Kolkata)
IT5	09:30-10:00	Dr. Sanjib Banerjee (IIT Bhilai)
IT6	10:00-10:30	Prof. C. R. Bhattacharjee (Assam University)
IT7	10:30-11:00	Dr. Ritu Gupta (IIT Jodhpur)

December 15 11:00-13:00

Session 2C (M1)		
Chair: Prof. Siddhartha S Ghosh		**Bio material**
IT12	11:00-11:30	Prof. Samir K. Maji (IIT Bombay)
IT13	11:30-12:00	Prof. Biman B. Mandal (IIT Guwahati)
IT14	12:00-12:30	Dr. Shaikh M. Mobin (IIT Indore)
IT15	12:30-13:00	Prof. Ehud Gazit (TAU, Israel)

BREAK

December 15 14:00-15:30

Session 2E (M1)		
Chair: Dr. Uttam Manna		**Nano material**
IT20	14:00-14:30	Dr. Abhijit Patra (IISER Bhopal)
IT21	14:30-15:00	Prof. Raja Shunmugam (IISER Kolkata)
IT22	15:00-15:30	Prof. Gopinath Packirisamy (IIT Roorkee)

December 15 15:30-18:00

Session 2G (M1)			
Chair: Dr. Arun Tej M			
G1008	15.36- 15.43	FT8	Debojit Paul
G1024	15.44- 15.51	FT9	CHING THIAN MOI
C1053	15.52- 15.59	FT10	Sravani Kaja
G1028	16:00-16:07	FT11	Praveen Kumar
G1030	16:08-16:15	FT12	Hemanth K Beere
G1034	16:16-16:23	FT13	Srijon Ghosh
G1036	16:24-16:31	FT14	Kritiman Marjit
G1047	16:32-16:39	FT15	Prangya Bhol
G1048	16:40-16:47	FT16	Raktim Gogoi
G1052	16:48-16:55	FT17	Soniya Agarwal
G1061	16:56-17:03	FT18	ANUSRI MEDDA
G1076	17:04-17:11	FT19	KIRAN MAYAWAD
G1077	17:12-17:19	FT20	Rishi Verma
C1098	17:20-17:27	FT21	Ramesh Babu Y
G1090	17:28-17:35	FT22	Zahir Abbas
G1110	17:36-17:43	FT23	Meenakshi Sharma
C1012	17:44-17:51	FT24	Sabyasachi Das
C1118	17:52-18:00	FT25	Kasturi Gogoi

M1 - Meeting 1@ICANN2021

DAY 2 -M2

December 15 09:00-11:00

Session 2B (M2)

Chair: Prof. Pravat Kumar Giri		Material for device
IT8	09:00-9:30	Prof. Zachary M. Hudson (UBC, Canada)
IT9	09:30-10:00	Prof. Shyam S. Pandey (KIT, Japan)
IT10	10:00-10:30	Prof. Mohd. Qureshi (IIT Guwahati)
IT11	10:30-11:00	Dr. Poulomi Roy (CSIR-CMERI)

December 15 11:00-13:00

Session 2D (M2)

Chair: Dr. Kalyan Raidongia		60th Birth Day Prof. AK Ganguli
IT16	11:00-11:30	Prof. Amitava Patra (INST, Mohali)
IT17	11:30-12:00	Prof. Arun Chattopadhyay (IIT Guwahati)
IT18	12:00-12:30	Prof. Hirendra Ghosh (INST Mohali)
IT19	12:30-13:00	Prof. Ashok K. Ganguli (IIT Delhi)

BREAK

December 15 14:00-15:30

Session 2F (M2)

Chair: Dr. Harshal B Nemade		Device
IT23	14:00-14:30	Dr. Shaibal Mukherjee (IIT Indore)
IT24	14:30-15:00	Prof. Rajadurai Chandrasekar (Univ. Hyd.)
IT25	15:00-15:30	Dr. Soumitra Satapathi (IIT Roorkee)

December 15 15:30-18:00

Session 2H (M2)

Chair: Dr. D Pamu			
A1011	15.36- 15.43	FT26	Shilpi Jaiswal
A1013	15.44- 15.51	FT27	NEHA CHOUDHARY
A1015	15.52- 15.59	FT28	Swarnalata Swain
A1037	16:00-16:07	FT29	Paulami Bose
A1040	16:08-16:15	FT30	Angana Borbora
D1145	16:16-16:23	FT31	RAJIB SHOME
A1043	16:24-16:31	FT32	Arpita Shome
A1055	16:32-16:39	FT33	SARITA KOLAY
A1058	16:40-16:47	FT34	Vishal Kumar
A1064	16:48-16:55	FT35	Bhavya M.B.
A1067	16:56-17:03	FT36	Debasish Borah
A1162	17:04-17:11	FT37	Debasish Barman
A1092	17:12-17:19	FT38	Manideepa Paul
A1093	17:20-17:27	FT39	Puja Saikia
A1095	17:28-17:35	FT40	AVIJIT PATRA
B1057	17:36-17:43	FT41	eepthi Priyanka Damer
B1087	17:44-17:51	FT42	SUVODEEP SEN
B1121	17:52-18:00	FT43	Sanjib Kumar Baglari

DAY3- M1

December 16 09:00-11:00

Session 3A (M1)

Chair: Dr. P Gopinath		Bio-Material
IT26	09:00-9:30	Prof. Robert Flavell (UCSF, USA)
IT27	09:30-10:00	Dr. Apurba Lal Koner (IISER Bhopal)
IT28	10:00-10:30	Prof. Rohit Srivastava (IIT Bombay)
IT29	10:30-11:00	Prof. Chittaranjan Patra (IICT Hyderabad)

December 16 11:00-13:00

Session 3C (M1)

Chair: Prof. Mohd. Qureshi		Material for Device
IT34	11:00-11:30	Dr. Mukesh Kumar (IIT Ropar)
IT35	11:30-12:00	Prof. Monica Katiyar (IIT Kanpur)
IT36	12:00-12:30	Dr. Santhosh Babu Sukumaran (NCL Pune)
IT37	12:30-13:00	Dr. Abhay Sachdev (CSIR-CSIO)

BREAK

December 16 14:00-15:30

Session 3E (M1)

Chair: Prof. P. K. Giri		Materials
IT42	14:00-14:30	Prof. Mahesh Hariharan (IISER Thiruvananthapuram)
IT43	14:30-15:00	Prof. Ramanathan Vaidhyanathan (IISER Pune)
IT44	15:00-15:30	Prof. Vivek Polshettiwar (TIFR)

December 16 15:30-18:00

M1 - Meeting 1@ICANN2021

Session 3G (M1)

Chair: Dr. P Gopinath

D1049	15.36- 15.43	FT44	Dencil Basumatary
D1074	15.44- 15.51	FT45	Navpreet kaur
D1089	15.52- 15.59	FT46	Ankit Samanta
D1106	16:00-16:07	FT47	Maharshi Thalla
D1144	16:08-16:15	FT48	Muktashree Saha
D1147	16:16-16:23	FT49	Debashree Debasmita
D1116	16:24-16:31	FT50	MITALI BASAK
J1082	16:32-16:39	FT51	Himadree Das
J1085	16:40-16:47	FT52	AKBAR ALI
J1094	16:48-16:55	FT53	Suditi Neekhra
K1026	16:56-17:03	FT54	Randeep Kaur
K1054	17:04-17:11	FT55	SHIVASISH DAS
K1108	17:12-17:19	FT56	Nehal Zehra
A1126	17:20-17:27	FT57	Neeraj Kumar Sah
A1133	17:28-17:35	FT58	sakshi bawa
A1006	17:36-17:43	FT59	SHANKHA BANERJEE
A1007	17:44-17:51	FT60	Subhadeep Das
A1010	17:52-18:00	FT61	Bharti Koshti

DAY3- M2

December 16 09:00-11:00

Session 3B (M2)

	Chair: Dr. Arun Tej M	Device
IT30	09:00-9:30	Prof. Aditya D Mohite (Rice University, USA)
IT31	09:30-10:00	Dr. Abhijit Hazarika (IICT Hyderabad)
IT32	10:00-10:30	Dr. Vijayakumar Chakkooth (CSIR-NIIST)
IT33	10:30-11:00	Dr. Anuja Datta (IACS, Kolkata)

December 16 11:00-13:00

Session 3D (M2)

	Chair: Prof. Parameswar K Iyer	Device
IT38	11:00-11:30	Dr. Ratheesh K. Vijayaraghavan (IISER Kolkata)
IT39	11:30-12:00	Dr. V Aravindan (IISER Tirupati)
IT40	12:00-12:30	Dr. Satyaprasad P. Senanayak (NISER)
IT41	12:30-13:00	Dr. Rohit John Abraham (ETHZ, Switzerland)

December 16 14:00-15:30

Session 3F (M1)

	Chair: Tapas Kumar Mandal	Inorganic Materials
IT45	14:00-14:30	Dr. Chandana Rath (IIT BHU)
IT46	14:30-15:00	Dr. Neha Hebalkar (ARCI)
IT47	15:00-15:30	Dr. Somenath Garai (BHU)

December 16 15:30-18:00

Session 3H (M2)

M2 - Meeting 2@ICANN2021

Chair: Dr. Mahima Arrawatia			
G1141	15.36- 15.43	FT62	Rabindranath Garai
G1128	15.44- 15.51	FT63	Richa Tiwari
G1131	15.52- 15.59	FT64	GAURAV SINGH
C1016	16:00-16:07	FT65	Srimanta Pal
C1119	16:08-16:15	FT66	Riya Sebait
C1120	16:16-16:23	FT67	Madalasa Mondal
G1027	16:24-16:31	FT68	SOURAV BHOWMICK
F1123	16:32-16:39	FT69	Ritupan Borah
F1045	16:40-16:47	FT70	PUSHPANJALI PATRA
C1124	16:48-16:55	FT71	Himangshu J. Gogoi
A1003	16:56-17:03	FT72	Vivekshinh Kshtriya
A1004	17:04-17:11	FT73	ARIJIT JANA
E1051	17:12-17:19	FT74	Angira Das
E1080	17:20-17:27	FT75	Jahnabi Gogoi
E1081	17:28-17:35	FT76	ANKITA DEB
E1097	17:36-17:43	FT77	Aviti Katare
I1031	17:44-17:51	FT78	Ankit Nagar
	17:52-18:00	FT79	

DAY 4 M1

December 17 9:00-11:58

Session 4A (M1)

Chair: Dr. Salil Kashyap

A1086	09:00-09:07	FT80	Biswajit Hudait
A1070	09:08-09:15	FT81	KANISKA MURMU
A1102	09:16-09:23	FT82	Manoj K Mohanta
A1071	09:24-09:31	FT83	Pronoy Dutta
A1072	09:32-09:39	FT84	Prerona Gogoi
A1073	09:40-09:47	FT85	Tapas Pal
A1078	09:48-09:55	FT86	Bipasha Saikia
A1114	09:56-10:03	FT87	Priyalakshmi Devi
A1125	10:04-10:11	FT88	Shankab Jyoti Phukan
B1107	10:12-10:19	FT89	Smita Das
B1150	10:20-10:27	FT90	Deepa Garg
E1112	10:28-10:35	FT91	Anand Maurya
E1113	10:36-10:43	FT92	Abrar Ahamad
E1127	10:44-10:51	FT93	Riu Riu Wary

DAY 4 M2

December 17 9:00-11:58

Session 4B (M2)

Chair: Dr. Ravindra Kumar Jha

C1160	09:00-09:15	ST1	Dipjyoti Das
H1059	09:16-09:30	ST2	Subhamoy Singha Roy
K1065	09:31-09:38	FT96	Neha Barnwal
K1029	09:39-09:46	FT97	MANPREET KAUR
K1032	09:47-09:54	FT98	Pillalamarri Srikrishnarka
K1033	09:55-10:02	FT99	Tanvi Gupte
K1035	10:03-10:10	FT100	MD TOUSIF ALAM
K1060	10:11-10:18	FT101	Barsha Rani Bora
K1063	10:19-10:26	FT102	KABYASHREE PHUKAN
A1142	10:27-10:34	FT103	Ritesh Kant Gupta
K1069	10:35-10:42	FT94	Nirmiti Mate
K1091	10:43-10:50	FT95	MIHIR MANNA
K1025	10:51-10:58	FT96	Geetika Bhardwaj

BREAK

Session 4B (M1)

December 17 11:00-12:30

Chair: Dr. Ashok K Dasmahapatra

IT47	11:00-11:30	Prof. Satish A. Patil (IISc Bangalore)
IT48	11:30-12:00	Dr. Satish K. Dubey (IIT Delhi)
IT49	12:00-12:30	Prof. Dipankar Bandyopadhyay (IIT Guwahati)

December 17 12:30-13:00

Flash Talk(FT) Award and Valedictory Session

Prof. Parameswar K Iyer	Flash talk prize announcement, ICANN2023 announcement
Prof. Siddhartha S Ghosh	Vote of thanks

Content

Invited Speaker

Flash Talk

Secondary Phases, Defects and Interface Engineering in Earth Abundant CZTS Solar Cells

Mukesh Kumar*, Nisika, Kumwinder Kaur

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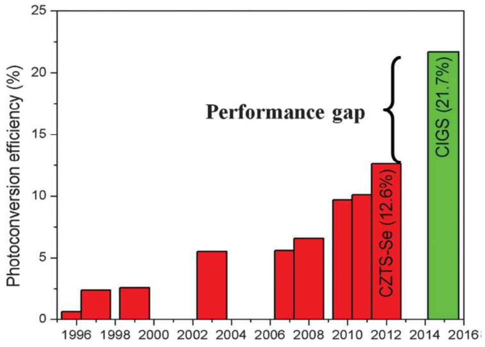
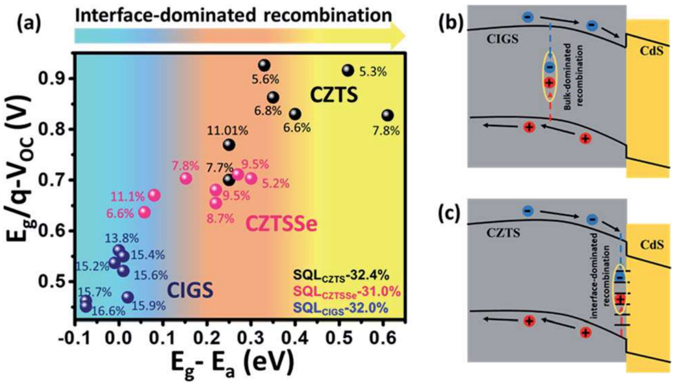
Almost 80% of the world's energy demand is fulfilled by fossil fuels which produces greenhouse gases upon combustion and are primary contributors of global warming. Moreover, the rarity and scarcity of these energy resources will lead to catastrophic state to meet future energy demands. Meeting the global energy demands in a sustainable fashion needs nonpolluting and an abundant resource of energy. Solar energy can provide a substantial fraction of global energy demands in near future. International Energy Agency (IEA) estimated 11% of global electricity production through photovoltaics (PV) by 2050 that would dodge 2.3 Gigatons (Gt) of CO_2 emissions per year [1] Thin-film solar cell technology is considered to play an important role to meet this terawatt (TW)-scale PV power demand at an affordable price. Cost-effective kesterite copper-zinc-tin-sulfide–selenide (CZTS–Se) and perovskite are considered as cost-effective solution for next generation solar cells. However, current CZTS–Se and perovskite solar cells have many open challenges for their commercialization.

The narrow phase stability and non-stoichiometry in CZTS leads to formation of secondary phases and substantial amount of localized defects such as vacancies and antisites. The existence of highly conducting phases on the CZTS surface often results in non-performing devices as it offers shunting paths to current. Therefore, suppression of highly conducting phases and defects on CZTS surface urges a great challenge to further optimize the CZTS films and CZTS/buffer interface quality for better device performances. The interface engineering and probing using nanoscale charge transport and replacing conventional buffer layer is considered as a path forward for next generation CZTS solar cells.

Keywords: CZTS solar cells, secondary phase, defects, AFM and interface engineering





CMOS-compatible and Low Variability Memrisitve Crossbar Array for Medical Image Processing

Shaibal Mukherjee

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Indian Institute of Technology Indore, Simrol, Indore-453552, M.P., India

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Currently, transition metal-oxides play a very significant role to realize complementary metal-oxide-semiconductor (CMOS)-compatible memristive crossbar array for varied applications such as neuromorphic computation, image processing, storage and logic operations. However, there are several hinders such as low device throughput, high device-to-device (D2D) and cycle-to-cycle (C2C) variability to develop high-density memristive crossbar array for aforementioned applications. Here we present a successful fabrication of a stable, scalable, reproducible, and CMOS-compatible Y_2O_3-based memristive crossbar array of size 15×12 on silicon by utilizing dual ion beam sputtering (DIBS) system. The fabricated memrisitve crossbar array shows intrinsic nonlinear resistive switching characteristics with high endurance ($\sim 7.5\times10^5$ cycles), high inter-state resistance ratio (>200), high retention properties (2.25×10^5 sec), high device throughput, low D2D (0.25) and C2C (0.6080) variability parameters in the switching voltages. An analytical model is developed based on the fabricated memrisitve crossbar array, which is further deployed to analyze the biomedical images, specifically computed tomography (CT) scan and magnetic resonance imaging (MRI) images, by utilizing 2-dimensional (2D) image decomposition technique and discrete wavelet transform (DWT). To evaluate the performance of the memrisitve crossbar array-based image processing, various performance parameters such as peak signal-to-noise ratio (PSNR), structural similarity index (SSIM), and mean square error (MSE) of the reconstructed images have been analysed. The results are promising in the development of the Internet of Things (IoT), analog computation, in-memory computation, image processing and logic operations.

Keywords: Crossbar array, variability, image computation, CMOS-compatibility

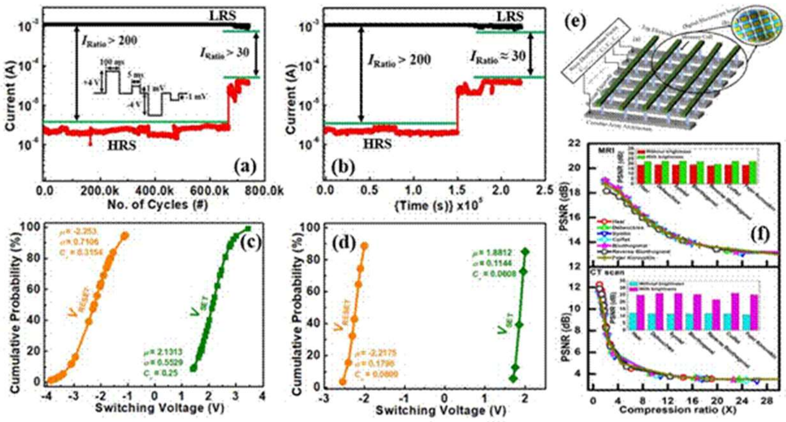

Figure: (a-b) Endurance and retention properties, (c-d) D2D and C2C variability, (e) image storage mechanism, and (f) PSNR vs compression ratio analysis of computed image.

Design and Development of NIR Dyes for Immense Solar Energy Harvesting based on Combined Theoretical and Experimental Approaches

Shyam S. Pandey*

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Kyushu Institute of Technology, $^{2-4}$, Hibikino, Wakamatsu, Kitakyushu, Japan

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Dye-sensitized solar cells (DSSCs) have attracted the huge attention of the materials science community not only due to environment-friendly and cost-effective solar energy harvesting but also their aesthetic vibrant colour tunability and tremendous potential for building integrated photovoltaics (BIPV) due to controllable transparency. Bi-facial solar cells are another area, where DSSCs find a tremendous application potential too. State-of-art DSSCs have reached photoconversion efficiencies (PCE) beyond 13 % despite photon harvesting window mainly in the visible wavelength region covering only 45 % photon flux of the solar spectrum. Sensitizing dyes can be considered as the heart DSSCs owing to their pivotal role in controlling the PCE as well as the stability of the devices. Design and development of near-infrared (NIR) dyes are inevitable for further improvement in the PCE by the panchromatic photon harvesting. The design of optimal sensitizers of DSSCs needs an amicable consideration about the presence of a suitable anchoring group, their energetic matching, high molar extinction coefficient and good electronic coupling between the excited dye molecules. Owing to the huge possibilities of molecular structures, quantum chemical (QC) calculations have emerged as one of the potential tools for the prediction of their energetics and spectral behaviour. Our group is involved for >10 years in the development of NIR dyes aiming towards the enhancement of the PCE of DSSCs. A series of NIR dyes from the Squaraine (SQ) family has been designed considering aspects like energetic control, wavelength tenability and implication of nature of anchoring group on the photovoltaic performance of DSSCs based combined theoretical (QC) and experimental approaches. Nature of the anchoring groups not only control the PCE by controlling the efficiency of electron injection but also controls the stability of DSSCs by controlling the extent of binding on the TiO_2 surface. Recently, we have demonstrated the design of novel NIR dyes bearing dual anchoring group with differential functionalities such one making strong binding while other imparting efficient electron injection aiming towards development of sensitizers for improved stability as well as stability of DSSCs. In the mean time DSSCs have also shown their potentiality towards BIPV applications owing to their transparency and aesthetic colour. Recently we have shown that judicious selection of colour of sensitizers play a dominant role in controlling the transparency and PCE of the transparent DSSCs, where we have demonstarted that red colour of the dyes are not suitable for such applications owing to the very high sensitivity of the human eye for the red colour. At the same time, use of NIR sensitizers along with yellow dye imparted transparent DSSCs not only with improved transparency but also the improved PCE. Similarly, utilization of NIR dyes have also demonstarted their suitability for the fabrication of bifacial DSSCs. In my lecture, emphasis will be given to the design and development of novel NIR dyes aiming towards not only enhancing the efficiency and stability of DSSCs but also their suitability in the colourful transparent as well as bifacial solar cells.

Keywords: NIR Dyes, Dye-sensitized solar cells, Quantum chemical calculations, Transparent solar cells, Bi-facial solar cells.

Hot Carrier Relaxation in $CsPbBr_3$-based Perovskites: A Polaron Perspective

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Long-standing interpretations for the exceptional photovoltaic and optoelectronic properties showcased by the perovskite family pertain to the underlying complicated interplay of polaron formation and hot carrier cooling. This Perspective primarily focuses on reassessing the existing status of polaron studies conducted on CsPbBr3-based systems in particular, in the framework of transient absorption investigations. The role of the key aspect that is ultimately accountable for deciding the fate of polaron formation, i.e., the carrier−longitudinal optical phonon coupling, has been comprehensively evaluated in terms of diverse factors which affect this Fröhlich interaction-mediated coupling. The study provides a detailed discussion regarding the alterations in lattice polarity, surrounding dielectric medium, lattice temperature, and system dimensionality which can influence the charge screening extent and thereby the polaron formation. Such studies concerning strategies for achieving easily attainable modulations in polaron formation in CsPbBr3-based systems are highly relevant for technological advancement.

Halide Perovskite Memristors as Flexible and Reconfigurable Physical Unclonable Functions

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Physical Unclonable Functions (PUFs) address the inherent limitations of conventional hardware security solutions in edge-computing devices. Despite impressive demonstrations with silicon circuits and crossbars of oxide memristors, realizing efficient roots of trust for resource-constrained hardware remains a significant challenge. Hybrid organic electronic materials with a rich reservoir of exotic switching physics offer an attractive, inexpensive alternative to design efficient cryptographic hardware, but have not been investigated till date. Here, we report a breakthrough security primitive exploiting the switching physics of one dimensional halide perovskite memristors as excellent sources of entropy for secure key generation and device authentication. Measurements of a prototypical 1 kb propyl pyridinium lead iodide (PrPyr[PbI3]) weak memristor PUF with a differential write-back strategy reveals near ideal uniformity, uniqueness and reliability without additional area and power overheads. Cycle-to-cycle write variability enables reconfigurability, while in-memory computing empowers a strong recurrent PUF construction to thwart machine learning attacks.

Keywords: Physical Unclonable Functions (PUFs), Halide Perovskite, Memristors

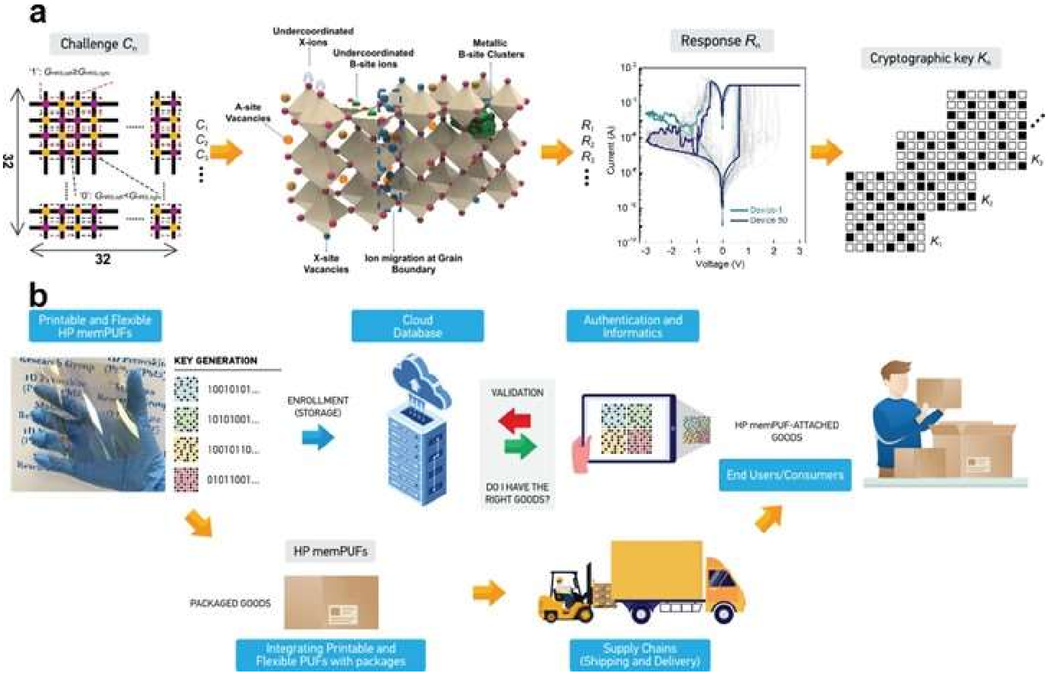

Figure: **a** HPs possess a rich reservoir of intimately coupled charge transport properties that could serve as sources of entropy to design new kinds of PUFs. **b** Concept schematic of product authentication

Benignant Electron Carrier Traps in Organic Semiconductors for Electrical Bistability

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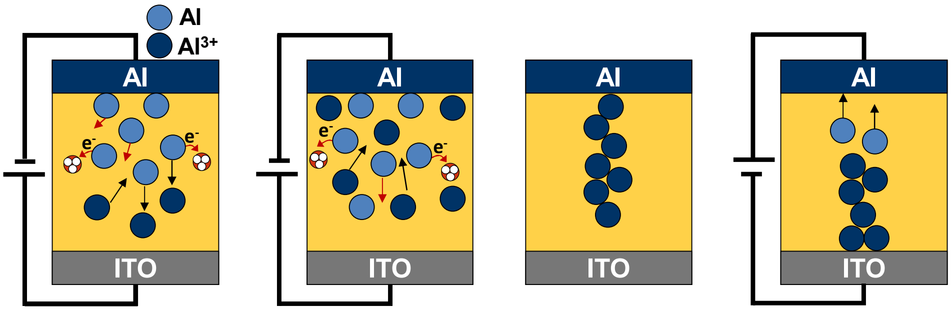
Charge carrier traps (**CCT**) are considered to be highly detrimental for the performance of most of the organic semiconductor (OSC) devices such as Organic Field Effect Transistors (**OFETs**), Organic Solar Cells (**OSC**) comprising OSC active layer (**AL**) processed under ambient environmental conditions. The present talk will describe our attempt of the functional utilization of this highly derogatory attribute (CCT) of tailored organic semiconductors to yield high performance organic memristor devices. The idea of translating the bulk charge traps as the cause to nucleate switchable electrical bistability (bistable conducting states) in metal-semiconductor metal (MSM) sandwich devices. Switching between two conducting state is the primary requisite of memristors or resistive memory devices that are considered as an essential electrical component in data processing and information technology. The bistable and switchable conductive states (ON & OFF or '0' & '1') can be assigned as the binary data storage and if it is reversible, it could be rewritable as well. Having a non-volatile nature to the stored data would make such devices superior over the volatile one with respect to the wide range of use. Here, we demonstrate the switching mechanism bases on the initial results of trap assisted control on the resistive state switching in Metal-Semiconductor-Metal devices with a precise control over the trap density by carefully designed chemical structures resulted in regulating the formation of conductive filaments persuaded in tuning the ON/OFF current ratio in resistive memory devices.

Keywords: Electron traps, Organic Semiconductors, Memristors



- Atom difusion Ion migration
- Accumulation at Top electrode (Electrodeposit)
- Non-volatile Conductive state
- Dissolution of the conductive channel under reverse bias

Scheme: Mechanism of the bistable electrical conductance inducted.

Engineering of Orientational Orders in Liquid Crystal Nanodroplets as Phototunable Softmasks

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A self-organized pathway is harnessed to generate large-area and high-density liquid crystal micro/nano droplets. The experiments reveal a transition from a spinodal to the heterogeneous nucleation pathway of dewetting when the surfactant loading is modulated in the aqueous phase. A host of unprecedented drop formation modes such as dewetting and contact-line instability (DeCI), random ejection (RanEj) and 'fire cracker' toroid splitting (FiCTS), have been uncovered. Such liquid crystal micro/nano droplets are employed as photomasks to decorate a host of mesoscale three-dimensional features on the photoresist films. In such a scenario, phase transition of LC droplets under solvent vapor annealing is employed to control the movement of photons through drops and subsequently modulate the light exposure on the photoresist surface. The orientation of nematogens within liquid crystal droplets and at the three-phase contact-line provide additional handles in controlling the transmission of photons, which facilitates such unique pattern formation. Importantly, with a minor modification to the same experimental setup, we could also measure the variation in the order parameter of micro/nano droplets during its phase transitions from nematic to isotropic state.

Multiblock Nanofibers from Organic Electronic Materials

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Techniques for the assembly of hierarchical nanostructures from soft matter have opened the door to many new applications of nanotechnology. Despite these achievements, nanoscale syntheses which rely on self-assembly can be highly dependent on conditions such as solvent and temperature if the integrity of the nanomaterial is to be maintained. Bottlebrush copolymers provide a compelling bottom-up approach to the synthesis of hierarchical nanostructures from soft material, allowing for the preparation of multicompartment structures that remain nanosegregated by virtue of their covalent chemistry. Here we describe methods for the preparation of fiber-like nanomaterials that mimic the multilayer structure of organic electronic devices on individual polymer chains. Narrowly dispersed fibers are prepared from materials commonly used as the hole transport, electron transport, and host materials in organic electronics, with molecular weights on the order of 10^6 Da. Finally, we use this approach to prepare nanofibers with the structure of multilayer organic devices on single macromolecules, and to reveal new photophysical properties enabled by this unique morphology.

Keywords: Bottlebrush polymers, ring-opening metathesis polymerization, organic light-emitting diodes, charge transfer, thermally activated delayed fluorescence

Gold, Silver and Copper Nanoclusters: From synthesis to applications

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Gold, silver and copper nanoclusters belong to a unique class of nanomaterials showing molecule-like behaviour and excellent fluorescent property. Gold nanoclusters was made by core-etching method from a gold precursor using a dipeptide L-cysteinyl-L-cysteine and mainly 7 atom Au clusters were observed. These blue emitting clusters have been successfully applied for very selective and ultra-sensitive sensing of AsIII ions in the presence of other bivalent and trivalent metal ions in aqueous solution with a lower limit of detection (LOD) is 53.7 nM.[1] Other examples of preparing a few atoms fluorescent gold clusters include formation of clusters from gold nanorods and the use of these clusters for Fe (III) ions sensing slectively[2], synthesis of various-coloured different sized fluorescent gold clusters from blue to NIR and cancer cell-imaging by the NIR gold cluster [3], making of peptide capped different colour emitting gold quantum clusters with modulating photo switching property[4]. A recent example includes in situ the formation of fluorescent Au nanoclusters over the graphene sheet to create a novel trihybrid system consisting of C dots, rGO and carbon dots, in the presence of GO and gold salt and a blue light-emitting diode (LED) irradiation [5] and the application of this newly prepared nanohybrid system with C dots as a good photo-switching material and also a nanocatalyst. Blue, green and red emitting Ag clusters have been made by using a bioactive peptide and the red emitting clusters were used for selective and sensitive detection of toxic HgII ions in water by using even naked eyes, fluorometric, and calorimetric studies [6]. Different colour emitting Cu nanoclusters have been prepared by varying reaction conditions and orange-red emitting clusters have been used for overial cancer cell imaging [7]. A fascinating study includes the bulk scale synthesis of red emitting Cu nanoclusters and their use as a catalyst for the transformation of aromatic nitro to aromatic amino compounds with the reusability for several times [8].

A Model Approach to the Fermi Energy under Size Quantization with Nanostructured Systems

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During recent time, through the advent of MBE, MOCVD, FLL and other investigational method, low dimensional structures having quantum confinement in one, two and three dimensions such as ultra-thin films, inversion layers, quantum wires and dots, have attracted much attention, not only for their potential in uncovering new phenomena in nanostructured electronics but also for their interesting devices application in heterostructure based various materials, that are being currently studied because of the enhancement of carrier mobility and such quantum confined systems find ex-digital networks, optical modulators and also in other devices. In this paper, an effort is made to study the Fermi-Dirac distribution function in degenerate semiconductors forming band tails (f_s) on the basis of a newly formulated electron dispersion law (f_0) the well Fermi-Dirac function) and also it will be of much more interest, to investigate the Fermi-Dirac distribution function under the condition of carrier degeneracy, since it will help my revise in transport coefficients and electron dynamics in electronic devices ready of degenerate n-GaAs materials.

Keywords: Heterostructure materials, Fermi-Dirac distribution function, electron dispersion law.

Nanomaterials for Micro-Energy Harvesting: Successes and Challenges

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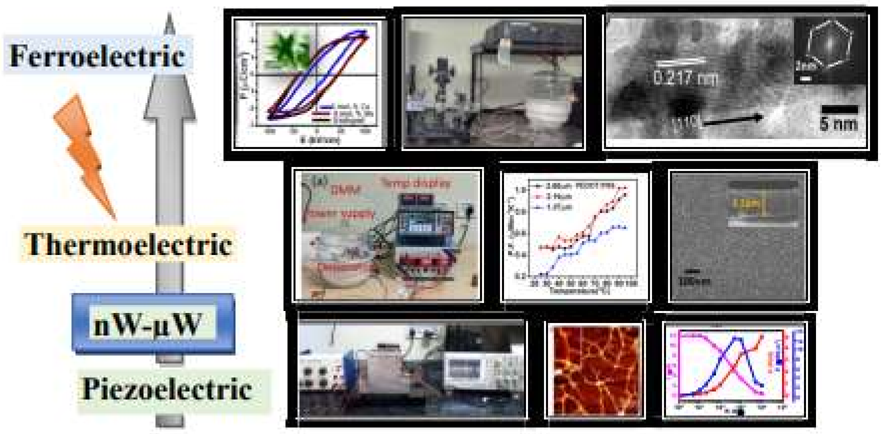
Dependencies on batteries are increasing exponentially as the sole choice of power source, with the increasing global reliance on electronic devices and gadgets in everyday life. Batteries require regular charging and eventually replacement, slowing down device performances and add to the materials wastage and pollution. [1] Harvesting or scavenging micro-energies is the conversion of ambient energy present in the environment such as heat (thermoelectric, pyroelectric), vibration (piezoelectric), static charges (triboelectric), magnetic (thermomagnetic, magnetoelectric) etc. into usable electrical energy for powering autonomous electronic devices or circuits and are suitable to run persistently through downsizing in nanoscale. [1-3] With increasing research and industrial interest in micro-energy harvesting, largely for sensing, and smart flexible electronics, latest aspect of energy harvesting in current technology is focused on the use of environment friendly inorganic oxides and organic materials that are commonly durable, light weight, temperature sensitive, can be easily manufactured without heavy cost and should be easily transferred to any workable surface. [3] In this talk, I will first build on the importance of materials development in improving micro-energy harvesting technologies, then will detail on inorganic/organic hybrid nano-thermoelectrics, and vibrational piezoelectric energy harvesting via. nanocomposites and oxide based ferroelectric nanostructures for micro-energy applications (using Zn- and Sn- based titanates and stannates perovskites), their facile synthesis and properties, which are currently the active research areas in micro-energy harvesting, carried out in my research group. [2,3]

Keywords: Energy Harvesting, Micropower, Thermoelectrics, Piezoelectrics, Ferroelectrics.



Colloidal Metal Halide Perovskite Quantum Dots: Opportunities and Challenges in PV Application

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Among all emerging photovoltaic (PV) technologies, metal halide perovskite (MHP) PV is undoubtedly the most promising technology for efficiently harvesting the solar energy in the near future. MHP semiconductors, with general chemical formula ABX3 (where A= Cesium-Cs, methylammonium-MA, formamidinium-FA etc.; B= Pb or Sn; X= Cl, Br, I), have already shown to inherently possess almost all the characteristics like high light absorption coefficient, long-range charge carrier diffusion and low exciton binding energy, which are highly desired in an ideal solar absorber material. In lower dimensions, 3D colloidal Quantum Dots of these unique materials offer some additional advantages which, otherwise are not achievable in their bulk or thin-film counterparts.1,2 For instance, although geometrical factors like Goldschmidt Tolerance Factor (GTF) do not favor formation of 3D structure of CsPbI3 with corner-shared [PbI6] 4- octahedra in ambient conditions, such structure can be stabilized in colloidal nanocrystalline form due to surface strain.3 Similarly, alloy compositions, like Cs1-xFAxPbI3 or Cs1-xFAxPb(Br1-xIx)3, can be synthesized in colloidal nanocrystalline form for any arbitrary value of "x", and such freedom is often lacking in the corresponding bulk/thin film.4,5 Such synthetic control and capabilities not only allow to tune the optical properties by expanding the compositional space of metal halide perovskites in general, but also offer unique opportunities to design Quantum Dot Solar Cells (QDSCs) that may complement the MHP PV technologies. All-inorganic CsPbI3 perovskite quantum dot based solar cells showed certified record efficiency of 13.4%6 in 2017 and just after a couple years, Cs1-xFAxPbI3 based QDSCs achieved a certified record efficiency of 16.6%7 in laboratory scale cells. Perovskite QD based solar cells also exhibit high VOC reaching ~ 90% of Shockley-Quiesser limit.4 Compatibility with environment friendly low boiling point solvents like hexane, octane, etc., has made the perovskite QDSCs ideal candidate for roll-to-roll processing for large-area fabrication. In this talk, we will discuss about suitability of colloidal perovskite quantum dots for PV applications by highlighting the above-mentioned advantages, and the challenges for future progress of this technology.

Keywords: Colloidal Perovskite Quantum Dots, Composition tuning, Perovskite Solar cells.

Development of World Class Thermal Insulation Product Based on Nanoporous Silica Aerogel

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Silica aerogel is known as world's most efficient thermally insulating material. The most attractive physical features of aerogels are its ultralow density, porosity as high as 99% and the pore size less than 100 nm, giving rise to the best thermal, electrical and acoustic insulation property in it. Due to these extraordinary properties in single material, the application areas are wide spread. However, being fragile in nature, these were unexplored for actual commercial applications for several years. We developed a fiber-aerogel composite product in the flexible sheet form having thermal conductivity as low as 0.01 W/Mk, which can serve as thermal insulator at high temperatures in many industrial applications. The other features of the product are resistance to fire, chemicals and corrosion, breathable and hydrophobic in nature. This product competes with globally available equivalent products and will be commercialized soon in India. The presentation will give the highlights of the journey during product development from lab scale to commercially viable product.

Keywords: aerogel, nanoporous, silica, thermal insulation, light weight.

Nitrogen-rich Mesoporous Carbon Nanoparticles: Design, Synthesis and Applications

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Increasing levels of CO_2 in the atmosphere has led to global warming, neceaastiating extensive research and development towards the development of new materials/technologies for CO_2 capture. On the water hand, controlling the rising level of water pollution has emerged as a major concern. We have developed a straightforward and cost-effective strategy for the synthesis of novel template-shape-replicated nitrogen-rich mesoporous carbon nanospheres (NMCN) with high surface area, pore volume and ordered pore geometry. NMCN demonstrated efficient ability for (a) CO_2 capture and (b) contaminant removal from wastewater.

Keywords: nanoparticle; global warming; water pollution; mesoporous; CO_2 capture

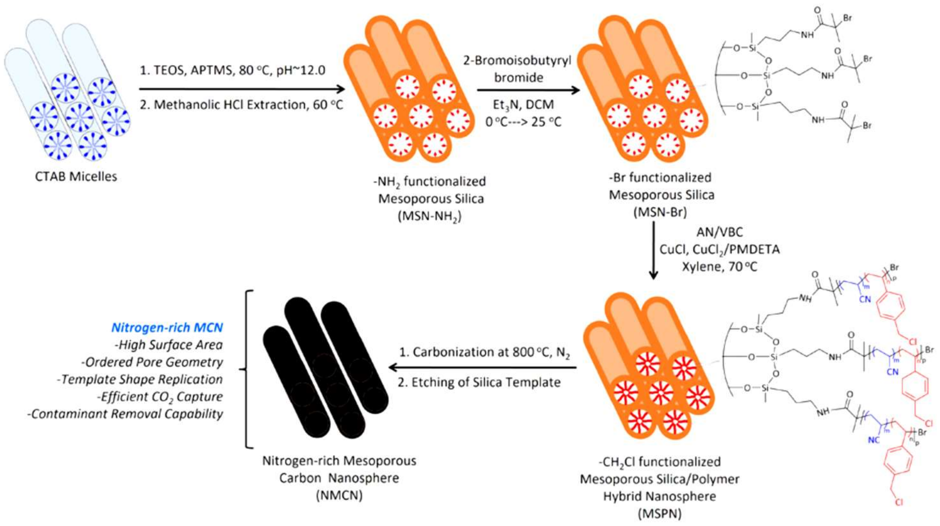

Figure: Synthesis of Nitrogen-rich Mesoporous Carbon Nanoparticles.

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Mimicking the Bio-Functions Inside the i-cells: A Next Generation Nanocavity for Studying Rehabilitated Kinetics for Catalysis Under Nano-Confinement of Inorganic Superfullerene

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The unique spherical nanocapsules/Keplerates of the type $[\{(Mo)Mo_5\}_{12}M'_{30}]$ ($M' = \{Mo^{V}{}_{2}\}$, V^{IV}, Cr^{III}, Fe^{III}) (more generally: (pentagon)$_{12}$(spacer/ligand)$_{30}$) allow versatile chemistry and applications as well as the option to study new phenomena of interdisciplinary interest due to their exceptional structural features and easy variations/derivatizations (Chem. Soc. Rev., 2012, 41, 7431 & Front Cover: Angew. Chem. Int. Ed., 2016, 55, 6634). The self-assembly of the $\{Mo^{VI}(Mo^{VI})_5O_{21}(H_2O)_6\}^{6-}$ -type pentagonal and $\{Mo^{V}{}_{2}O_4(H_2O)_2\}^{2+}$ -type diamond shaped dinuclear building blocks lead to the formation of icosahedral $[\{Mo^{VI}(Mo^{VI})_5O21(H_2O)_6\}^{12}\ \{Mo^{V}{}_{2}O_4(RCO_2)\}_{30}]^{42-}$ nanocluster (where R = H or alkyl); the central pentagonal bipyramidal $\{MoO_7\}$-subunits of 12-$\{Mo(Mo)_5\}$-type pentagons, are placed at the vertices of an icosahedron and are connected by 30 $\{Mo^{V}{}_{2}\}$-type dinuclear linkers to form the "Inorganic Superfullerene" or even "Inorganic Nano-football". Astonishingly, the cavity internal catalytic uptake of CO_2 via. the 30 $\{Mo^{V}{}_{2}\}$-receptors effects the formation of $[\{(Mo^{VI})Mo^{VI}{}_{5}O_{21}(H_2O)_6\}_{12}\ \{Mo^{V}{}_{2}O_4(CO_3)\}_{30}]^{72-}$ 2a (Angew. Chem. Int. Ed., 2012, 51, 10528) which has been proved to be a potential starting reagent for the synthesis of the novel Keplerates for e.g. the encapsulation of the weakly coordination ligands such as fluoride ions to form the $[\{(Mo^{VI})Mo^{VI}{}_{5}O_{21}(H_2O)_5F\}_{12}\{Mo^{V}{}_{2}O_4(F)(H_2O)\}_{30}]^{69-}$ 3a (VIP: Angew. Chem. Int. Ed., 2015, 54, 5879) even from the aqueous solution with absolute selectivity. The molecular level snapshot of the itinerary for the coordination expansion of tetrahedral oxo-anions to their Oh-coordination is one of the most eminent advancement to the fundamental principles (J. Am. Chem. Soc. 2019, 141, 9170).

Keywords: Polyoxometalate, Encapsulation Chemistry, High Efficiency CO_2/SO_2 Uptake, Aqueous Solution F - scavenger, TBP-Coordination Capture, Azatobacter Modelling, Reverse Micellar Scaffold

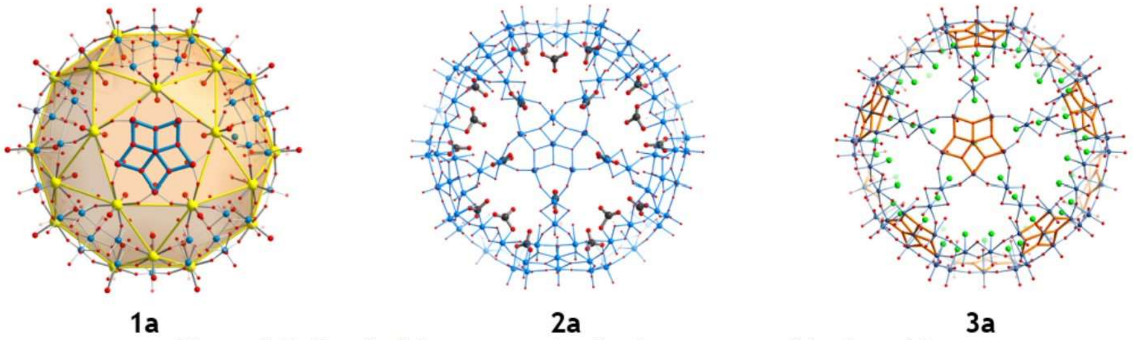

Figure: Ball-and-stick representation for the structures of **1a**, **2b** and **3a.**

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A Roadmap to All-Organic Photonic Integrated Circuits from Nano/Micro Organic Solids

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Recently, nano/micro organic solids have emerged as promising materials for producing miniaturized organic photonic components, such as optical waveguides (active/passive), lasers, resonators (including chiral ones), filters, and modulators suitable for constructing organic photonic integrated circuits (OPICs).[1-2] Miniature crystal (rigid/flexible) optical waveguides[1-8] are useful for controlling and manipulating light propagation down to microscale. In optical resonators,[4] their mirror-like geometry allows them to trap the photons tightly by repeated total internal reflection at the air-matter interface and produce multimodal optical emissions. Low-optical-loss (high Q) resonators are good optical gain media, therefore potential elements for microlasers. The guided light-intensity and- speed can be modulated using light-driven refractive index changes in photochromic optical waveguides.[10(iii)] Selective reabsorbance of broad-band optical emission in microcrystal waveguides lessens the bandwidth of the propagating light signal producing a long-pass filter effect.[8]

Atomic force microscopy (AFM) is an effective technique to mechanically micromanipulate miniature organic photonic components towards OPICs - an approach known as Mechanophotonics.[1,2,8] I will introduce examples of miniature organic photonic (optically linear and nonlinear) components in my talk. I will also discuss the construction of OPICs with active, passive, and energy-transfer attributes using mechanophotonics. The fabricated OPICs switch, split, direct, and filter optical signals useful for signal enhancement, sensing, information processing and switchable photonic device applications.

Keywords: Mechanophotonics, Organic Photonic Integrated Circuits

High Energy Li-Ion Capacitors: An approach Beyond Intercalation

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Li-ion capacitor (LIC)/hybrid electrochemical capacitor assembly comprises the battery-type electrode as the energy component and capacitive electrode as the power component to realize the high energy and power capability in the presence of aprotic organic solvents. This LIC assembly is anticipated to deliver the combined features of both high power and high energy density. Unfortunately, the LIC failed to render the necessary energy density as that of Li-ion batteries, but without much compromise in the power density. This is mainly originated from the limited capacity and Li-ion kinetics. On the other hand, the hybrid configuration delivered a satisfactory power density. Approach beyond intercalation, such as conversion and alloying materials as battery-type electrodes, is one of the efficient approaches to improve the energy density. Although we demonstrated various electrodes employed for the LIC applications, however, in the present talk mainly deals with the conversion (Fe_3O4) and alloy (SnO_2) based electrodes. Further, the combination of interesting features like insertion and alloying will be discussed.

Keywords: Battery; supercapacitor; energy; power; intercalation.

In Pursuit of Green Hydrogen by Electrocatalytic Water Splitting

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To address the ever-increasing energy demand, electrochemical water splitting has attracted tremendous attention these days for the production of hydrogen as clean fuel avoiding environmental pollution. The role of catalyst for oxygen evolution reaction (OER) cannot be ignored as the kinetics can be modulated not only by choosing the materials with their intrinsic catalytic properties, electronic structure but also by designing the morphology in nanoscale level offering large number of active sites. While the number of active sites is important, easy diffusion of electrolytes and access to the active sites is also crucial for exhibiting high activity. Furthermore, insertion of catalytically active foreign elements enhances the catalytic activity into many folds. Therefore, manipulation of intrinsic properties of material is highly desirable by designing different nanoarchitectures as well as by optimum doping with transition metals. Even though conventional OER catalysts are available; their extensive use in industrial application has been limited due to their expensive nature. In purview of this a number of novel electrocatalysts have been rationally designed and developed to facilitate OER as well as HER mechanism.

Further, often fresh water is used for electrocatalytic water splitting. It is needless to say that we have been going through tremendous scarcity of water. To avoid the use of fresh water, seawater can be considered as a futuristic approach for producing green hydrogen by electrocatalytic water splitting. However, the presence of chloride limits the use of seawater due to dominating chlorine evolution reaction over OER, especially under high current region. Thereby, rational design of noble metal free electrocatalysts for seawater splitting blocking the CER and allowing OER at anode is one of the most ambitious approach to meet energy demand without wasting usable water.

The presentation will discuss about the rational designing electrocatalysts, modification of their intrinsic properties and detailed electrochemical analyses to generate green hydrogen effectively not only using fresh water but also possible use seawater.

Keywords: Hydrogen, Electrocatalysis, Electrocatalyst, Oxygen evolution reaction, Water splitting.

Bioengineered Human Tissues & Organs: The Way Forward

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Every year, millions of patients suffer loss or failure of an organ or tissue as a result of accidents or disease. Tissue or organ transplantation is a commonly accepted norm under these circumstances. However, constant shortage of donor tissue and organ transplants coupled with high morbidity and mortality has spurred great interest for lab grown bioengineered tissues/organs as promising substitute. Our laboratory at IIT Guwahati specifically focuses on recreating these functional tissues, organs and implants at an affordable cost using naturally derived biodegradable biomaterials i.e., Indian endemic silk in combination with stem cells. We have developed methods using conventional and latest 3D bioprinting techniques to intricately mimic the architecture of organs/tissues in great details in an attempt to understand the underlying cell-material crosstalk and its role in tissue regeneration. As an outcome of our research endeavor at IITG, we have developed a number of affordable prototypes which are in various phases of animal/clinical validation. These include smart wound dressings for diabetic foot ulcers, skin grafts for burn injuries, vascular grafts for by-pass surgery, vascularised bone grafts as orthopaedic implants, beating cardiac patch for myocardial infarction, bioartificial pancreas releasing insulin for type-1 diabetes, 3D printed intervertebral disc and knee meniscus as orthopaedic grafts and minimally invasive anti-cancer drug eluting injectable gels for cancer treatment. Similarly, we have developed multiple in vitro human disease models which can contribute to Industry in high throughput drug screening and drug development.

Keywords: Silk, Tissue Engineering, Biomaterial, Bioengineered Organs, 3D Bioprinting.

Molecular Architectonics

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Molecular architectonics has its essence in the custom design and engineering of molecular assemblies by judicious exploitation of noncovalent forces to construct ordered architectures with novel properties and functions. This concept of designing noncovalent systems enable us to focus on distinct functional aspects of designer molecules for biological and non-biological applications, which strengthen our efforts in understanding the art of controlled molecular assemblies. However, the art of mastering the programmed molecular assemblies is a challenging task owing to complex factors that govern recognition events at the molecular level. In this context, biomolecules with in-built information for molecular recognition can guide the molecular architectonics. We adopted the tailorability of molecular assemblies by employing biomolecules as auxiliaries with functional-core modules. Molecular architectonics of functional modules and the derived nanoarchitectures that are developed in our group have led to understanding homochirality, protein folding, organic electronics, high-mechanical strength (bio)organic materials, self-cleaning, (bio)sensors and tissue engineering applications. In this talk, I shall present exquisite designer molecular units with amino acids and peptides developed in our group to construct well-defined molecular and material architectures with range of functional properties and applications.

Simultaneous One Pot Synthesis of Fe Doped Carbon Dots and Fe_3O_4 Nanoparticles; Heteroatom-Doped Carbon Dots as Label Free Fluorescent Probe for Sensing and Light Induced Bacterial Inactivation

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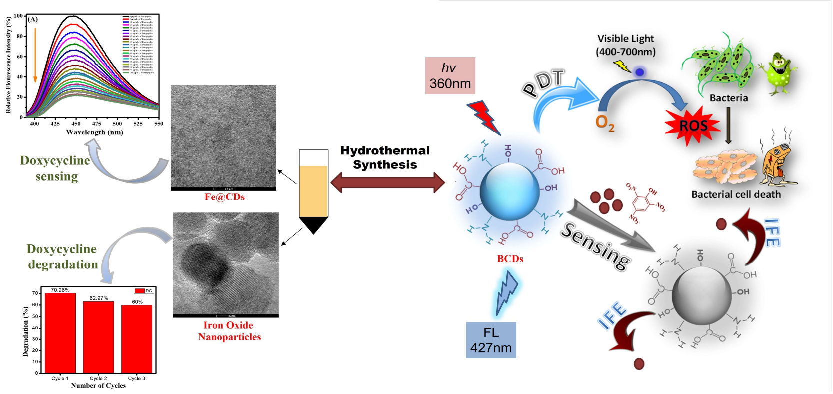
To improve the fluorescent properties of carbon dots metal ion doping is less explored in comparison to non-metallic element doping in carbon dots. In this work, we demonstrate a novel strategy to fabricate Fe doped carbon dots (Fe@CDs) using a mixture of $FeCl_2.6H_2O$, citric acid and ethylene diamine, yielding Fe_3O_4 nanoparticles during the hydrothermal process. To investigate the formation of magnetite (Fe_3O_4) and successful doping of Fe in carbon dots the material has been characterized extensively. Detailed magnetic properties of Fe_3O_4 were explored using vibrating sample magnetometer (VSM). The proposed sensing system has been successfully used for the assay of doxycycline in raw milk samples. In other work, water soluble nitrogen, silver and gold co-doped bimetallic carbon dots (BCDs) were prepared using one pot hydrothermal method with citric acid as a sole carbon source. As prepared BCDs showed size in the range of 4-8 nm and excitation independent emission behaviour with maximum emission observed at 427 nm. Additionally, these BCDs showed very high quantum yield value of 50% and fluorescence life-time value of 10.1 ns respectively. Interestingly, as prepared BCDs selectively sense picric acid (PA) by exhibiting “selective fluorescence turn-off” behaviour in the presence of PA with a limit of detection value (LOD) of 46 nM. Further, as prepared BCDs were explored for photodynamic therapy to inactivate bacterial growth in the presence of light (400-700 nm) by generating singlet oxygen. Thus, as prepared BCDs offer lots of potential to use a nanoprobe to detect picric acid in aqueous medium and to design next generation antibacterial materials.

Keywords: Carbon dots; Photosensitizer; Sensing; Singlet oxygen; heteroatom doping



Halide Perovskite Nanocrystals: Photophysics and Applications

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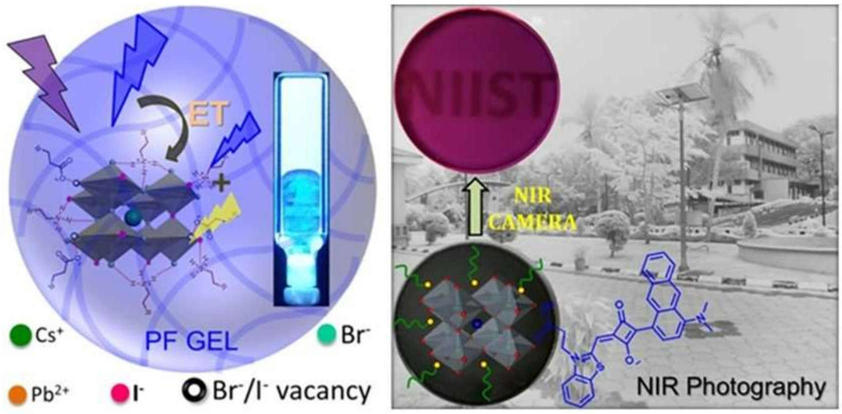
Halide perovskite nanocrystals (PNCs) are among the most attractive functional materials because of their composition/size/morphology tunable optical and photonic characteristics. They are promising for optoelectronic devices such as light-emitting diodes, solar cells, photodetectors, lasers, memories, and sensors. Recent studies suggest that the functional properties of these nanostructures are superior to traditional semiconducting inorganic quantum dots. Nevertheless, the underlying photophysics of these materials is still not well studied. A better and in-depth understanding of the photophysical properties is necessary for further development in this area and to push the present efficiency limits of perovskite-based optoelectronic devices. In this context, recently, we have studied the excitation energy migration, electron transfer, and energy transfer properties of PNCs.[1] We have also demonstrated the passivation of PNC surface with luminescent polymers to suppress the halide ion migration and generate stable and efficient white-light emission through controlled excitation energy transfer.[2] Consequently, the non-radiative recombination of photogenerated charge carriers has significantly reduced, resulting in the overall enhancement of their luminescence characteristics. We have recently developed visibly opaque and near-infrared transmitting filters suitable for security and NIR photography applications using a composite of PNC and squaraine dye.[3]



Understanding the Charge Transport in Lead Halide Perovskite

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Development of novel semiconducting materials with the ability to outperform conventional semiconductor is required for the demonstration of futuristic technologies. Among various materials developed lead halide hybrid perovskites have been attractive due to the possibility of demonstrating > 25% photovoltaics and > 20 % efficient color pure LEDs. Despite the development of these high efficiency optoelectronic devices, a clear understanding of the charge transport, scattering mechanism and knowledge of the instabilities in the perovskite is lacking. Field effect transistors (FETs) are an effective platform to probe the charge transport mechanism. However, demonstration of a room temperature operating field effect transistor has been difficult with lead halide perovskite. We describe the development of the room temperature operating field effect transistor with perovskite and use it as platform to develop a microscopic understanding of the charge transport behaviour in this class of materials. With a combination of electrical, magnetic and spectroscopic measurement we bring out the role of the crystal structure, cationic dipolar disorder, ionic defects and dynamic disorder of the inorganic octahedron cage in deciding the overall transport behaviour of these class of materials.

Keywords: Perovskite, field effect transistor, ionic defects, charge transport, mobility.

Molecular Imaging and Radionuclide Therapy of Cancer: Potential Role for Nanotechnology

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In recent years, advances in molecular imaging using positron emission tomography (PET) and radionuclide therapy have given rise to the new field of theranostics. By combining high resolution imaging with potent targeting molecules, the theranostic principle allows physicians to “see what they treat.” In this strategy, a molecular imaging technology such as prostate specific membrane antigen (PSMA) PET scanning allows for precise determination of target expression, prior to the delivery of a target therapy. The success of this strategy has been demonstrated in large multi-center trials such as the VISION or NETTER-1 trials, for 177Lu-PSMA or DOTATATE, respectively. These imaging methods and treatments have changed standard of care in the field of cancer imaging and treatment. With these milestones now accomplished, several new questions have emerged. For example - how can patients who become refractory to these treatments be best managed? Can the theranostic imaging principle be applied beyond radionuclide therapies as a more general strategy for cancer treatment? Can this strategy be applied beyond standard biomolecules such as peptides and proteins to include nanotherapeutics? We have recently described advances to overcome some of these challenges. For example, one key strategy to overcome theranostic resistance is to instead rely upon lineage independent targets which are upregulated upon loss of expression of other targets such as PSMA in prostate cancer. Another direction in our laboratory is the development of new methods for imaging and studying nanoparticle distribution. For example, by incorporating a positron imaging strategy utilizing ^{89}Zr labelled nanoparticles, we can better understand targeted nanoparticle therapies in preclinical models. These new methods may be used in future clinical trials to help improve patient care for those with prostate cancer or other diseases.

Keywords: Theranostics, positron emission tomography, imaging, clinical translation

Advanced Modelling of Materials for Clean Energy Applications : Hydrogen Storage Materials And Next-Generation Batteries

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Energy storage has been a theme for scientists for two hundred years. The Lead acid battery research on batteries occupied some of the best minds of the 19th century. Gaston Plante in 1859 invented the lead acid battery which starts your car and ignites the internal combustion which takes over the propulsion. Although the lead battery is over 150 years old but the origin of its open circuit voltage (OCV) of 2.1 V is still known. In present talk, I will show how one can explain the origin of OCV of 2.1 V based on foundations of relativistic quantum mechanics. Surprisingly, seems to be the first time its chemistry has been theoretically modelled from the first principles of quantum mechanics. The main message of this work is that most of the electromotoric force (1.7-1.8 Volts out of 2.1 V) of the common lead battery comes from relativistic effects. While the importance of relativistic effects in heavy-element chemistry is well-known since over two decades, this is a striking example on "everyday relativity". We believe that the fact that "cars start due to relativity."

The purpose of this talk is to provide an overview of the most recent studies in the field of hydrogen storage materials & rechargeable battery research with the focus how computational material science can play an important role in search and design of new hydrogen storage materials & next generation battery materials. On specific examples, the application of density functional theory calculations and molecular dynamics simulations will be illustrated to show how these computational methods can be of great use in the effort to reach a better understanding of materials and to guide the search for new promising candidates.

Keywords: Energy, Hydrogen storage, Materials Science

New Possibilities of Metal Clusters for Bio-Applications

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Atomically precise metal nanoclusters (MNCs) is an emerging area of research due to their potential applications.[1-7] We will discuss about DNA-based logic gate by probing the DNA-metal base pair in the presence of suitable additive such as metal nanoclusters and metal ions. We investigated the conformation of DNA by a photoexcited energy transfer process where the Au cluster is covalently attached with AlexaFluor 488 (A488) dye tagged DNA. Blue luminescent, pepsin-templated copper nanoclusters (Cu NCs) are synthesized for an effective peroxidase mimic. The development of Cu NC-based artificial enzymes will pave the way for versatile biomedical, environmental, and clinical applications.

Freeze-resistant Cadmium-free Quantum Dots for Live-cell Imaging

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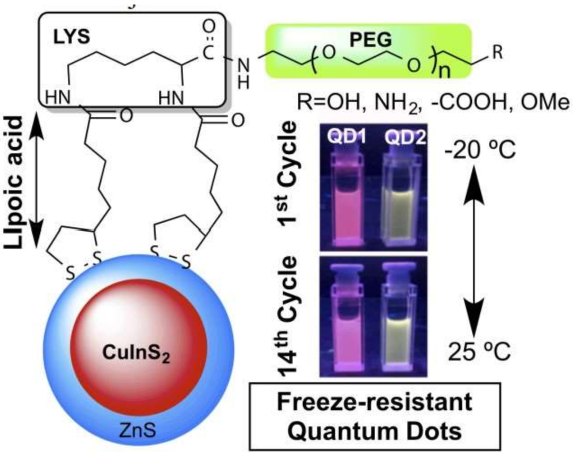
Semiconductor quantum dots (QDs) have gained enormous popularity as a fluorescent marker for their unique photophysical properties and composition-based tuning of emission properties ranging from visible to near-IR spectrum.1 A general route for QDssynthesisfrom organometallic precursors involves using high-boiling long-chain hydrophobic molecules. 2 These molecules, also acting as surface-passivating ligands, are attached to the outer surface of the QDs and are essential for their colloidal stability. A variety of strategies has been introduced already to make the QDs soluble in aqueous media like encapsulation in micelles, coating with silica, and ligandexchange (LE) with small molecule, etc. Among all these methods, LE of the hydrophobic ligands with hydrophilic ligands containing thiols, amines, pyridines, histidines, and phosphine derivatives as the coordinating ligand are well-documented. 3 Recent studies reveal the cadmium toxicity of core/shell CdSe/ZnS QDs on biological systems, and the poor colloidal stability under different storage conditions are major concerns.

Keywords: Cadmium-free quantum dots, Live-cell imaging, Freeze-resistance, Tetrathiolate ligand, Bioconjugation



Scheme: Freeze-resistant CuInS2/ZnS QDs for bioconjugation and live-cell imaging To overcome the aforementioned problems, a new class of multifunctional and tetra-coordinating ligands has been synthesized using lipoic acid, starting from lysine.4 The synthesized ligands provide facile ligand exchange of CuInS2/ZnS quantum dots and offer exceptional colloidal stability upon freezing, robust photophysical properties in various aqueous media across a wide pH range buffer composition with a tunable surface charge for the QDs (see Scheme). The QDs after ligand exchange is easily amenable to covalent modification with biotin-binding traptavidin protein exclusively by employing simple carbodiimide coupling chemistry. The QDs also showed excellent biocompatibility and low nonspecific binding to the cells and, thus, are suitable for livecell imaging of cell-surface receptors.

Functional Polymers for Theranostic Application

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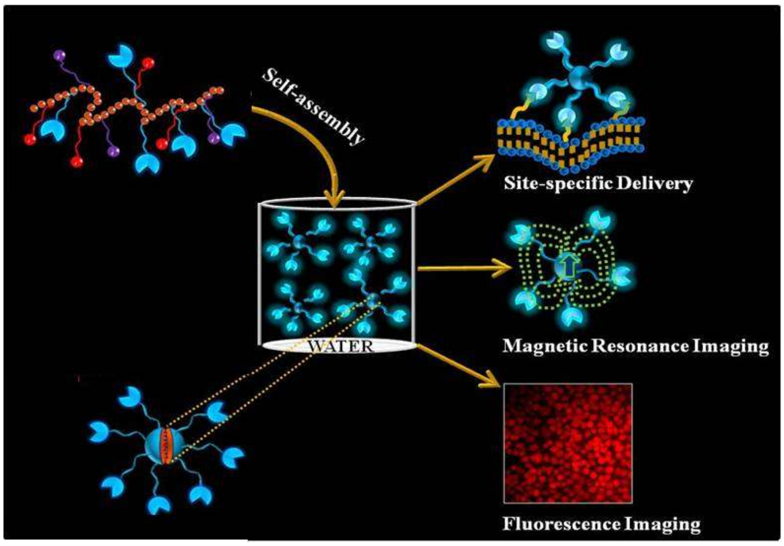
Theranostic based nanomedicine plays a crucial role in the field of cancer therapy. This is due to having the capability to combine both therapy and diagnosis in a single system. Herein a new class of metal-ligand based nanocarrier in a polymer backbone has been designed as a theranostic system. To prove the MRI capabilities of copolymer nano-aggregates, NMR experiment is performed at room temperature. Cell viability studies suggest the biocompatibility nature of the copolymer. Flow cytometry, as well as epi-fluroscence microscope experiments, clearly demonstrate the dual-imaging ability of the newly designed copolymer. The much higher relaxivity ratio (r_2/r_1) of the present method establishes the superiority of our system as one of the best contrast agent known to the practitioners of magnetic resonance imaging.

Keywords: Amphiphilic polymers, cancer therapy, imaging, drug-delivery



Structural Phase Transition and Spontaneous Exchange Bias in Fe doped $NiCr_2O_4$ Nanoparticles: EXAFS and Magnetic Measurements

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Transition metal based spinel oxides, ACr_2O_4, Cr^{3+} ions forms a pyrochlore sublattice, surrounded by octahedral network of oxygen anions, while A^{2+} ions occupy tetrahedral network of oxygen anions and forms a diamond sublattice. What makes these chromium based spinel oxides so important, is the ability to tune their structural and magnetic properties in an additional way by adjusting the magnetic and chemical nature of A^{2+} ions. In $NiCr_2O_4$, when A^{2+}cations are $Ni^{2+,}$ the orbital degeneracy induced cooperative Jahn-Teller distortion results in a cubic to tetragonal structural transition above 320K and transforms into an orthorhombic phase at Curie temperature (TC ~ 71 K). Below TC, distortion within orthorhombic structure gives rise to a spin spiral ordering at ~ 31 K, known as spiral ordering temperature (TS). Thus, the competition between AFM between Cr^{3+} ions and FM ordering among A^{2+} ions results in some peculiar magnetic properties like negative magnetization, exchange bias effect etc. Here, in this report, the structural and magnetic phase transitions in $NiCr_2O_4$ nanoparticles of size ~60 nm after doping Fe show a stable cubic phase at RT in contrast to tetragonal phase in bulk $NiCr_2O_4$. Below RT, a complete tetragonal symmetry is observed at 50 K, followed by a coexistence of cubic and tetragonal phases in the intermediate temperature range. Interestingly, no tetragonal to orthorhombic phase transformation has been observed down to 12 K. The plausible structural transformation examined from temperature dependent EXAFS. Magnetic studies demonstrate two-fold increase in para to long range ferrimagnetic transition, TC, due to increase in A-B exchange interaction and no change in spiral ordering temperature, TS indicating strong B-B interaction. Unusually high spontaneous exchange bias of ~1.265 kOe at 60 K and tunable exchange bias observed with temperature highlight the potential applications of these materials in spintronics devices.

Self-Assembly of π-Conjugated Molecules and Nanoporous Organic Polymers

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The intriguing self-assembled architectures in nature fascinate researchers to tune the morphology of the synthetic materials.[1] Morphology and textural features of materials are essential parameters to influence their physicochemical properties, such as porosity, adsorption, diffusion kinetics, and optoelectronic properties.[2] Morphological tunability of any supramolecular/ macromolecular architectures demands detailed elucidation of the molecular self-assembly processes. In the present talk, I will discuss the evolution of the self-assembly processes of π-conjugated fluorophores through fluorescence correlation spectroscopy coupled with electron and atomic force microscopy.[3] Such self-assembled nanostructures have been used for optical sensing and cellular imaging. In addition, I will also present the morphological evolution of hypercrosslinked porous organic polymers from nanosphere to nanosheets obtained through solvent knitting process and the impact of morphology towards polar molecule separation from water.[4]

Keywords: Self-assembly, nanofibers, nanosheets, fluorescence, porous organic polymers

Figure: Schematic illustration of deciphering the self-assembled nanostructures through spectroscopic and microscopic approach.

Gold Nanoparticles Based Drug Delivery System for Ovarian Cancer

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Ovarian cancer is the second most common gynecologic cancers in India and USA. It is one of the most common cancers that has the highest mortality rate in women. Traditional therapies for the treatment of ovarian cancer comprise surgery, chemotherapy and radiation therapy. However, these strategies have several limitations including damaging of healthy cells, non-specificity, toxicity of anticancer drugs, poor bioavailability, fast clearance and restrictions in case of metastasis. In this context, nanotechnology can make a significant role. Very recently, nanotechnology dealing with metal-based nanomaterials is widely applied in almost every filed of science and technology including biomedical applications due their unique fundamental properties. To this context, our group at IICT is currently pursuing various nanomedicine research projects aimed at developing advanced nanomaterials and nanoparticles-based drug delivery systems (DDS) for treatment of cancers and angiogenesis. My talk will mainly focus on gold nanoparticles-based drug delivery systems for the treatment of ovarian cancers.

In the present talk, using a combinatorial approach, we designed and fabricated a drug delivery system by combining gold nanoparticles (AuNPs) with an engineered bi-functional recombinant fusion protein TRAF(C)(TR), loaded with an anticancer drug namely doxorubicin (DX) and erbB2-siRNA (si), to mediate target specific delivery into SK-OV-3, a model human ovarian cancer cell line overexpressing HER2 receptors, (i.e. human epidermal growth factor receptor-2). The nanoparticles-based targeted drug delivery system, designated as TDDS (Au-TR-DX-si), was found to be stable and homogenous as revealed by physicochemical and biochemical studies in vitro. In addition, TDDS was functional upon evaluation in vivo. Intraperitoneal administration of TDDS at 2.5mg/kg of DX and 0.25mg/kg of erbB2 siRNA into SK-OV-3 xenograft nude mice, revealed target specific uptake and consequent gene silencing resulting in significant tumor suppression. We attribute these results to specific co-delivery of erbB2 siRNA and DX mediated by TDDS into SK-OV-3 cells via HER2 receptors. Additionally, biodistribution of TDDS, as quantitated by ICP-OES, confirmed tumor-specific accumulation of AuNPs primarily in tumor tissues, which firmly establishes the efficacy of nanomedicine-based combinatorial approach for the treatment of ovarian cancer in a non-toxic manner. Based on these findings, we strongly believe that the nanomedicine-based combinatorial approach can be developed as a universal strategy for treatment of HER2+ ovarian cancers.

Roughened gold films by cold argon plasma as SERS-active substrate for detection of explosives in trace quantities

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Surface-enhanced Raman scattering (SERS) spectroscopy is one of the most powerful analytical techniques which can be used for the identification of molecular species, with the potential to reach single-molecule detection under ambient conditions. It provides complete vibrational information of the molecular system under study and, since the output is essentially a Raman scattering spectrum, it is highly sensitive toward conformational changes. SERS based detection is non-destructive, rapid, permits detection of several analytes simultaneously, allows on-site analysis by using portable instruments. The underlying mechanism of SERS is broadly classified into two effects- the electromagnetic (EM) effect and the chemical (CM) effect. It can be used for quantifying a broad range of chemical and biological analytes down to ultra-low/trace levels with promising applications in diverse fields, including chemistry, food safety, drug detection, narco-analysis, explosive detection and medical diagnostics.

One of the challenges is to fabricate affordable, stable, and reproducible SERS-active substrates with a sufficient number of hotspots to achieve sensitive detection. The potential of SERS spectroscopy has been explored aggressively leading to the development of several methods to produce SERS-active substrates with either ordered and uniform nanostructures or chemically synthesized nanoparticles/composites, using different materials and fabrication techniques.

We have provided the design of a large-area SERS-active substrate, theoretically (via simulations) and experimentally validated it. It constitutes of modified thin gold (Au) film on silicon (Si). This was achieved by irradiating the Au film with argon ions (Ar+) at optimized parameters. Such a design can neither be classified as ordered nanostructure nor as randomized colloids of nanoparticles or nanostructures, it lies somewhere between the two broad classification, providing the combined advantage of high sensitivity (enhancement factor of ~108 for the most prominent Raman mode) and ease of fabrication. The hotspots are uniformly distributed all over the surface which ensures an efficient substrate with easy and quick detection of analytes with a high order of repeatability. The fabrication included roughening of the surface under controlled environment which supports high reliability, reproducibility cost-effectiveness and high-fidelity of the proposed design/substrate. The proposed SERS substrates has the potential to measure up to picograms levels of compounds constituting nitro-based explosives which has been validated using analytes such as urea and p-nitrobenzoic acid (PNBA).

Keywords: SERS, thin gold film, argon plasma, explosives.

Nanomaterial-based Microfluidic Platforms for Bioanalytical Applications

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Nanomaterials possess distinct physicochemical attributes that make them excellent sensing systems for biomolecules. They are bringing important advantages in the design of novel biosensing systems or improvements of the existing devices in terms of high response time, improved signal-to-noise ratio and lower limits of detection. Sensitive and selective sensing systems based on electrochemical methods have been explored extensively. Specifically, most of such applications are based on solution assay formats. Although efficient, it is difficult to incorporate these formats into a miniaturized device which hinders their practical applications. Therefore, it is imperative as well as challenging to design a robust solid sensing platform. Such platforms can securely hold the nanosensors and minimizes the analyte-independent effects caused by sample conditions with the ability to operate for low quantities of sample volume. Water swellable, 3-D structured hydrogels have become popular for sensing applications. Immobilization of nano-bioreceptors into their porous structure is a logical approach for constructing qualitative/quantitative detection platforms with multiple features: high loading capacity; tunable geometries; and their regulating viscoelastic properties. On the other hand, integration of electrochemical sensors within the microfluidic channels for creating lab on chip devices offers several inherent benefits of miniaturization, portability, reusability, low cost, and ease of operation over conventional methods. Overall, the combination of several such powerful techniques could be leveraged to create lab-on-a-chip paradigm with detection capabilities which offer the possibility to build new bioanalytical devices.

Keywords: Nanomaterial, Hydrogels, Microfluidic, Electrochemical, Lab-on-a-chip, Sensing

Nanostructured Electrodes using Ni-Co Functional Inks for Electrochemical Energy and Sensing Applications

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The design of electrode, device architecture, and functional properties of the material play an important role in fabrication of energy devices and sensors. The literature is bound with various examples of nanomaterials including metal oxides and spinels as electrocatalysts in energy-efficient systems and sensing applications. The conventional methods for synthesizing these nanomaterials are well established; however, they often fail to address the stability, durability, reproduciblity and scalability issues that are stringent requirements for practical application. In this prospect, the large-scale fabrication of electrocatalytic materials with controllable and flexible preparation remains a challenge since various processes are multistep, instrumentation-dependent and often result in loss of activity during synthesis. For commercial applications, it is important to synthesize solution-processable inks that can be coated on the choice of conductive support system for the fabrication of active electrodes. In the laboratory, Ni and Co-based alkanethiolate complexes with lamellar structure are used as functional inks that could be directly coated on the desired substrates, and the processing conditions are rigorously optimized for application as electrocatalyst in oxygen evolution reaction (OER),[1-2] development of glucose sensors[3], biomolecular and chemical sensors[4] and as a catalyst in the synthesis of graphite for the fabrication of supercapacitors.[5]

High-Temperature CO_2 Capture using Lithium Silicate Nanosheets

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An excessive amount of CO_2 is the leading cause of climate change, and hence, its reduction in the Earth's atmosphere is critical to stop further degradation of the environment. Although a large body of work has been carried out for post-combustion low-temperature CO_2 capture, there are very few high temperature pre-combustion CO_2 capture processes. Lithium silicate (Li_4SiO_4), one of the best known high-temperature CO_2 capture sorbents, has two main challenges, moderate capture kinetics and poor sorbent stability. In continuation of our work in carbon capture and utlization,[1-5] in this work, we have designed and synthesized lithium silicate nanosheets (LSNs), which showed high CO_2 capture capacity (35.3 wt% CO_2 capture using 60% CO_2 feed gas, close to the theoretical value) with ultra-fast kinetics and enhanced stability at 650 °C.[6] Due to the nanosheet morphology of the LSNs, they provided a good external surface for CO_2 adsorption at every Li-site, yielding excellent CO_2 capture capacity. The nanosheet morphology of the LSNs allowed efficient CO_2 diffusion to ensure reaction with the entire sheet as well as providing extremely fast CO_2 capture kinetics ($0.22\ g\ g^{-1}\ min^{-1}$). Conventional lithium silicates are known to rapidly lose their capture capacity and kinetics within the first few cycles due to thick carbonate shell formation and also due to the sintering of sorbent particles; however, the LSNs were stable for at least 200 cycles without any loss in their capture capacity or kinetics. The LSNs neither formed a carbonate shell nor underwent sintering, allowing efficient adsorption–desorption cycling. We also proposed a new mechanism, a mixed-phase model, to explain the unique CO_2 capture behavior of the LSNs, using detailed (i) kinetics experiments for both adsorption and desorption steps, (ii) *in situ* diffuse reflectance infrared Fourier transform (DRIFT) spectroscopy measurements, (iii) depth-profiling X-ray photoelectron spectroscopy (XPS) of the sorbent after CO_2 capture and (iv) theoretical investigation through systematic electronic structure calculations within the framework of density functional theory (DFT) formalism.

Keywords: CO_2 capture, Lithium Silicates, Nanosheets, CCU, Climate Change

Fabrication of Nanofibers for Biomedical Applications

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Nanofibers have gained profound application in tissue engineering, wound healing and anticancer therapy. In the recent past, anticancer drug-loaded nanofibers have been sought extensively as post-operative implants to prevent cancer recurrence and metastasis. In this quest, although numerous nanofiber-based drug delivery systems have been realized, they unfortunately remain largely ineffective due to certain disadvantages. One such drawback is their incompetence to attain controlled and sustained drug release profile which could also be effectively tuned to meet personalised medications of diverse patient. Thus, to overcome these drawbacks, we have developed differentially crosslinkable polymeric nanofibers to deliver various therapeutic agents for anticancer and wound dressing applications. Apart from this, we have also developed novel nanofibrous scaffolds to overcome the drawback associated with the existing scaffolds for tissue engineering applications.

Keywords: Nanofibers; Cancer Therapy; Wound Healing; Tissue Engineering

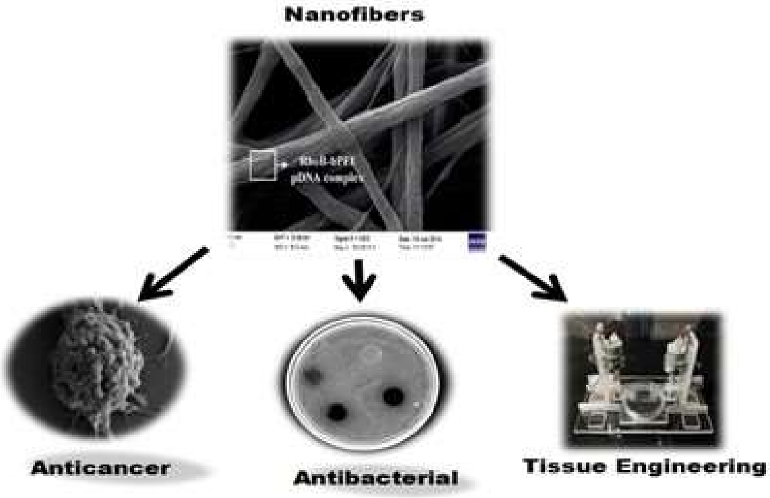

Figure: Biomedical applications of nanofibers

Functionalised Schiff Base Ligands for Accessing Novel Multifunctional Materials

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Design and synthesis of Schiff bases derived from the condensation reaction of aromatic/aliphatic aldehydes and amines continue to spawn great interest amongst chemists and physicist alike even after more than 150 years of their discovery. Structural and binding flexibility along with their potential applications in the areas of catalysis, novel materials and wide range of biological activities, including antibacterial, antifungal, antidiabetic, antitumor, antiproliferative, anticancer, anticorrosive and anti-inflammatory activities renders this class of compounds highly attractive materials for exploring their properties and applications.

Complexation of polydentate and functionalized Schiff base with metal ions and/or formation of self assembled nanohybrids proved to be quite significant allowing steric and electronic properties to be easily tailored, formation of modular building blocks in the construction of more complex architectures. Schiff base with appropriate functional groups may also lead to noncovalent interaction-driven self-assembly of molecular entities which offers attractive strategy for constructing new interesting supramolecular materials. The present paper describes the design strategies and self-assembly possibilities of some functionalized Schiff base ligands and their metal complexes with structural versatility and multifunctional properties.

Keywords: Schiff base, self-assembly, supramolecular, multifunctional

Design of Nanoheterostructures for Energy and Environmental Applications

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An outstanding challenge in the realm of photocatalysis is the development of functional nanomaterials in the visible region of the electromagnetic spectrum. We have investigated the tunability of electronic and optical properties of semiconductor nanostructures by control of their shape, size[1] and which have applications in water splitting, photocatalysis and dye degradation.[2] Core-shell, doped and composite heterojunction have been designed for renewable energy production and environmental remediation under visible spectrum. Coupling of wide band gap semiconductor such as ZnO, $NaNbO_3$ with narrow band gap semiconductors like Ag_2S, In_2S_3, $CuInS_2$ etc. (which acts as sensitizer) forms efficient heterostructures for the separation of photogenerated charge carriers and makes it a good candidate for visible-light photocatalysis.[3] We have also fabricated double heterojunction nanostructures (with 2D MoS_2 and rGO) for extended stability, suppressing the charge recombination and enhance the life time of photogenerated charge carriers at the interface.[4-6]

Low Equivalent Oxide Thickness (EOT), High-κ $Hf_xZr_{1-x}O_2$ Capacitors for Next Generation DRAM

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Achieving low equivalent oxide thickness (EOT), preferably below 5Å, with lower leakage current density ($<10^{-7}A/cm^2$) is of prime importance for further miniaturization of DRAM technology. Despite several efforts being made in this regard, especially by using high dielectric constant (κ) materials, utilization of novel electrodes to counterfeit the high leakage current, limits its immediate implementation. In this presentation, an effective way to achieve high κ, low EOT HZO capacitors for next generation DRAM application by utilizing the less explored morphotropic phase boundary (MPB) region of HZO and high pressure annealing (HPA) technique will be discussed. Usually, rapid thermal annealing (RTA) is the most common technique used by ferroelectric research community for crystallization of HZO films. Although MPB can be achieved by precise optimization of process parameters such as HZO composition and thickness, it emerges at a higher physical thickness for HZO capacitors annealed using RTA. This mitigates the advantage of high-κ value which could otherwise be helpful for achieving lower EOT value. By introducing the HPA, the physical thickness at which MPB emerges can be significantly reduced. The smaller physical thickness of HPA together with the demonstration of significantly high-κ value (> 50) by HZO in the vicinity of MPB was therefore found to be very effective in reducing the EOT. By careful optimization, an EOT value of 5.7 Å for HZO [1:2] capacitors in TiN/HZO/TiN structure with leakage current density $<10^{-7}A/cm^2$ was demonstrated by using HPA. In addition, by introducing rapid cooling together with HPA, the thickness of emergence of MPB was further reduced. Faster cooling resulted in more o-phase and reduced leakage current in the fabricated capacitors by controlling the grain size and their distribution inside the HZO layer. A maximum dielectric constant (κ) of ~49 was achieved for 6.0 nm HZO [1:2] films for 500 ˚C HPA-RC resulting in an EOT as low as ~4.8 Å. The demonstration of such low EOT using CMOS compatible HZO films with leakage current $<10^{-7}$ A/cm^2 using TiN as both top and bottom electrode and can be of significant importance for the future DRAM technology.

Keywords: DRAM, HZO, MPB, HPA, HPA-RC

Greek Cross (+) Aggregate: A Paradigm for Exciton Isolation

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The exciton theory formulated by Kasha and co-workers and Davydov independently gave the fundamental understanding of the photophysics of molecular aggregates.[1] Kasha demonstrated exciton splitting for various geometrical orientations of molecular transition dipoles based on the long-range Coulombic coupling employing the point dipole approximation. The molecular exciton theory highlighted the significance of the orthogonal arrangement of transition dipoles in isolating the exciton and subsequent null exciton coupling mediated monomer-like optical properties.[2] The emergent photophysical properties from the crafted architectures were explored using both experimental tools and the state-of the-art computational methods for understanding the aggregates beyond the Kasha's model.[3,4] The ability of selective activation of one of the charge transfer couplings occasioned ultrafast dissociation of null exciton and evolution of charge separated state in polar solvent facilitated by the selective hole transfer coupling in the edge-to-edge arranged perylenediimide (PDI) dimer Greek cross (+), providing a way forward in fundamental understanding as well as to identify the emergent properties of null aggregates.[5]

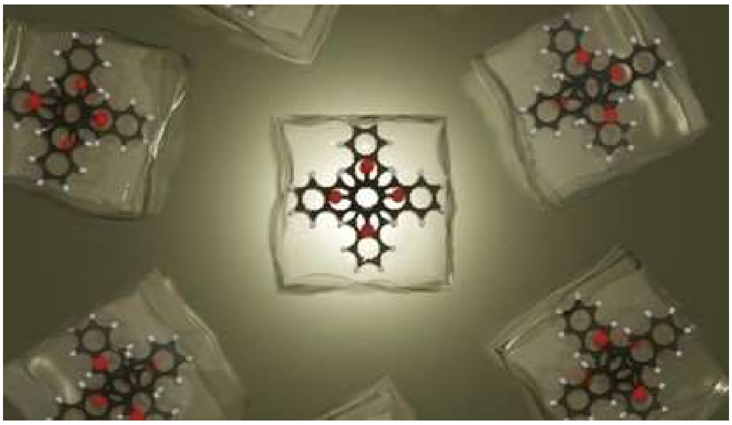

Figure . Depicts the Greek cross arrangement of the pentacene chromophore

Realization of Mott-Wannier Exciton in Organic Semiconductors: An Agnostic Approach

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In conventional inorganic semiconductors, the Coulomb interaction between electron and hole is strongly screened via the large dielectric constant. However the electron and the hole are tightly bound to each other within the same or nearest-neighbour unit cells in molecular semiconductors due to low dielectric constant. The low dielectric constant of organic semiconductors limits the efficiency of organic solar cells (OSCs). In this talk, I will discuss molecular design approaches to improve the dielectric constant for realization of Mott-Wannier exciton in molecular semiconductors. Our findings suggest that utilizing the polar side-chains enhances the dielectric constant in a frequency regime of megahertz. However, it is not sufficient to reduce the Coulombic interaction between hole and electron in excitonic solar cells.

Amyloid-like Structures Formed by Single Amino Acid Self-assemblies of Cysteine and Methionine

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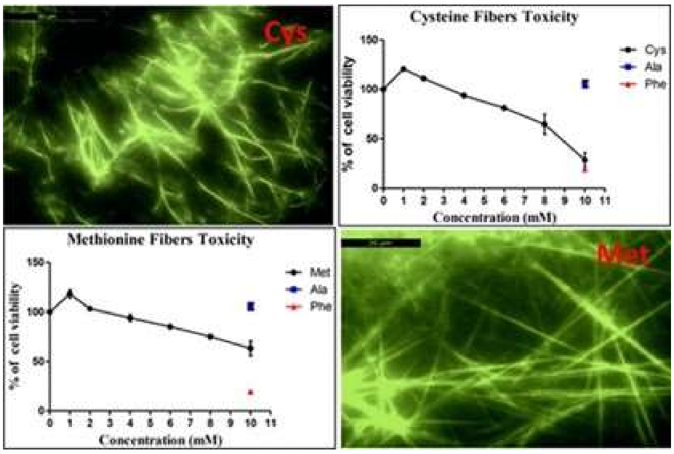
We report for the very first time the discovery of amyloid-like self-assemblies formed by the nonaromatic single amino acids cysteine (Cys) and methionine (Met) under neutral aqueous conditions. The structure formation was assessed and characterized by various microscopic and spectroscopic techniques such as optical microscopy (OM), phase contrast microscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM). The mechanism of self-assembly and the role of hydrogen bonding and thiol interactions of Cys and Met were assessed by Fourier transform infrared spectroscopy, thermogravimetric analysis, X-ray diffraction, and solid-state NMR along with various control experiments. In addition, molecular dynamics simulations were carried out to gain insight into assembly initiation. Further, Thioflavin T and Congo red binding assays with Cys and Met structures indicated that these single amino acid assemblies may have amyloid-like characteristics. To understand the biological significance of the Cys and Met structures, cytotoxicity assays of the assemblies were performed on human neuroblastoma IMR-32 cells and monkey kidney cells (COS-7). The results revealed that both Cys and Met fibers were cytotoxic. The cell viability assay further supported the hypothesis that aggregation of single amino acid may contribute to the etiology of metabolic disorders like cystinuria and hypermethioninemia. The results presented in this study are striking, and to the best of our knowledge this is the first report which demonstrates that nonaromatic amino acids like Cys and Met can undergo spontaneous self-assembly to form amyloidogenic aggregates. The results presented are also consistent with the established generic amyloid hypothesis and support a new paradigm for the study of the etiology of single amino acid initiated metabolic disorders in amyloid related diseases.

Keywords: Single amino acid, amyloid, cysteine, methionine, self-assembly, cytotoxic



Carborane Thiol Protected Hexagonal Propeller-shaped Silver Nanomolecule with Bidirectional Rotational Orientation

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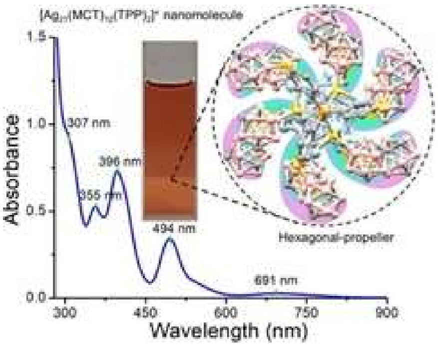
We presented a hexagonal propeller-shaped Ag_{21} nanomolecule protected with meta-carborane-9-thiol (MCT) and triphenylphosphine (TPP) ligands. Single crystal structural analysis reveals that the nanomolecule has an Ag_{13} central icosahedral core with six directly connected silver atoms and two more silver atoms connected through three Ag-S-Ag bridging motifs. While twelve MCT ligands protect the core through metal-thiolate bonds in a 3-6-3 layered fashion, two TPP ligands solely protect the two bridging silver atoms. Interestingly, the rotational orientation of silver sulphide staple motif is opposite to the orientation of carborane ligands, resembling the existence of bidirectional rotational orientation in the nanomolecule. There are multiple absorption peaks in its UV-vis absorption spectrum, as characteristic of a quantized electronic structure. The spectrum appears as a fingerprint for the cluster. High-resolution electrospray ionization mass spectrometry proves the structure and composition of the nanocluster in solution and systematic fragmentation of the molecular ion starts with the loss of surface-bound ligands, upon increasing the collision energy. Its multiple optical absorption features are in good agreement with the theoretically calculated spectrum. The cluster shows a narrow NIR emission at 814 nm with a Stokes shift of 355 nm. The Ag21 nanomolecule is thermally stable at ambient conditions up to 100 °C. However, white light illumination (lamp power =120-160 W) shows photosensitivity and this induces structural distortion as confirmed by changes in Raman and electronic absorption spectra. Femtosecond and nanosecond transient absorption studies reveal an exceptionally stable excited state having a lifetime of 3.26±0.02 μs for the charge carriers, spread over a broad wavelength region of 500-650 nm. The formation of core-centered long-lived charge carriers is responsible for the observed light activated structural distortion.

Keywords: Atomically precise clusters • Silver nanocluster • Carborane • NIR emission • Thermostable • Photo responsive • Electron dynamics



Active Pharmaceutical Ingredient (API) Based Ionic Liquids (ILs): Characterization and *In Vitro* Assessments

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Ionic liquids (ILs) are organic salts comprising of bulky organic cations and organic/inorganic anions with low melting points and high thermal stability1. Due to their other unique properties, such as superior pharmacokinetics and pharmacodynamics, ILs have been proposed as novel compounds in future drug design and synthesis. Active pharmaceutical ingredient (API) based ILs give higher activity and longer lifetime compared to API based drugs[2].

In this work, we report the synthesis and toxicity study of API based ILs having tetramethylguanidinium [TMG] and cholinium [CH] cations. [TMG] cation based protic ILs with diclofenac [DIC], and acetylsalicylate [ASP] anions and [CH] cation based aprotic IL with N-acetyl para amino phenolate [PCM] anion were synthesized at high purity. Results obtained from toxicological evaluation with HEK-293, MOLT4 and K562 cell lines show that all three ILs are non-toxic and bio-compatible. Future work will involve the permeability test of these API based ILs through membranes, followed by animal model studies.

Red Thermally Activated Delayed Fluorescence in Dibenzopyridoquinoxaline-Based Nanoaggregates

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All-organic thermally activated delayed fluorescence (TADF) materials, with long-lived emissive properties, have gained much popularity in recent years for their diverse applications in optoelectronic devices and biomedical applications.[1,2] However, it is challenging to synthesize TADF materials that can be applied to biological systems to produce background-free images due to their low-solubility, aggregation caused quenching in the aqueous medium and non-radiative deactivation of triplet state at ambient conditions.[2] In this regard, red-emitting TADF molecular materials (λem> 600 nm) with donor-acceptor architecture and high quantum yield are promising candidates for intracellular sensing and imaging. Herein, we designed a donor-acceptor-donor (D–A–D) type molecule with dibenzopyridoquinoxaline (PQ) as an acceptor and 3,6 di-t-butyl carbazole as an electron-donor (Fig. 1).[3] The T-shaped molecule (PQACz-T) showed triplet harvesting phenomenon along with environment-sensitive photophysical properties such as solvatochromism, fluorescence enhancement in the viscous medium, etc. Though the long-lived emission is sensitive to environmental parameters (air) in the solution phase, it was stabilized in the aggregated state. The long-lived component of the nanoaggregates of PQACz-T in the THF/H2O binary mixture was attributed to the TADF phenomenon, supported by the time-resolved emission spectra (TRES) analysis. The enhanced rate of reverse intersystem crossing (RISC) in the nanoaggregates facilitated the delayed fluorescence emission. Furthermore, an aqueous dispersion of the smaller-sized, homogeneous distribution of fluorescent nanoparticles (PQNPs) was fabricated upon encapsulating PQACz-T in a triblock copolymer, F-127. Cytocompatible, polymer encapsulated PQACz-T nanoparticles with large Stokes shift, excellent photostability were demonstrated for the specific imaging of lipid droplets in HeLa cells.3c The present study further paves the path for exploring self-assembly processes in TADF nanoaggregates for specific intracellular sensing and imaging.

Keywords: TADF, dibenzopyridoquinoxaline, nanoaggregates, fluorescence imaging, lipid droplets.

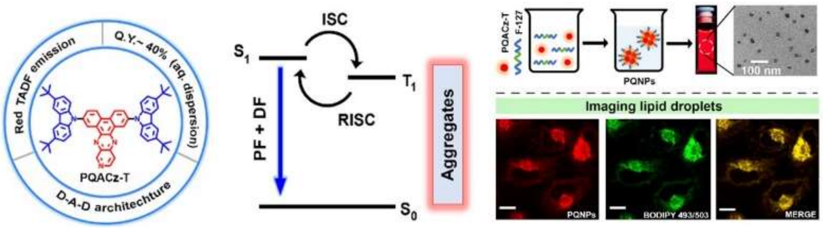

Fig. 1: Schematic illustration of the prompt fluorescence (PF) and delayed fluorescence (DF) in PQACz-T nanoaggregates. The fabrication of triblock polymer F-127 encapsulated particles, PQNPs and their specific organelle targeting ability was also depicted. Scale: 20 µm

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Unusual Aggregates Formed by the Self-Assembly of Proline, Hydroxyproline, and Lysine

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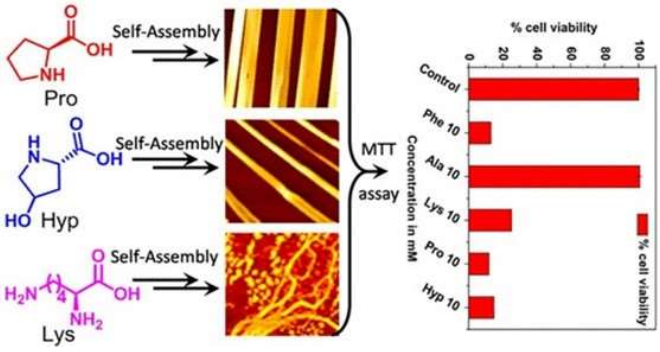
There is a plethora of significant research that illustrates toxic self-assemblies formed by the aggregation of single amino acids, such as phenylalanine, tyrosine, tryptophan, cysteine, and methionine, and their implication on the etiology of inborn errors of metabolisms (IEMs), such as phenylketonuria, tyrosinemia, hypertryptophanemia, cystinuria, and hypermethioninemia, respectively. Hence, studying the aggregation behavior of single amino acids is very crucial from the chemical neuroscience perspective to understanding the common etiology between single amino acid metabolite disorders and amyloid diseases like Alzheimer's and Parkinson's. Herein we report the aggregation properties of nonaromatic single amino acids L-proline (Pro), L-hydroxyproline (Hyp), and L-lysine hydrochloride (Lys). The morphologies of the self-assembled structures formed by Pro, Hyp, and Lys were extensively studied by various microscopic techniques, and controlled morphological transitions were observed under varied concentrations and aging times. The mechanism of structure formation was deciphered by concentration-dependent 1H NMR analysis, which revealed the crucial role of hydrogen bonding and hydrophobic interactions in the structure formation of Pro, Hyp, and Lys. MTT assays on neural (SHSY5Y) cell lines revealed that aggregates formed by Pro, Hyp, and Lys reduced cell viability in a dose-dependent manner. These results may have important implications in the understanding of the patho-physiology of disorders such as hyperprolinemia, hyperhydroxyprolinemia, and hyperlysinemia since all these IEMs are associated with severe neurodegenerative symptoms, including intellectual disability, seizures, and psychiatric problems. Our future studies will endeavor to study these biomolecular assemblies in greater detail by immuno-histochemical analysis and advanced biophysical assays.

Keywords: Self-assembly, Proline, Hydroxyproline, Lysine, Amyloid



A Hybrid Upconversion Nanoprobe for Ratiometric Detection of Aliphatic Biogenic Amines in Aqueous Medium

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Nanomaterials have been employed for real-time sensing and white light-emitting lighting devices.[1] The unique feature of lower energy excitation (NIR excitation) and higher energy emission (visible region) makes the upconversion-based nanoprobes exciting to the scientific community over the last few years.[2] Considering the non-specificity of pristine upconversion nanoparticles (UCNP), the inorganic-organic hybrid upconverting nanoprobe through the judicious integration of small organic molecules with UCNP has emerged as a smart sensor platform for detecting different analytes.[3,4] In the present study, we developed the hybrid upconversion nanoprobe for the ratiometric detection of aliphatic biogenic amines in an aqueous medium. The hybrid upconversion nanoprobe consists of the fluorescent π-conjugated organic molecule, TDPM and near-infrared light-absorbing silica-coated UCNP (UCNP@mSiO_2@TDPM). The mechanism of ratiometric detection through inorganic-organic hybrid nanoprobe is governed by resonance energy transfer (RET). Yb^{3+}, Tm^{3+} doped upconversion nanoparticles act as energy donors and TDPM as an acceptor due to a significant spectral overlap between the TDPM absorption and the emission band of UCNP at 475 nm (Fig. 1). The emission of UCNP at 475 nm was found to decrease with the increasing concentration of TDPM due to the energy transfer. Further, the inhibition of the RET process with the gradual addition of aliphatic biogenic amines in the TDPM loaded UCNP@mSiO_2 led to the turn-on emission of UCNP. Moreover, we explored the detection of aliphatic biogenic amines in real samples like adulterated milk and rotten fish.[5]

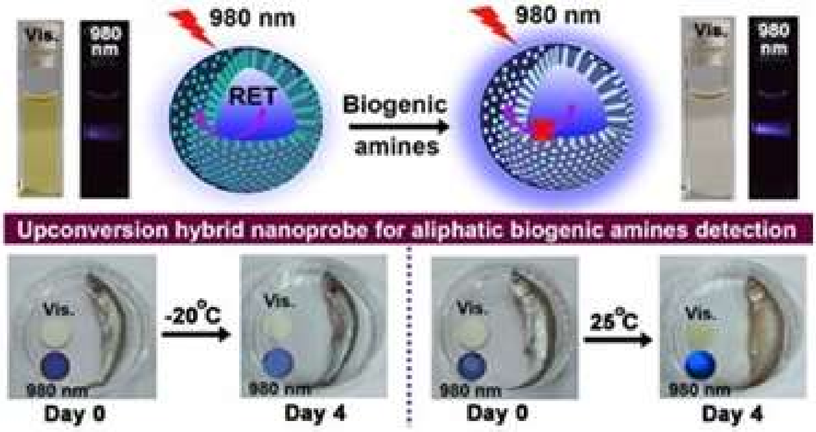

Fig. 2: Schematic representation depicting the detection mechanism of the aliphatic biogenic amines involving organic-inorganic hybrid upconversion nanoprobe (UCNP@mSiO_2@TDPM) through the concept of resonance energy transfer (RET).

New Mechanistic Pathways for Direct Carboxylation by Employing CuNi Bimetallic Nanocatalyst

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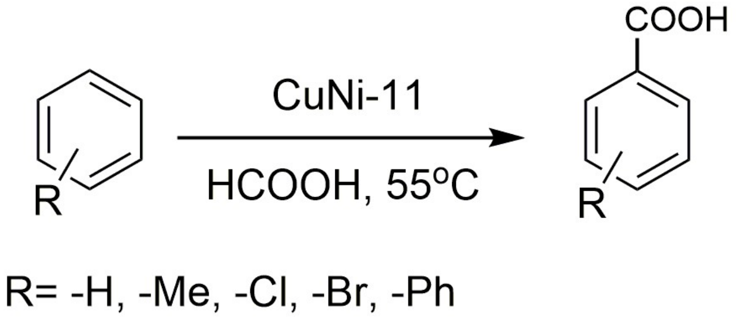
Herein, we report the bimetallic CuNi-11 nanocatalyst for direct carboxylation of arenes with excellent yield. Combined catalytic experiments and Density Functional Theory (DFT) calculations provide mechanistic insights revealing the interplay of the individual metals in the formation of the corresponding acids. The mechanistic pathway involves benzene and formic acid C-H bond activation, benzoic acid and H_2 formation with the benzene C–H activation being the rate-determining step. Further, the bimetallic CuNi-11 nanocatalyst exhibits a high surface area of 58.993 m^2/g with excellent reusability (up to 6 cycles) and the carboxylation reaction is activator-, additive- and solvent-free taking place at mild conditions. The CuNi-11 (molar ratio of Cu:Ni = 1:1) was characterized by Powder X-ray diffraction study, Thermogravimetric analysis, N_2-adsorption desorption analysis, VSM magnetic study and morphogical study by SEM, HR-TEM and oxidation state study by XPS analysis.

Keywords: Carboxylation reaction, CuNi nanocatalyst, Magnetic nanoparticles, bimetallic nanocatalyst, Recyclable catalyst.



Facets Dependent Catalytic Activity of Pd Nanocrystals for the Remedy of Organic Pollutant: A Mechanistic Study

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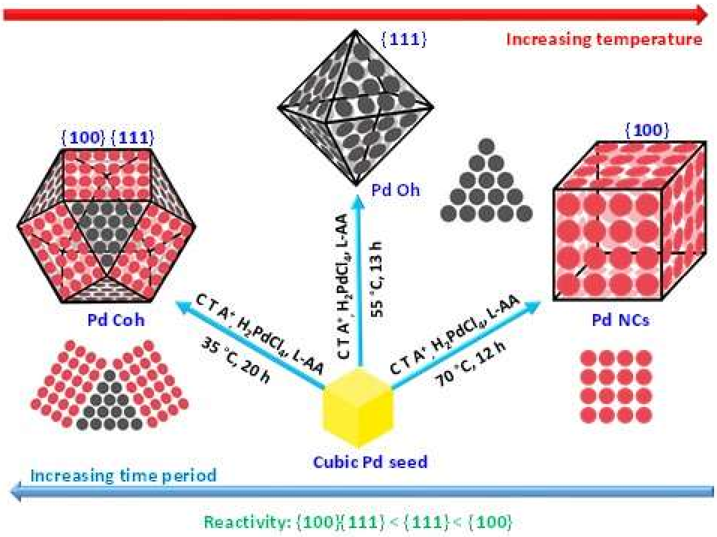
Facet dependent catalytic activities of Palladium (Pd) nanocrystals have great significance in the field of catalysis. In this report, the robust seed-mediated synthesis method has been used to synthesize cuboctahedral (Coh), octahedral (Oh), and cubic Pd nanostructures. Optimizing the reaction time and temperature, the growth of nanocrystals directed along different low index planes such as {100} for Pd NCs, {111} for Oh and mixed planes of {100} and {111} assigned for Coh structure. To understand the role of different facets, nanocrystals were employed for the reduction of organic pollutant *4*-Nitroaniline (*4*-NA) to *4*-Phenylene diamine (*4*-PDA), and substituent effect of nitro (–NO_2) group such as *3*-NA and *2*-NA were studied. By keeping the total surface area of particles, the same, different volumes of nanocrystals were taken into account to carry out an accurate facet-dependent analysis. To extend the catalytic activity, degradation of cationic dye, Rhodamine B (Rh B), and anionic dye, Methyl Orange (MO) were studied. The reduction and degradation process were monitored through UV-Visible absorption spectroscopy. It was confirmed from the absorption spectra that the efficiency of Pd NCs was higher than Oh and Coh nanocrystals, which established the depiction of the best role of {100} planes out of the other two planes exposed on the surface. The catalytic trends of low index planes follow the order NCs {100}> Oh {111}> Coh {100} {111} for Pd nanocrystals was confirmed from the analytical model.

Keywords: Palladium nanocrystals; Low index planes; Organic pollutant; Cationic dye, Anionic Dye.



Synthesis and Characterization of Metal Halide Perovskite-Gold Nano Rod

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In recent years, metal halide perovskites have become a burgeoning field of research due to their applications in solar cells, light emitting diodes (LEDs), photodetectors, and lasers[1,2]. Lead-halide perovskite materials are widely recognized for their strong potential as photovoltaic materials though due to its toxicity and instability; main focus has inclined towards synthesis of lead-free perovskite materials amongst which double perovskites are one of the best candidates[3,4]. In this work, a nanoheterostructure, involving a lead free halide double perovskite (DP) $Cs_2AgBiBr_6$ and Gold nanorod (AuNRs) has been synthesized linkingthrough a bifunctional ligand 1,4-aminothiophenol (4-ATP). Gold nanorods (AuNRs) are of intense technological interest due to their broadly tunable surface plasmon resonances (SPR), also a promising material for SERS[5]. It shows broad range of Longitudinal Surface Plasmon Resonance (LSPR) band around 600-1100nm[6]. Since most of double perovskites and perovskites are high band gap materials, hence unable to absorb low energy photons (visible and IR regions) which are the main constituents of solar energy. The main purpose to synthesize the hybrid material (AuNR/4-ATP/DP) is that it would absorb a broad range and would be a promising material for photovoltaic devices.

Keywords: Gold nanorod, Perovskite, Double Perovskite, Surface Plasmon Resonance

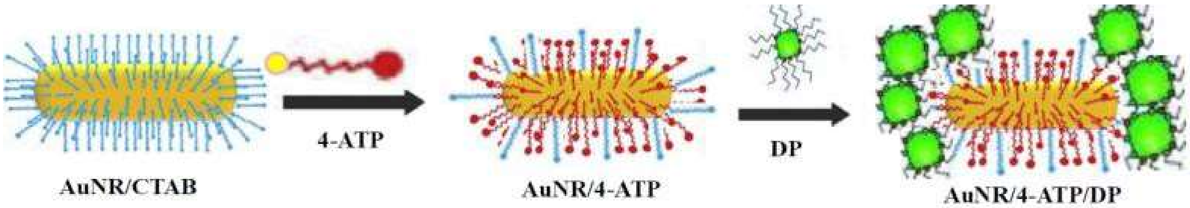

Figure: Schematic representation of preparation of the heterostructure AuNR/4-ATP/DP

Polyacrylonitrile (PAN)/Aminoclay- Based Self-Cleaning Membranes for Multiple Emerging Pollutant Separation and Wastewater Treatment

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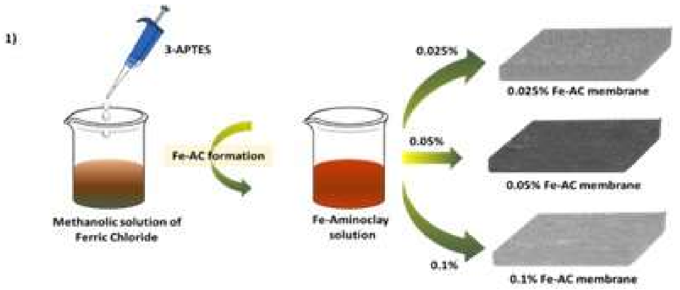
The rapid development of manufacturing technology after the industrial revolution has improved the standards of living significantly but it is becoming a factor that is threatening human health and environment. Increased industrialization has led to contamination of various water sources. These toxic effluents have great carcinogenic and mutagenic effects on aquatic life as well as other life forms thus resulting in imbalance in the ecosystem. Thus, treatment of such contaminated waters becomes a priority. From the past few decades, membrane technology is emerging as one of the promising techniques which addresses the concern towards wastewater treatment. Some of the conventional membrane materials such as Polyacrylonitrile (PAN) are being used in commercial filtration processes, while high flux at low pressure and high fouling tendency limits its widespread utility towards water purification. Herein, for the first time, self-cleaning aminoclay (AC) based PAN membranes are produced by a cost-effective and sustainable process. A remarkable increase in flux rate was achieved without compromising the rejection efficiency of the solutes and chemical structure of PAN. The structural and functional properties of the as prepared AC PAN membranes were thoroughly characterized using ATR-IR, FE-SEM, PXRD, contact angle and zeta potential measurements. Performance testing for optimized membranes using various feed streams under different testing conditions showed > 90.0% rejection for most of dyes (anionic, cationic and neutral), humic acid and > 40.0% for $MgSO_4$ with 50.0-70.0 $Lm^{-2}h^{-1}$ flux at 4 bar pressures. The study was extended using pharmaceutical wastes as feed solutions and >90.0% rejection was achieved. Moreover, long-term studies revealed to compare commercial RO to different Fe-AC membranes which showed high flux without compromising rejection of humic acid. The membranes were stable even after repeated operating cycles without any significant reduction in flux and rejection, thus manifesting their potential to be used as an effective pre-treatment media for various pharmaceutical wastewater treatment. Therefore, Fe-AC membrane can be anticipated as both high rejection and self-cleaning via cost-effective and eco-friendly approach.

Keywords: Membrane, Aminoclay (AC) Fe-aminoclay (Fe-AC), Polyacrylonitrile (PAN), blend.



Atom Transfer Between Precision Nanoclusters and Polydispersed Nanoparticles: a Facile Route For Monodisperse Alloy Nanoparticles and Their Superstructures

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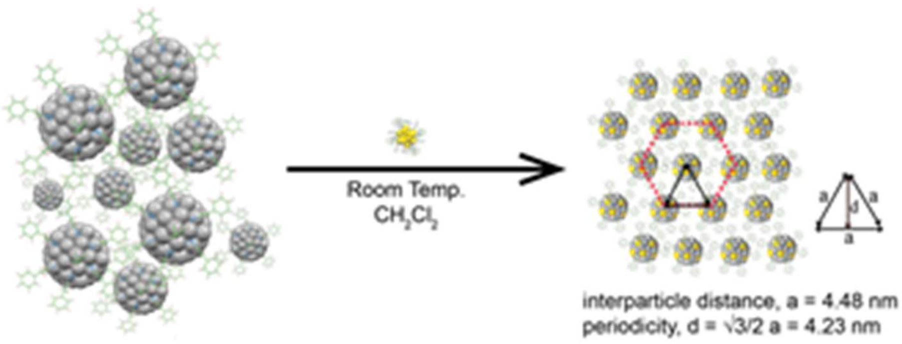
Reactions between atomically precise noble metal nanoclusters (NCs) have been studied widely in the recent past, but such processes between NCs and plasmonic nanoparticles (NPs) have not been explored earlier. For the first time, we demonstrate spontaneous reactions between an atomically precise NC, $Au_{25}(PET)_{18}$ (PET = 2-phenylethanethiol), and polydispersed silver NPs with an average diameter of 4 nm and protected with PET, resulting in alloy NPs under ambient conditions. These reactions were specific to the nature of the protecting ligands as no reaction was observed between the $Au_{25}(SBB)_{18}$ NC (SBB = 4-(tert-butyl) benzyl mercaptan) and the very same silver NPs. The mechanism involves an interparticle exchange of the metal and ligand species where the metal–ligand interface plays a vital role in controlling the reaction. The reaction proceeds through transient $Au_{25-x}Ag_x(PET)_n$ alloy cluster intermediates as observed in time-dependent electrospray ionization mass spectrometry (ESI MS). High-resolution transmission electron microscopy (HRTEM) analysis of the resulting dispersion showed the transformation of polydispersed silver NPs into highly monodisperse gold–silver alloy NPs which assembled to form 2-dimensional superlattices. Using NPs of other average sizes (3 and 8 nm), we demonstrated that size plays an important role in the reactivity as observed in ESI MS and HRTEM.

Keywords: Nanocluster, reactions, alloy, gold, silver, nanoparticles



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Tolerant and Hard Superhydrophobicity: Restricting Physical Deformation

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Lotus leaf-inspired superhydrophobicity emerged as a prospective avenue for developing various functional materials. But the durability of such nature-inspired artificial materials remains a significant concern and thus restricts its future applications at outdoor settings. Multiple strategies have been introduced in the last few years to develop abrasion tolerant and mechanically durable superhydrophobic coatings.Although some of these seminal reports achieved durable superhydrophobic coatings on rigid substrates, most reported approaches followed complex fabrication processes or required sophisticated setups. Moreover, the previously reported strategies could not tailor the mechanical properties of the soft and geometrically complex (fibrous and porous) substrates. In this work, we have reported facile 1,4-conjugate addition reaction under ambient conditions between selected reactants, i.e. [3-(2-aminoethylamino)propyl]trimethoxysilane (AEAPTMS) and octadecyl acrylate (ODAc), in the presence and absence of crosslinker molecules [pentaerythritol triacrylate (3-Acl) or dipentaerythritol penta-acrylate (5-Acl)] to develop either non-deformable or deformable (compressible/stretchable) superhydrophobic coatings on selected soft and deformable respectively, as shown in Schematic. The compressive and tensile moduli of the selected soft substrates increased by 2.2 × 104 % and 1.8 × 104 %, respectively, after the deposition of the appropriate reaction mixtures. Moreover, the integration of the crosslinkers in the reaction mixture provided a facile basis to resist the physical erosion/rupture of the selected soft substrates under severe abrasive conditions. Hence this current approach is likely to open up the possibilities for using prospective bio-inspired wettability in different and relevant outdoor applications in the future.

Keywords: Superhydrophobicity, Cross-linker, Physical deformation, Tolerant

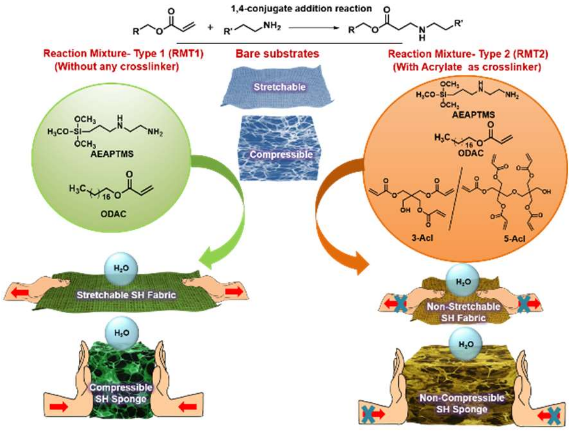

Figure Schematic illustration for the preparation of deformable and non-deformable superhydrophobic materials

ICANN2021 **ID: A1040**

Fabrication of Orthogonally Reactive Micron/ Sub-Micron Capsules

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Hollow polymeric capsules tailored with different desired chemical functionalities are of particular interest due to their potential application in confining various cargo, liquid crystal, and bioactive enzymes for the various relevant application. One of the most versatile and facile approaches for the fabrication of mono-disperse hollow capsules is the layer-by-layer (LbL) deposition process, where appropriately selected polyelectrolytes- or polymers-pairs having complementary functional groups that can mutually interact or react, are sequentially deposited on the sacrificial colloidal templates. The LbL method provides precise control over the size, shape, shell thickness, composition of the resulting hollow multilayered capsules. In the past, mostly weak interactions/bondings, such as electrostatic interactions, hydrogen bonds, disulfide bonds, host-guest interactions etc., between two different polymers, were used to synthesize multilayered microcapsules. In our approach, a single polymer derived covalently crosslinked microcapsule loaded with orthogonally-reactive residual functional groups- acrylate and amine, is synthesized by the facile LbL deposition process following the catalyst-free 1,4-conjugate addition reaction at ambient conditions. Further, this single polymer derived microcapsule is tailored with different desired functionalities using various selected nucleophiles and electrophiles, following two orthogonal reaction pathways at ambient conditions.

Keywords: Microcapsule, layer-by-layer, 1,4-conjugate addition reaction

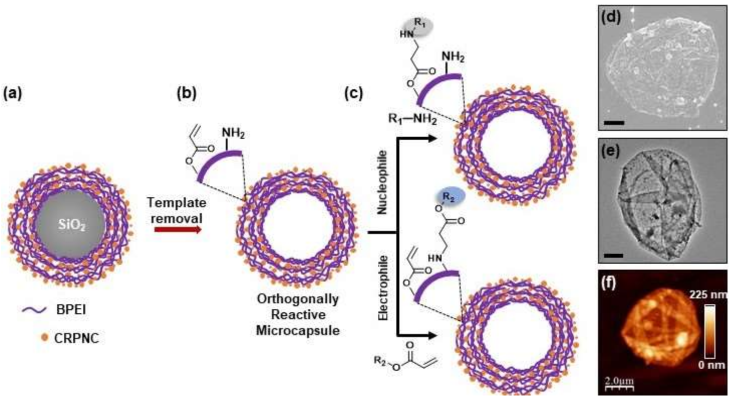

Figure. (a-c) Schematic representation of (a) CRPNC/BPEI coated silica microparticles, (b) dually reactive microcapsules of CRPNC/BPEI loaded with residual acrylate and amine groups after core dissolution, (c) 1,4-conjugate addition reaction of residual acrylate and amine with nucleophile and electrophile, respectively. (d-f) FESEM (d), FETEM (e), and AFM (f) images of microcapsules made of multilayers (5 bilayers) of CRPNC/BPEI. Scale bar 2 µm for (d) and e).

ICANN2021 **ID: A1041**

Chitosan-PVA Composite Film as a Local Drug Delivery System for Pancreatic Cancer Treatment

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Pancreatic cancer is a metastatic cancer with poor prognosis and diagnostic difficulty. Pancreatic tumor lacks necessary blood vessels, and hence it is difficult for anticancer drugs to reach there. By the time it is detected, it would have already spread to other body parts. So, removing the tumor through surgery becomes difficult. Until now, the main challenges in the treatment has been: (i) the toxicity caused by drugs going to healthy cells instead of the desired cancer cells, (ii) drug resistance and overdose of a single drug causing inefficiency in destroying the tumor completely and thus increasing the chances of recurrence, (iii) gemcitabine (GEM), the stand-alone drug for pancreatic cancer treatment is highly hydrophilic and hence, difficult to have its controlled release.

To overcome the above challenges, there is a need for a local drug delivery system. In this direction, we have made a composite film loaded with both GEM and curcumin (CUR), by solvent casting method. Chitosan was mixed with PVA in an equal volume ratio for improved mechanical strength of the film. It resulted in a drug-loaded film with modulus of elasticity of 0.65 MPa, which reduced to 0.19 MPa after crosslinking with sodium tripolyphosphate (TPP). As expected, the composite film showed a higher strength than pure chitosan and displayed a desirable, controlled release of both CUR and GEM, with only 50% and 70% release, respectively, in acidic pH, after two weeks. Cytotoxicity results in pancreatic cancer cells have shown more than 50% killing, when both the drugs were used in conjunction in the film. Based on MTT results, none of the polymers were toxic to healthy cells.

GEM is administeredintravenously or through adrug-loaded carrier, from which it is released within a day. A rapid releasebecomes problematic for healthy tissues and also compromises itseffectiveness on tumor cells.However, so far, the approach of delivering dual anticancer drugsthrough a biodegradable polymer composite gel for local delivery, has not been tried. Our results indicatethat the gel can be used for efficient delivery of dual anticancer drugs in the treatment of pancreatic cancer

Keywords: Chitosan, PVA, Curcumin, Gemcitabine, and TPP

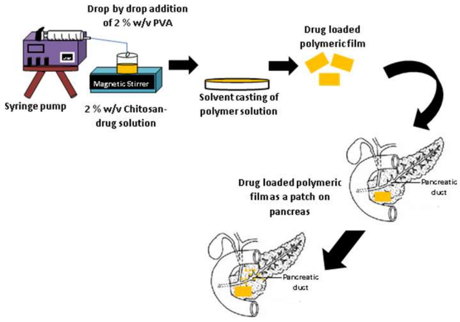

Figure 1: Drug loaded chitosan-PVA composite filmfor local drug delivery

Mechanically Tailorable, Superhydrophobic Silk Sponges for Environmental Remediation

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Silk cocoon derived silk fibroin (protein) and silk microfibers have been widely used for prospective biomedical, energy, and environmental applications. Deformable silk sponges have been fabricated in the past associating different nanomaterials. However, reports on controlling the mechanical property of silk sponges is scarce. Moreover, the chemical modification of silk protein requires extremes of temperatures and catalysts. In this approach, facile tailoring of both mechanical property and induction of chemical reactivity at ambient conditions has been introduced. The ethanol-assisted induction of β-sheets in the silk protein network provided scope to modulate the beta sheet content as desirable which in turn affected the mechanical property. The additional silk microfibers as reinforcements imparted mechanical stability to the sponges and aided in self-recovery after compression. Simultaneously, the 1,4-conjugate addition reaction between amine residues of silk (fibre and fibroin) and acrylate groups of a multifunctional cross-linker provided residual chemical reactivity. Further, the chemically "reactive" sponge was post modified with the selected alkylamines to introduce a wide range of water wettability (from 36 to 161°) without affecting the mechanical property. Thereafter, the silk cocoon-derived and extremely water-repellent sponge was used for environment-friendly remediation of oil spillages through selective absorption-based and filtration-based oil/water separation at different and severe aqueous conditions. This silk cocoon-derived mechanically tailorable and chemically reactive sponge could also be useful for various biomedical and energy-related applications.

Keywords: silk, mechanically tailorable, superhydrophobic sponges, oil−water remediation

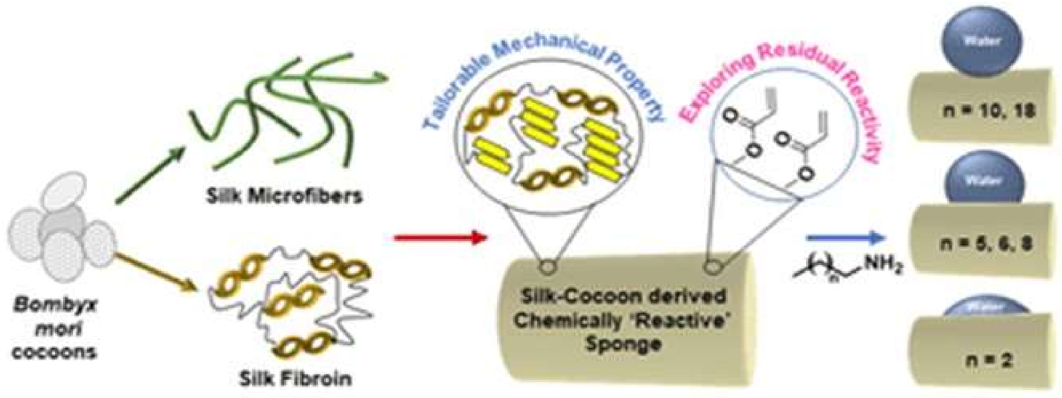

Figure: Schematic representing the fabrication of silk sponges using silk microfibers and silk protein such that the mechanical property can be tailored and chemically 'reactive' is induced. The residual chemical reactivity would provide an avenue to further functionalize the sponges with alkylamines to tailor the water wettability

ICANN2021 **ID: A1051**

Surface Modified Nanoparticle Impregnated Activated Carbon for Disinfection of Water

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Availability of safe drinking water is one of the current global challenges affecting millions of people and the situation is projected to worsen in coming decades. Conventional disinfection techniques used in the urbanized world has limitations, such as generation of toxic by-products or they require high capital investments. One of the most promising solutions to this problem is through the use of cheap, autonomous point-of-use water disinfection systems. In our work we have aimed to develop a nanoparticle (NP) conjugated activated carbon (AC) hybrid that can be used in column-based water decontamination. We have prepared copper nanoparticles (CuNP) with a mean diameter of 4.37 nm using green synthesis protocol and deposited them on the surface of acid functionalized AC to prepare the AC-NP hybrid. The exact chemistry behind the acid functionalization of AC was investigated using FTIR and XPS, while the impregnation of CuNP was characterized, both qualitatively using SEM and EDX, and quantitatively though ICP-AES. A maximum loading of 0.8 ± 0.08 wt% of CuNP is obtained in case of 48-hour acid treated AC hybrid. Further, batch killing studies performed with the hybrid shows complete inactivation of E. coli in contaminated water within 35 minutes of residence time, thus demonstrating good antibacterial performance of the hybrid and its potential for use in column-based systems for water disinfection.

Keywords: nanoparticle, synthesis, bacteria, water, disinfection

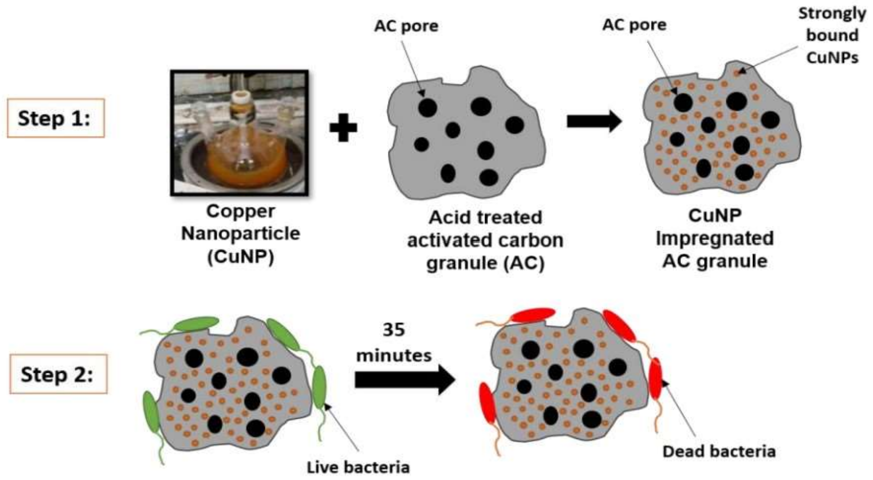

Figure: Schematic illustration of the proposed methodology for decontamination of drinking water by nanoparticle conjugated activated carbon hybrid

Copper Sulfide Nanostructures: Synthesis and photocatalytic activities

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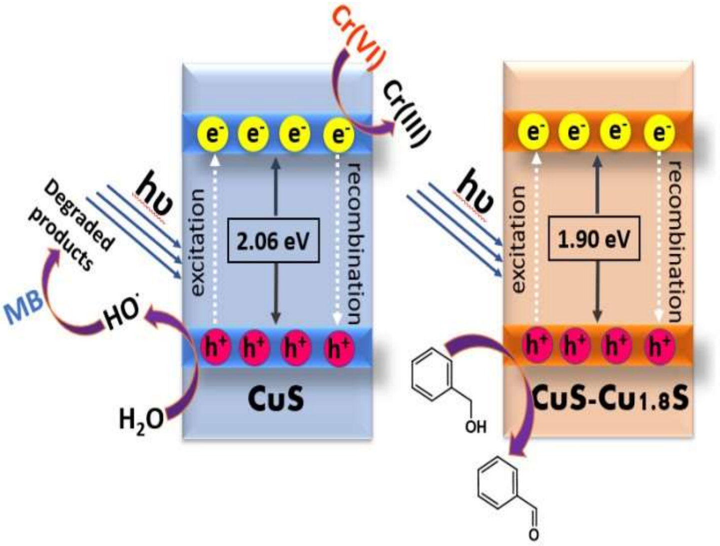
Multifunctional and eco-friendly photocatalyst is the demand of 21st century for a sustainable living without compromising its efficiency and activity. A low cost, greener and versatile nanomaterial was developed as a bifunctional catalyst for the synthesis of industrially concerned benzaldehydes and removal of water pollutant. Pure (CuS) and mixed phase copper sulfide (CuS-Cu1.8S) nanostructures were designed through a simple and green protocol through hydrothermal route. Sodium dodecyl sulfate in the synthesis is employed as the growth directing reagent to obtain hexagonal nanoplates and broken nanosheets. The optical study revealed the UV-visible absorption in the near UV and visible region with band gap of 2.06 and 1.90 eV for pure and mixed phase copper sulfide respectively. The synthesized pure hexagonal covellite CuS turned out to be highly efficient in the removal of water pollutant (MB degradation and Cr(VI) reduction) while the mixed phase exhibited photocatalytic conversion of benzyl alcohols to corresponding benzaldehydes with ~99% selectivity.

Keywords: Bifunctional, copper sulfide, photocatalyst, benzaldehyde.



Bimetallic Ag-Cu Alloy Microflowers as SERS Substrates with Single Molecule Detection Limit

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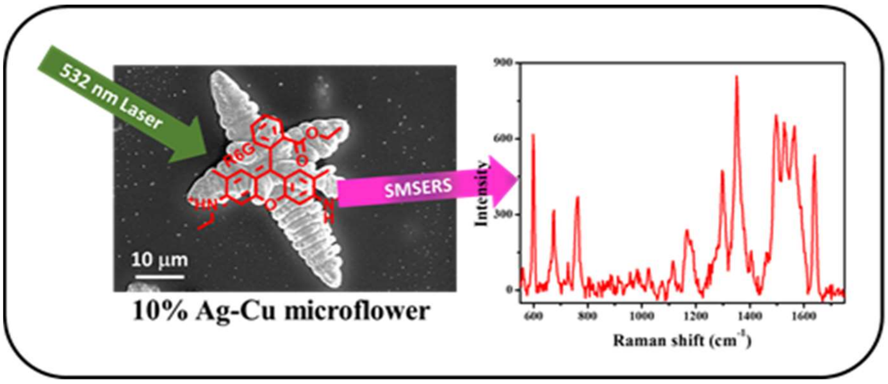
Bimetallic Ag-Cu alloy microflowers with tunable surface compositions were fabricated as SERS substrates with a limit of detection in the zeptomolar range for the analyte molecule Rhodamine 6G (R6G). The substrates were prepared on a glass coverslip through a bottom-up strategy by simple thermolysis of metal-alkyl ammonium halide precursors. The reaction temperature and composition of the alloy were varied sequentially to find out the maximum SERS efficiency from the substrates. While, UV-Vis spectroscopy were employed to characterize the optical properties of the substrates, the bulk and surface composition of the microflowers were determined using ED-XRF and XPS techniques, respectively. Also, the structural and morphological characterization of the substrates were performed by X-ray diffraction and SEM, respectively. For alloys, the ED-XRF studies confirmed that the bulk compositions matched with the feed ratio, while the surface compositions were found to be rich in copper in form of both elementary copper and copper oxide, as revealed by XPS studies. From the efficiency studies for different compositions prepared, it was found that 10% Ag-Cu alloy microflowers produced maximum SERS intensity for resonant R6G molecule as probe. In fact, R6G evidence 50-fold enhancement in SERS spectra with 10% alloy microflowers as against pure Ag microflower. Using 1, 2, 3-benzotriazole as a non-resonant Raman probe, uniform enhancement factors in the order of $\approx 10^8$ were achieved from different parts of the 10% Ag-Cu alloy microflower. The same substrate showed excellent Raman response for detecting R6G at very low concentrations such as 10 zM, leading to detection and analysis of SERS spectra from a single R6G molecule.

Keywords: SERS, Ag-Cu, bimetallic, alloy, Rhodamine 6G, single molecule.



ICANN2021 **ID: A1055**

Manifestation of Non-Covalent Interactions in Self-Assembled Copper Nanoclusters

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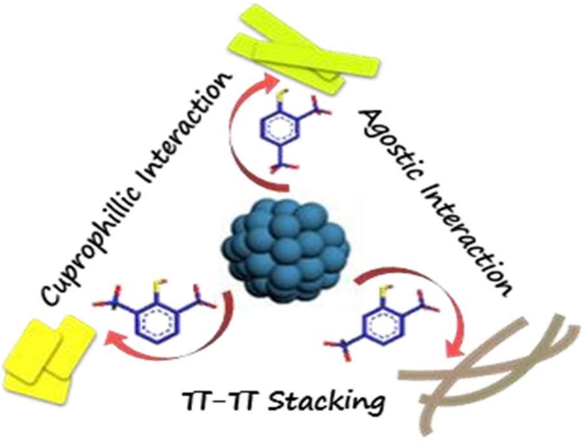
The family of directed self-assembly has found its pristine building block in sub-nanometer metal nanoclusters (NCs) owing to their precise composition and customizable surface environment. Herein, our findings will allow to understand how the non-covalent interactions direct the morphology with a subtle change of only one –CH_3 position in the capping ligand. We have designed three different self-assembled structures of Cu NCs with three isomers of dimethylbenzenethiol ligand resulted into rod, platelet and ribbon like assembly. Although the steric factor of the ligands are unlike, the building blocks are found to be identical, Cu_7L_6 NC for all the three assembled structures, thus eliminating the compositional effect on different morphology. Detailed investigation reveals that the interplay of cuprophilic, π-π stacking and agostic interaction (Cu-C···H) direct the organization of Cu_7 NCs into different ordered structures. The difference in –CH_3 position of the isomers significantly alters the extent of π-π stacking and agostic interaction among the NCs. The ribbon like assembly shows maximum extent of agostic interaction as the capping ligand has more ortho-CH_3 groups. The red emission and excited state relaxation dynamics for the three assembly structures strongly establish a relation with the degree of compactness and different extent of interactions amongst them. The insights into the tailored self-assembled structures and their tunable optical properties will pave the way for designing ordered structure with promising application.

Keywords: Self-assembly, Metal Nanoclusters, Isomers, Agostic Interaction.



Green Synthesis of Full-Color Fluorescent Carbon Nanoparticles from Eucalyptus Twigs for Sensing the Synthetic Food Colorant and Bioimaging

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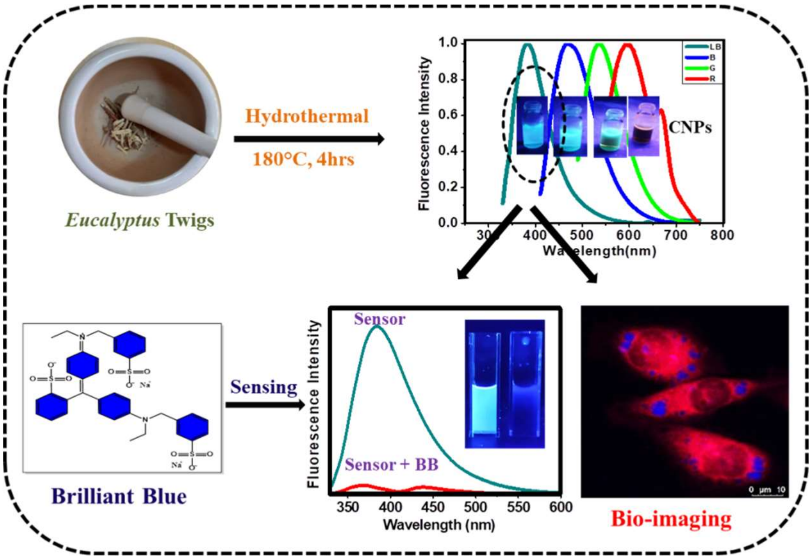
Full-color fluorescent carbon nanoparticles (CNPs) are produced by a facile and green hydrothermal method followed by the differential washing technique. *Eucalyptus* twigs are used as a precursor to synthesize multiemissive light blue, blue, green, and red CNPs. Brilliant Blue FCF (BB) is a widely used synthetic food colorant, which is toxic for the human body, when consumed beyond the permitted limit. Herein, we demonstrate light blue CNPs as a sensor for selective and sensitive detection of BB *via* a fluorescence quenching mechanism with a limit of detection of 200 nM. Temperature-dependent fluorescence and ^{1}H NMR studies confirmed the mechanism as combined dynamic and static quenching. To demonstrate the practical efficacy of the sensor, BB is effectively detected and estimated in selected food samples procured from the market. Moreover, the biocompatibility of light blue and blue CNPs is examined and confirmed by performing a cytotoxicity assay on MDA-MB-231 cell lines. Subsequently, the cellular imaging study is also carried out to explore the internalization process of the CNPs as a function of concentration. To the best of our knowledge, this is the first time that *Eucalyptus* twigs, a natural source of high abundance, are used as raw materials and valorized for sensing artificial food color and bioimaging purposes.

Keywords: *Eucalyptus* twigs, carbon nanoparticles, sensing, brilliant blue, Bioimaging



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Triboelectric Generator for Sustainable Synthesis of Nanoparticles and Nanoclusters

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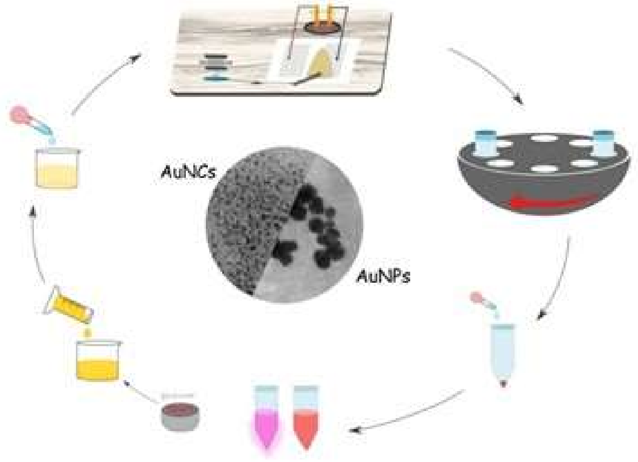
Here, we demonstrate a simple and affordable means to room temperature synthesis of plasmonic nanoparticles and luminescent nanoclusters of gold. The synthesis was performed using a robust, easy to build, and inexpensive triboelectric generator (TG). The electricity generated by the TG was transferred to the solution continuously to synthesize gold nanoclusters (AuNCs). The obtained AuNCs had an extremely narrow size distribution with a mean particle size of ~2 nm and showed a bright pink luminescence under UV light. The approach was also extended to synthesize plasmonic gold nanoparticles (AuNPs). With this method, the synthesis time could be reduced from hours to several minutes without requiring any reducing agents.

Keywords: Triboelectric generator, Gold nanoparticles, Gold nanoclusters



Ultrafast Carrier Relaxation Dynamics in 2D CdSe Nanoplatelets for Photodetector Applications

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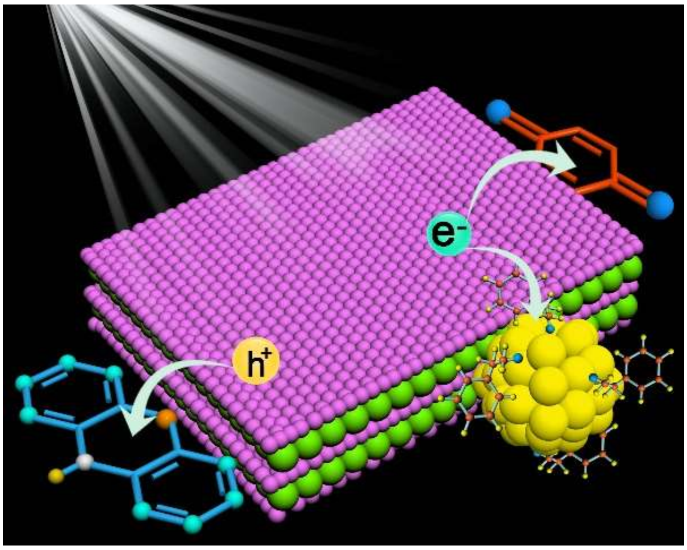
Two-dimensional (2D) atomically thin colloidal semiconductor nanoplatelets (NPLs) have recently emerged as a novel nanostructure exhibiting several unique photophysical properties such as large absorption cross-section and high exciton binding energy, very narrow emission line-width, tunable emission, high molar extinction coefficient, and high photo-stability. Designing of hybrids or heterostructures and understanding the ultrafast carrier dynamics is essential for optoelectronic and photocatalytic applications. We have designed heterostructure/hybrids based on 2D CdSe NPLs with metal nanoclusters and molecular acceptors. Transient absorption spectroscopy depicts ultrafast electron/hole transfer and the presence of radical ion in the transient absorption signal, confirming the efficient charge separation between CdSe NPLs and metal nanoclusters/molecular acceptors. The devices exhibit more considerable photocurrent enhancement, higher responsivity, detectivity than pure NPLs based devices. It holds promise for the future design of 2D NPLs-based materials for optoelectronic applications.

Keywords: 2D nanoplatelets, CdSe NPLs, Ultrafast charge transfer, Photodetectors



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Detection of Nuclear Hydrogen Peroxide in Living Cells by Carbon Dot-Based Nucleus Targeted Fluorescent Imaging

Kabyashree Phukan;[1], Ritwick Ranjan Sarma;[1], Somarani Das;[2], Rajlakshmi Devi*[2] and Devasish Chowdhury *[1]

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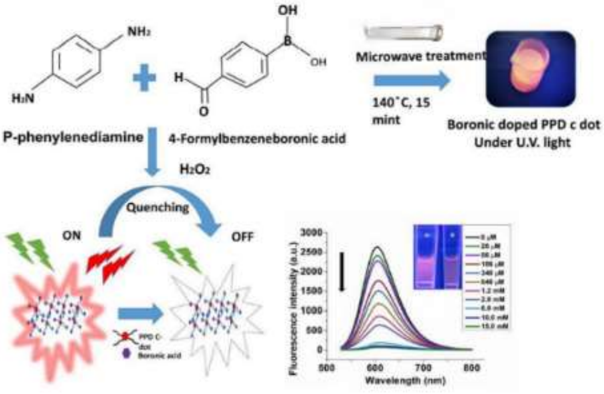
Among various reactive oxygen species (ROS), H_2O_2 is one of the major ROS produced by living cells. Under oxidative stress conditions, intracellular generation of H_2O_2 becomes high which indicates the beginning of inflammation-related various diseases. However, investigation of intracellular generation of H_2O_2 is crucial for preventing various diseases since it is closely linked with different physiological and complex cell signaling pathways. Despite the development of various fluorescent probes, the drawback of the majority of the fluorescent probes is that they cannot move across the nuclear membrane. However, detection of the nuclear level of H_2O_2 is very important since it can directly cause oxidative DNA damage which ultimately leads to various diseases. Therefore, in this study, *p*-phenylenediamine based carbon quantum dots (B-PPD CDs) have been synthesized and integrated with 4-formyl benzene boronic acid as a doping agent for the detection of H_2O_2. The detection mechanism showed that, upon exposure to H_2O_2, the fluorescence of the B-PPD CDs was immediately quenched. Further investigation has been done in the *in vitro* RAW 264.7 cell line by both exogenous and endogenous exposure of H_2O_2 to demonstrate the feasibility of the method. It is shown successfully that the exogenous presence and endogenous generation of H_2O_2 in RAW 264.7 cells can be detected using B-PPD CDs. The limit of detection (LOD) was determined to be 0.242 µM. Thus the synthesis of such fluorescent probes using carbon quantum dots will lead to the practical application in live-cell imaging as well as ROS detection in the nucleus of the cell.

Keywords: ROS, Exogenous, Endogenous, B-PPD CD, Fluorescence, H_2O_2 detection



Scheme: Schematic representation of the synthesis of B-PPD CDs and fluorescent switch on-off sensor for H_2O_2 detection.

A Unique Bridging Facets Assembly of Gold Nanorods for the Detection of Thiram Through SERS

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Concerns have grown in recent years about the widespread use of the pesticide thiram (TRM), which has been linked to negative effects on local ecosystems. This highlights the critical need for quick and accurate point-of-need pesticide analysis tools for real-time applications. The detection of TRM using gold nanorods (Au NRs) with a limit of detection (LOD) of 10^{-11} M (10 pM) and an enhancement factor (EF) of 2.8×10^6 along with 6.2% of signal homogeneity (with respect to peak at 1378 cm^{-1}) achieved through surface-enhanced Raman scattering (SERS). Spectroscopic analysis reveals the formation of the Au-S bond, which emphasizes the adsorption of TRM on Au NRs through Au-S bond. Addition of Au NRs to TRM of higher and lower concentration, yields side-by-side assembly (SSA) and bridging facets assembly (BFA), respectively and exhibited excellent hotspots for the ultra-low detection of TRM. Bridging facets of Au NRs, such as (5 12 0) and (5 0 12) planes are mainly responsible for the BFA. This kind of interaction is observed for the first time and not reported elsewhere. The detailed facets of Au NRs, namely side facets, bridging facets and pyramid facets, were discussed with the 3D model of Au NRs. The interaction of Au NRs with TRM is sensitive, and ultra-low detection of hazardous TRM through SERS makes an ideal technique for environmental protection, real-time applications and analysis of one-of-a-kind materials.

Keywords: Gold nanorods (Au NRs); Thiram (TRM), Surface-enhanced Raman scattering (SERS), Side by side assembly (SSA), and Bridging facets assembly (BFA)

Multifunctional N-Doped Carbon Dots for Bimodal Detection of Bilirubin and Vitamin B12, Living Cell Imaging, and Fluorescent Ink

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A N-doped carbon dot (NCD) has been synthesized via a simplistic one-step hydrothermal technique using L-aspartic acid and 3,6-diaminoacridine hydrochloride. The NCDs exhibit a high quantum yield (22.7%) and excellent optical stability in aqueous media. Additionally, NCDs display good solid-state yellowish-green emission and are suitable for security ink applications. The remarkable fluorescence (FL) properties of NCDs are further applied to develop a multifunctional sensor for bilirubin (BR) and vitamin B12 (VB12) via fluorescence quenching. We have systematically studied the FL quenching mechanisms of the two analytes. The primary quenching mechanism of BR is via the Förster resonant energy transfer (FRET) pathway facilitated by the H-bonding network between the hydrophilic moieties existing at the surface of BR and NCDs. In contrast, the inner filter effect (IFE) is mainly responsible for the recognition of VB12. The practicability of the nanoprobe NCDs is further tested in real-sample analysis for BR (human serum and urine samples) and VB12 (VB12 tablets, human serum, and energy drink) with a satisfactory outcome. The in vitro competency is also verified in the human cervical cancer cell line (HeLa cell) with negligible cytotoxicity and significant biocompatibility. This result facilitates the application of NCDs for bioimaging and recognition of VB12 in a living organism.

Keywords: N-doped carbon dots, bilirubin detection, vitamin B12 sensing, cell imaging, fluorescent ink.

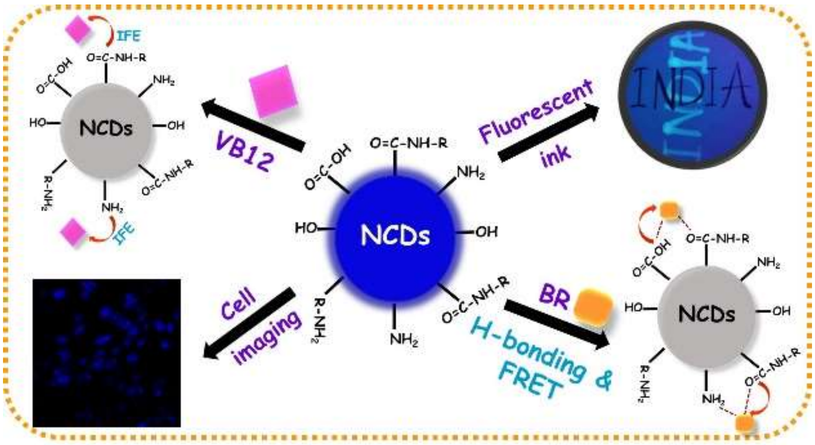

Figure: Blue emitting N-doped carbon dot for highly selective and sensitive detection of bilirubin, vitamin-B12, living cell imaging and fluorescence inlk

Synthesis of Surface Modified Carbon Nanotube Composite for Environmental Pollutant Sensing Application

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A great deal of research is directed towards real-time monitoring of environmental pollutants as their excessive presence has a negative impact on environmental and human health. With rapid urbanization and industrialization, the need for an affordable, rapid, reliable, and portable gas sensor is of paramount importance. This study reports the fabrication of a room temperature carbon monoxide (CO) sensor based on multiwalled carbon nanotube (MWCNT)-poly (diallyldimethylammonium chloride) solution (PDDA) composite. The surface of MWCNT is functionalized with PDDA, and confirmed with appropriate characterizations. Interdigitated electrodes of silver are patterned on glass substrates, and MWCNT-PDDA composite is used as a sensing material. The electrical conductivity of the sensor changes due to charge transfer from CO to the positively charged quaternary ammonium group present on PDDA. The developed sensors can detect very low concentrations of CO gas ranging from 1 to 20 ppm with high sensitivity and limit of detection (LOD) of 127 ppb. The influence of other interfering gases and volatile organic compounds on the sensor has been investigated. The stability and repeatability of the sensor are examined, and the sensor shows almost stable performance for two months with excellent reproducibility. The sensors have shown excellent potential for rapid CO gas sensing, and they can be used in wearable electronics applications.

Keywords: Carbon nanotubes; Carbon monoxide; Nanomaterial; Sensor

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Composition Controllable Green Synthesis of Manganese Dioxide Nanoparticles Using an Edible Freshwater Red Alga and Its Photocatalytic Activity Towards Water Soluble Toxic Dyes

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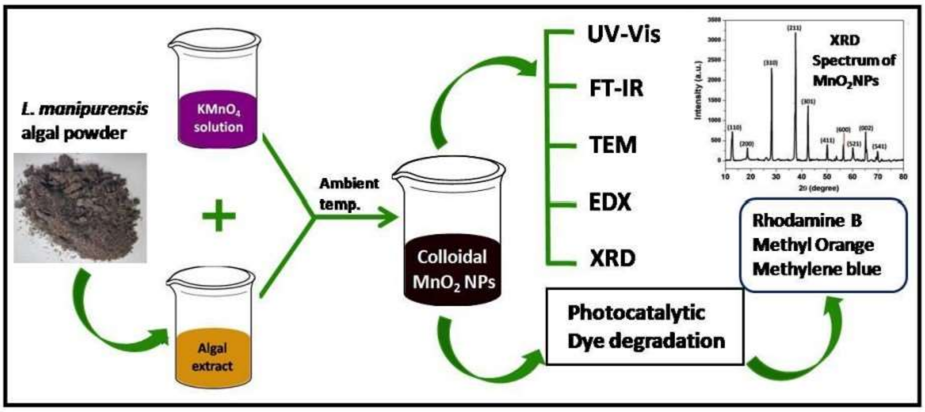
Composition controllable, facile and ambient temperature green synthesis of high purity manganese dioxide (α-MnO2) nanoparticles has been accomplished via reduction of an aqueous KMnO4 solution using aqueous extract of an edible freshwater red alga, Lemanea manipurensis. The phytochemicals present in the alga have served as both reducing and stabilizing agent. The as-synthesized nanoparticles were characterized by UV-vis, FT-IR, XRD, TEM, and EDX studies. The as-synthesized MnO2NPs showed excellent photocatalytic activity at ambient temperature for degradation of toxic dyes, rhodamine B (RhB), methyl orange (MO) and methylene blue (MB), the degradation rate being 0.082, 0.041 and 0.034 min-1 , respectively. The best photocatalytic performance was observed for RhB dye degradation under UV-visible light exhibiting almost complete degradation (91%) within 30 min of irradiation time. The photocatalytic degradation for all the dyes followed a pseudo-first order kinetics.

Keywords: Green Synthesis; Nanoparticles; Red alga; Lemanea manipurensis; Photocatalytic.



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Lichen Mediated Facile One-Pot Green Synthesis of Reduced Graphene Oxide (Rgo)-Ag@Mno2 Novel Ternary Nanohybrid

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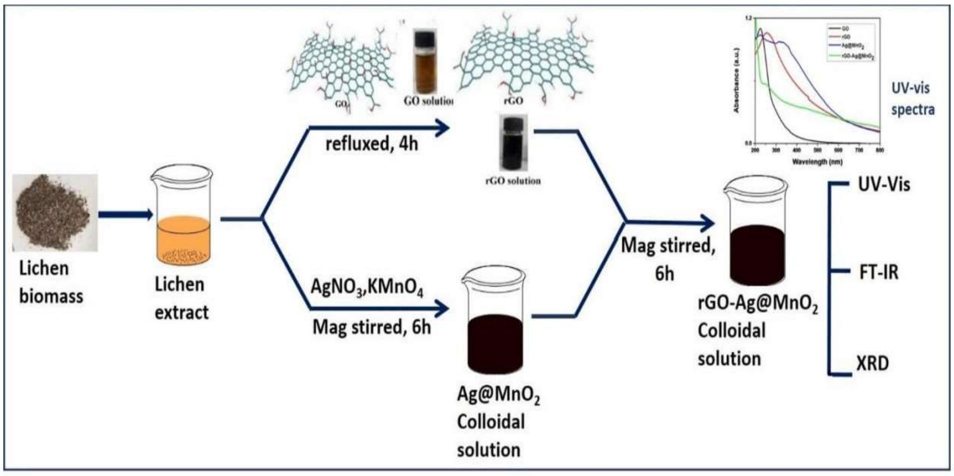
A novel ternary nanohybrid of reduced graphene oxide, (rGO)-Ag@MnO2 was prepared via a facile, low-cost, and green approach using aqueous extract of a lichen Acroscyphus spaerophoroides. In the first step, graphene oxide (GO) was prepared by a modified Hummer's method followed by reduction of exfoliated graphene oxide using the lichen extract. The lichen extract was further employed as reducing and stabilizing agent to synthesize Ag doped MnO2 nanoparticle (Ag@MnO2) from an aqueous solution of AgNO3 and KMnO4 in one step at ambient temperature. Finally, the rGO and as-synthesized Ag@MnO2 dispersed in aqueous medium were simply mixed by magnetic stirring for 6h to obtain the novel ternary nanohybrid material. The synthesized GO, rGO and nanohybrids were characterized using different spectroscopic techniques such as UV-Vis, IR and XRD etc.

Keywords: green synthesis, Graphene oxide, Acroscyphus spaerophoroides, Ag@MnO_2 .



A Banana Peel Derived Heteroatom Doped Green Carbon Dots and Its Reduced Form as an Efficient Fluorescence Sensor for Heavy Metal Ions and Pesticides

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Carbon dots with inherent optical property have diverging application in the fields such as catalysis, bioimaging, therapeutics, photovoltaics, electronics and sensing. Due to their facile synthesis method and tremendous fluorescent property, they have been utilized as a FL probe since last two decades. In the present work, a Co-doped (fluorine, boron and nitrogen) carbon dots (CBP) have been prepared from banana peel and further its reduced counterpart was prepared using $NaBH_4$ as a reducing agent (rCBP). After a thorough and systematic study of various optoelectronic and photophysical properties of two carbon dots they were utilized as an efficient nanosensor. Cobalt, mercury and Monocrotophos are among the wide range of contaminants present in the environment and food products which affects the human health as well as the eco-system. The fabrication of a cost effective and easy to use sensor for various contaminants is the need of the hour to solve our present environment predicaments. Therefore, to solve the present problem a fluorescence turn-off-on model was created. The FL turn-off system for Cobalt ion and mercury ion were static in nature. Importantly, CBP and rCBP have shown a highly sensitive and selective behaviour towards Co^{2+} and Hg^{2+} ions respectively by responsive fluorescence turn off behaviour. Monocrotophos, a pesticide was found to be responsible for the turn-on mechanism for both the system. The limit of detection was calculated to be 75.11nM and 190 nM for Co^{2+} and Hg^{2+}. The developed sensor was designed for Co^{2+} and Hg^{2+} and Monocrotophos sensing.

Keywords: Carbon dots, fluorescence, Metal ions, pesticides.

Patterning of Polymer Micro-Threads by Dynamic Contact Line Lithography; Guided by Chemically Patterned Surface

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Due to a huge demand on microelectronics industry, the fabrication of micro-nano structures has become more significant when microelectronics industry began to fabricate the integrated chips using different lithography techniques. Usually, there are three primary approaches to pattern surfaces like top-down approach, bottom-up approach and self-organization method. Compare to other two, self-organization method is not widespread. Many researchers have focused on this unconventional method to achieve ordered patternsfor more than a decade. Many de-wetted micro-nano structures have been reported while casting a polymer solution. Many have reported reproducible ordered patterns also by controlling several factors. De-wetting is a spatio-temporal phenomenon which, shows the rupture of thin liquid film on a solid substrate into liquid droplets. Here, thin films play a significant role in ongoing de-wetting process. This, self-assembled colloidal lithography is very promising technique in order to fabricate micro-nano featured surface. Though, there are several difficulties but, this method is technically better in some areas and much cost-effective than conventional lithography process like photolithography or e-beam lithography. The flexibility of this printing process is remarkable in various fields, like surface modification, creating templates, sensors, data storage devices etc. This type of fabrication method is based on the so-called self-arrange of solute particle from an evaporating solution. A simple drop-cast is quite effective to re-arrange the solute particles to the edge of the contact line by capillary force and to deposit on the surface. This phenomenon is widely known as “coffee-stain” effect. Also, some others fabrication methods like mechanically or chemically induced contact line allows one to control over the deposited pattern to fabricate different ordered patterns of stripe or micro-nano drop of solute particle. Nevertheless being inexpensive, do not need complicated and expensive printing equipment to fabricate ordered patterns, opens a new area to print complex patterns with functional polymers for multifunctional application.

Keywords: Self-assemble, colloidal lithography, dewetting, chemically patterned surface, dynamic contact line lithography

Critical-Density Controlled Self-Assembly of Mxene Into Freestanding Hydrogels with Optimised Surface-Controlled Properties For High Performance Energy Storage

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Solvated network of two-dimensional materials in the form of hydrogel offers a unique platform for full utilization of surface dominated properties at the macroscopic scale. However, development of such hydrogels with ceramic sheets of MXene is highly challenging, and thus, are often critically dried to aerogel form to make them self-standing. Here, we report a freestanding thin MXene hydrogel through spontaneous, quasi-ordered assembly over metal plate and concurrent partial surface de-functionalization. We have established that self-standing hydrogel can only be assembled from MXene solution above a critical dispersion concentration (Cct) depending on the size of the sheets. On behalf of ordered porous structure with intrinsic hydrated ion permeable channels, MXene hydrogels display very high surface capacitive contribution (>94%) in their pseudocapacitive energy storage performance. Consequently, asdeveloped hydrogels display excellent gravimetric capacitance of 391 F g-1 and rate performance, and continue to display outstanding performance (>337 F g-1) at high enough mass loading up to ~15 mg cm-2 . As a versatility of hydrogel structure, an electrolyte protected mechanical compression method was employed to obtain a compact yet ion channel decorated electrode. As a result, compact MXene hydrogels achieved excellent volumetric capacitance (1120 F cm-3) and rate capability (73% at 1000 mV s-1).

Keywords: MXene, freestanding hydrogel, self-assembly, critical density, supercapacitor.

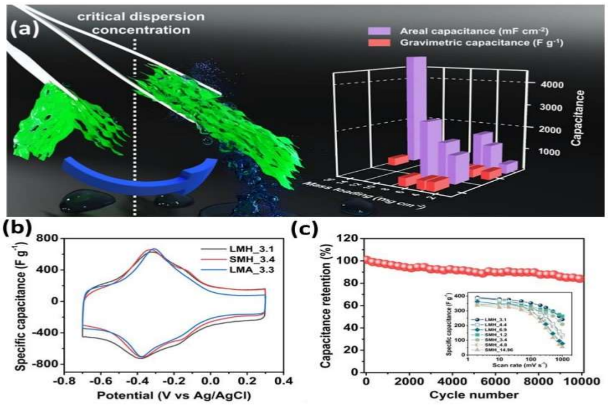

Figure: (a) Schematic illustration of critical concentration (Cct) dependence in freestanding MXene hydrogel development and its excellent capacitive performance; (b) Cyclic voltammetry profiles, (c) stability over 10000 charge-discharge cycles and rate performance (inset) of MXene hydrogel electrodes.

Chemically Modified Cloth Mask with Potential Efficiency Against COVID-19 Infections

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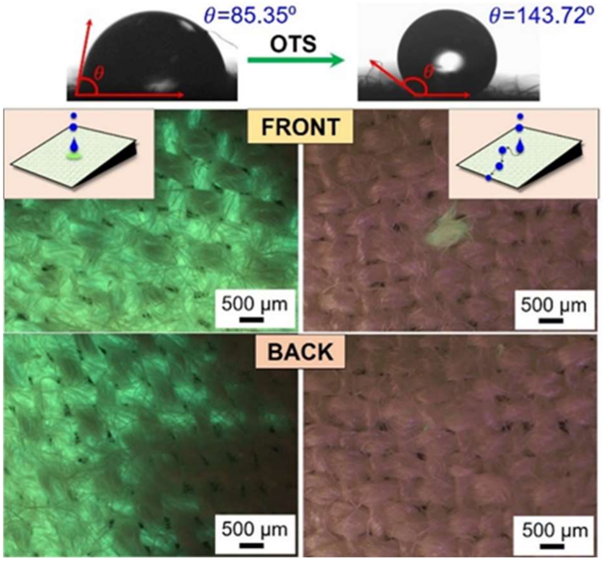
Presently wearing a mask has become necessary amongst every individual due to the ongoing COVID-19 pandemic. However, people are still experimental while choosing the suitable mask that will keep them safe from being infected by the coronavirus. N95 is indeed the best mask available in the market but the multi-layered sealed design of it makes it difficult to breathe through and uncomfortable for the person when worn for a longer period of time. Our findings say that the efficiency of a mask predominantly depends on the surface properties of the fabric. Even though the cloth masks are highly breathable, their ability to absorb the virus-laden droplets increases the plausible risk of getting infected easily. Hence, we converted the locally available hydrophilic Eri silk fabric into hydrophobic by depositing a nanometer-thick coating of OTS (octadecyltrichlorosilane) without compromising much the breathability of the mask. The modified hydrophobic Eri silk (contact angle of water is 143.7°) can repel back the incoming droplets without wetting the fabric and allow the easy flow of air through the three-layered treated Eri silk mask (breathability reduces by only 22% with respect to the pristine Eri silk, compared to 59% reduction by N95 mask), which makes this modified silk mask a better alternative to the N95 mask.

Keywords: masks, SARS-CoV-2, superhydrophobic, Eri silk, aerosol-driven infections.



Photophysical Investigation of a Sub-micellar Triblock Copolyme Cationic Surfactant Aggregate for Gold Nanoplate Synthesis

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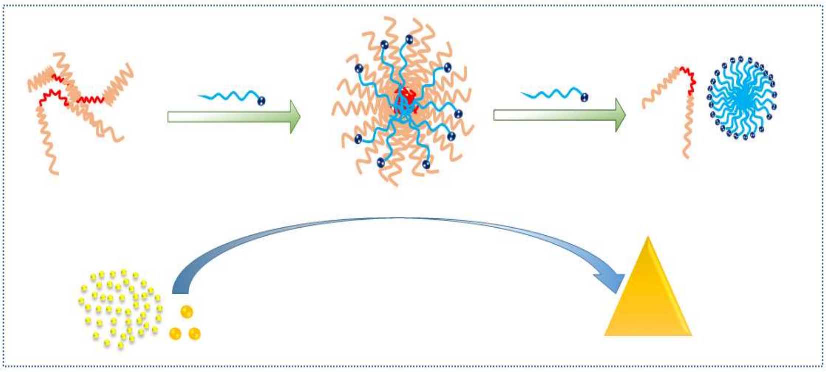
Surfactant assemblies are a popular medium for the synthesis of a variety of nanostructures. However, the requirement of large amounts of surfactants in these assemblies is detrimental to biological and medical applications. Herein, we optimized the size and interfacial packing of a sub-micellar aggregate of a triblock copolymer F127 (poly-(ethylene oxide)$_{101}$ (EO$_{101}$)−poly(propylene oxide)$_{56}$ (PPO$_{56}$)−PEO$_{101}$), and several cationic alkyl trimethylammonium surfactants at minute concentrations and demonstrated its feasibility in synthesizing gold nano-triangles.[1] We tracked various stages of the sub-micellar aggregate using time resolved dynamics of an ultrasensitive photoacid 8-hydroxypyrene-1,3,6-trisulfonate (HPTS or pyranine).[2] The emission intensity (protonated/deprotonated) ratio of HPTS follows an intricate pattern against the surfactant concentration displaying at least three transition points (T$_{1-3}$). The ratio starts to increase above an initial concentration (T$_1$), attaining a maximum at an intermediate concentration (T$_2$), and after that, decreases again before leveling off at a higher concentration (T$_3$). Fluorescence anisotropy measurements of the methoxy analog 8-methoxypyrene-1,3,6-trisulfonate (MPTS) further revealed that the most organized state is near the critical point T$_2$. Moreover, isothermal titration calorimetry (ITC) showed maximum enthalpy change at the same composition confirming optimum interaction. Finally, we show that the assemblies containing ultralow concentrations of both F127 and cationic surfactant can be a useful medium for synthesizing gold nano-triangles.

Keywords: Fluorescence; Gold nanoplates; TRANES; DLS; Triblock copolymer Surfactants.



Synthesis of Biocompatible Carbon Dots as Label Free Fluorescent Probe for Sensing and Preparation of 5-Fluorouracil-CD Nanoconjugate for In Vitro Antiproliferative Activity

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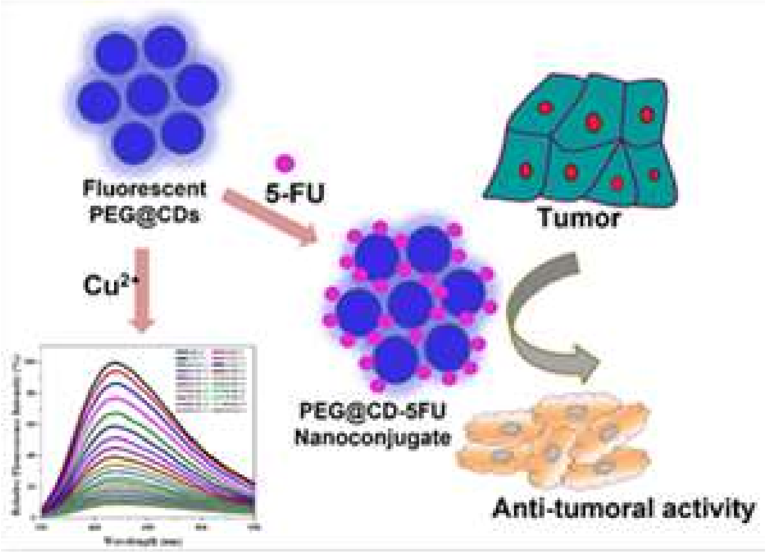
In this work we report one step eco-friendly route for the synthesis of biocompatible carbon dots (PEG@CDs). The as synthesised carbon dots were used successfully for loading and release of 5- Fluorouracil (5-FU). The photophysical and morphological characterization has been done using HR-TEM, XPS, XRD, FT-IR and UV-Vis spectroscopy. The results are indicative of improved photostability of the drug after conjugation with the carbon dots. The enhanced release of 5-FU in acidic environment makes it a selective antiproliferative drug carrier. The effective antiproliferative action of nanoconjugate has been explored using scratch assay, ROS generation assay and Hoechst staining. The reduced cytotoxicity of the carbon dot conjugated drug in comparison to free drug towards normal cells opens doors to explore the possibilities to design next generation antiproliferative drug delivery vehicle. The as synthesised PEG@CDs were further employed for assaying cobalt. The highly stable nature of PEG@CDs under various conditions such as different pH, high ionic strength, UV light irradiation, wide temperature range and prolonged storage time indicating their capabilities for expanding approach towards other applications.

Keywords: Carbon dots; Antiproliferative; Sensing; fluorescence; nanoconjugate.



Uphill Anion Pumping through Triangular Nanofluidic Device of Reconstructed Layered Double Hydroxide

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Numerous research efforts have been devoted to replicate the functioning of biological ion pumps in nanofluidic devices. Unlike previous reports of cationic pumps, positively charged CoAl layered double hydroxide (CoAl LDH) is exploited here for uphill pumping of anionic species. Nanofluidic membranes prepared by self-assembling exfoliated layers of CoAl LDH exhibit excellent anionic transport characteristics. At the surface-charge-governed regime, the positively charged CoAl LDH membrane (p-LDHM) showed a remarkable OH– ion conductivity of ~2 mS cm^{-1}. The remarkable mobility of OH– ions (4×10^{-4} cm^2 V^{-1} S^{-1}) in the atomically thin channel of p-LDHM is attributed to the tiny activation energy (0.09 eV) required for Grotthuss-like hopping of the ions between the positive charges of densely packed CoAl LDH layers. The lamellar p-LDHM was also found to be suitable for energy harvesting via salinity gradient, and a power density up to 0.7 Wm^{-2} was achieved under a 1000-fold concentration gradient. The triangular p-LDHM displays a diode-like nonlinear I–V curve, attributed to a combination of unipolar conductivity of counterions inside the two-dimensional (2D) nanochannels and geometrical asymmetry. The triangular p-LDHM pumps anions against the concentration gradient (up to 1000-fold), under fluctuating external potentials with a mean value of zero.

Keywords: Nanofluidics, Anion Pumping, ICR, Osmotic energy harvesting.

Smallest Shannon Radii Transition Metal Ion Ni (II) for Stabilizing α-$CsPbI_3$ Perovskite Nanocrystals

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Lead halide perovskite nanocrystals are recently emerged as one of the most efficient nanomaterial emitters having all visible colour tuneable emissions. However, the phase sensitivity of red emitting α-$CsPbI_3$nanocrystals remained the major concerned. Even though several reports already established with near unity photoluminescence quantum yields, but their phase and optical stability in ambient exposure had always some limitations. Ni(II) ions, having smallest transition metal Shannon radii were explored for B-site doping in red emitting α-$CsPbI_3$nanocrystals (fig. 1a). This successfully stabilized the cubic phase and retained the intense emission of nanocrystals for nearly two months (fig. 1b). The photoluminescence quantum yields also obtained ~80 % for the ~1% doping (atomic percentage). Being smallest ion, the halide octahedra in the perovskite lattice were expected to provide high restrain ability towards δ-$CsPbI_3$. Comparing with post synthesis iodide treatments, the importance of doping in high temperature reaction was discussed. Finally, these doped nanocrystals were explored for photovoltaic devices and showed comparable efficiency (9.1%) to different other similar doped nanocrystals.

Keywords: perovskite nanocrystals, Shannon radii, octahedral tilting

Facets Directed Connecting Perovskite Nanocrystal

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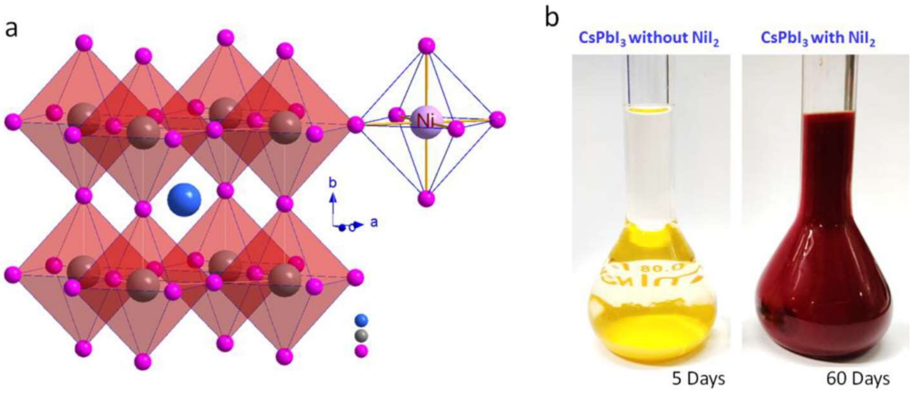
Perovskite nanocrystals have recently emerged as one of the most efficient energy materials in current research. From synthesis to optoelectronic and catalytic applications, these nanocrystals were extensively studied in the last five years and remained the workhorse in the field. Typically, ion migration for crystal deformation or connection with other nanocrystals needs a solvent as medium. However, on the contrary, this has been observed for CsPbBr3 perovskite nanocrystals in film where nanocrystals were swollen to get wider and fused with adjacent nanocrystals in self-assembly on film during solvent evaporation. Depending on precursor composition and exposed facets, again these connections could be programmed as both side-wise (**Fig.1a**) and corner-wise (**Fig.1b**) leading to different shapes. Aging further on solid substrate, these were also turned to continuous film of nanostructures eliminating all interparticle gaps on the film. This transformation could be ceased at any point of time, simply by heating or adding sufficient ligands. Analysis suggested that these unique and controlled connections were only observed with polyhedron shaped nanostructures with certain compositions and not with traditionally cubes. Details of this solid-surface transformation during solvent evaporation were analyzed, and an interparticle material transfer type mechanism was proposed. As these observations were not seen in chalcogenide and oxide nanocrystals and exclusively observed in perovskite nanocrystals, this would add new fundamentals to the insights of crystal growths of nanocrystals and would also help in obtaining films of connecting nanocrystals.

Keywords: Perovskite, Polyhedron, Shape modulation, Connection, Facet



Two Dimensional Luminescent Crystalline Assembly of Atomic Clusters - via Complexation Reaction for Recyclable Storage of Oxygen

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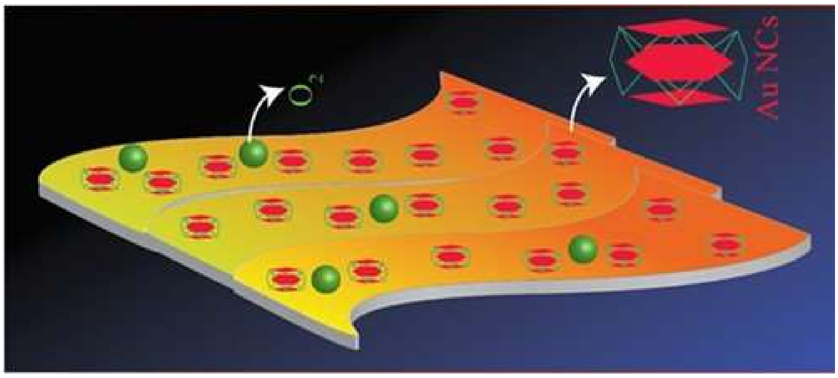
The storage of oxygen in two-dimensional (2D) crystalline nanosheets containing luminescent gold nanoclusters (Au NCs) is described in this work. The formation of crystalline assembly of Au NCs was generated by a complexation reaction between Au NCs (stabilised by l-phenylalanine and mercaptopropionic acid) and zinc ions. Transmission electron microscopy (TEM), high-resolution TEM, and selected area electron diffraction (SAED) analyses were used to demonstrate the crystalline character of the Au NCs assembly. The 2D nature of the assembly of the Au NCs was confirmed by atomic force microscopy (AFM) and field emission scanning electron microscopy (FESEM) analyses. The 2D crystalline nanosheets produced by the interaction of Au NCs with Zn2+ were found to have a near-uniform thickness of 3.8 ±1.65 nm on average. At ambient conditions of 20 °C and pressure 20 bar, these 2D nanosheets consisting mainly of hierarchically structured Au NCs were utilized for reversible oxygen storage.

Keywords: Zinc, Metal clusters, gold, Two-dimensional materials, Oxygen



Lichen Mediated Facile One-Pot Green Synthesis of Reduced Graphene Oxide (Rgo)-Ag@Mno2 Novel Ternary Nanohybrid

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A novel ternary nanohybrid of reduced graphene oxide, (rGO)-Ag@MnO_2 was prepared via a facile, low-cost, and green approach using aqueous extract of a lichen *Acroscyphus spaerophoroides*. In the first step, graphene oxide (GO) was prepared by a modified Hummer's method followed by reduction of exfoliated graphene oxide using the lichen extract. The lichen extract was further employed as reducing and stabilizing agent to synthesize Ag doped MnO_2 nanoparticle (Ag@MnO_2) from an aqueous solution of $AgNO_3$ and $KMnO_4$ in one step at ambient temperature. Finally, the rGO and as-synthesized Ag@MnO_2 dispersed in aqueous medium were simply mixed by magnetic stirring for 6h to obtain the novel ternary nanohybrid material. The synthesized GO, rGO and nanohybrids were characterized using different spectroscopic techniques such as UV-Vis, IR and XRD etc.

Keywords: green synthesis, Graphene oxide, *Acroscyphus spaerophoroides*, Ag@MnO2

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Tuning Facets and Controlling Monodispersity in Organic-Inorganic Hybrid Perovskite $FAPbBr_3$ Nanocrystals

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Lead halide hybrid perovskite nanocrystals are considered as one of the most efficient light harvesting materials in current research. However, unlike all inorganic perovskite nanocrystals, the quality optimization and synthetic progress for facets tuning of these hybrid nanocrystals could not be attended the same race. To meet the current demand of high quality, facet tuned and monodisperse nanocrystals, herein, surface A-site cations' population-controlled facet tuning of $FAPbBr_3$ nanocrystals are reported. Using specific alkylammonium ligands obtained from α-bromo ketones and comparing their concentration with FA^+, cube, dodecahedron and spherical like shapes in cubic phase are obtained having monodispersity compared to their best reports. In addition, by changing of surface ligands, spontaneous formation of self-assembled blue emitting platelets was also observed. As these materials are of high demand, these above findings would help for understanding more on fundamental understanding for hybrid perovskite nanocrystals and also for their wide spread applications.

Keywords: Hybrid perovskite, surface A-site cations', monodispersity, facet tuned, self-assembly

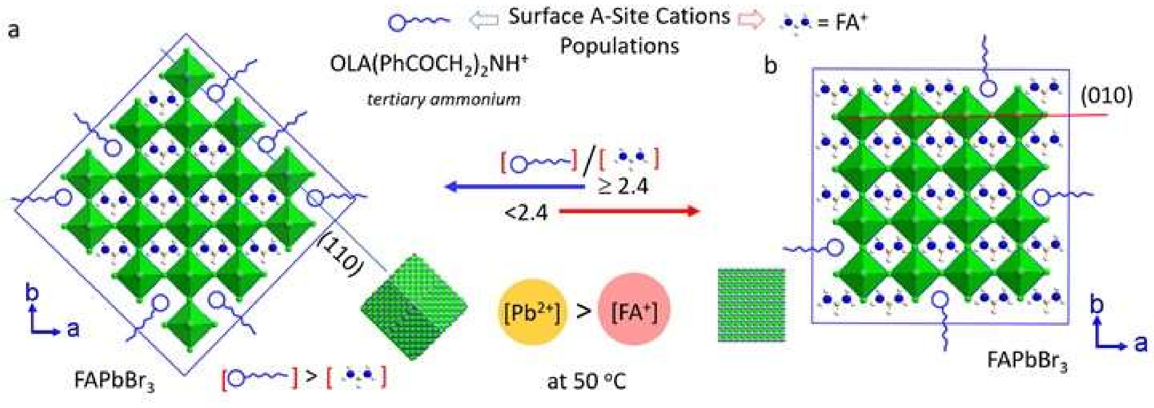

Figure 1. Schematic presentation of concentration variation of FA^+ and the tertiary ammonium ions obtained from the reaction of phenacyl bromide with oleylamine and the shape evolution of $FAPbBr_3$ nanocrystals. (a) Atomic models showing {110} group of facets with dominated tertiary ammonium ions bonding at the surface in dodecahedron shaped $FAPbBr_3$ nanocrystals. (b) Atomic model showing dominated FA^+ bonding at surface {010} facets. Concentration of FA^+ in all cases remained less than Pb^{2+}.

Tuning the Electronic Structure of Monoclinic Tungsten Oxide Nanoblocks by Indium Doping for Boosted Photoelectrochemical Performance

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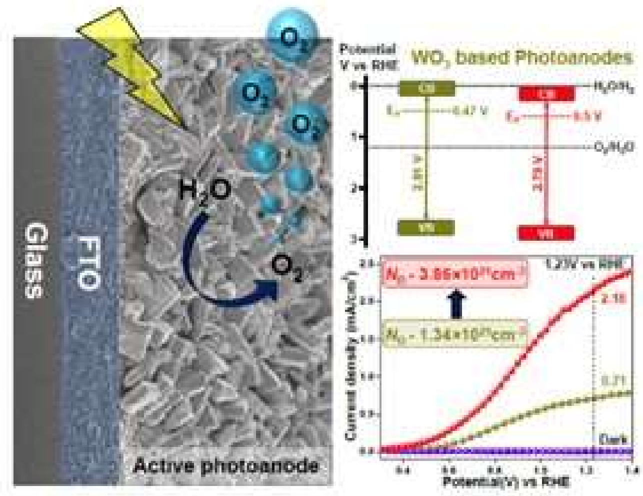
Photoelectrochemical (PEC) water oxidation, a desirable strategy to meet future energy demands has several bottle-necks to resolve. One of the prominent issues is the availability of charge carriers at the surface reaction site to promote water oxidation. Of the several approaches, metal dopants to enhance the carrier density of the semiconductors,is an important one. In this work, we have studied the effect of In-doping on monoclinic WO_3 nanoblocks, growing vertically over fluorine-doped tin oxide (FTO) without the aid of any seed layer. X-ray photoelectron spectroscopy (XPS)data reveals that In^{3+}ions are partially occupying the W^{6+}ions in In-doped WO_3 photoanode. In^{3+}ions are offering better performance by adding additional charge carriers for amplifying the expression of the number of carriers. The maximum current density value of 2.18 mA/cm^{2}has been provided by the optimized In-doped WO_3 photoanode with 3 wt% indium doping at 1.23 V vs. RHE, which is ~3 times higher than that of undoped monoclinic WO_3 photoanode. Mott-Schottky (MS) analysis reveals charge carrier density(ND)for In-doped WO_3photoanode has been enhanced by a factor of 3. An average Faradic yield of ~90 percent has been achieved which can serve as a model system using In^{3+}as a dopant for an inexpensive and attractive method for enhanced WO_3 based PEC water oxidation.

Keywords: Tungsten trioxide, In-doping, charge carrier density, charge separation, photoelectrochemical water oxidation



Aggregation Induced Emission Switching based Ultrasensitive Ratiometric Detection of Biogenic Diamines Using a Perylenedimide-based Smart Fluoroprobe

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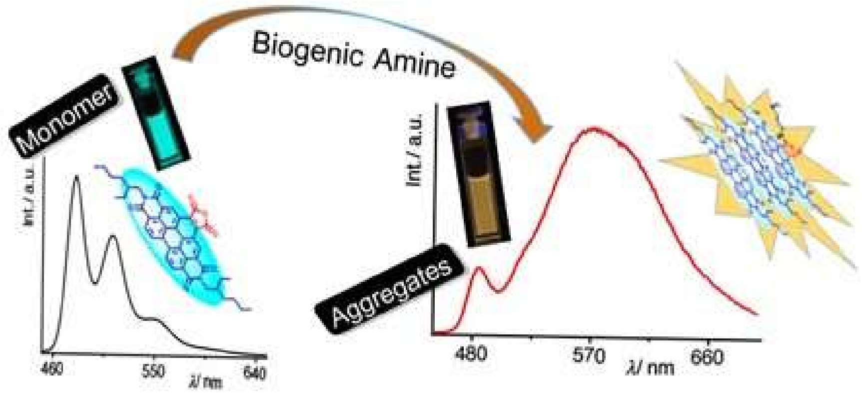
In recent years, the widely used concept "Aggregation induced emission (AIE) switching" has played an crucial role in the development of luminescent materials in organic light emitting diodes. Unfortunately, this concept has not been explored extremely in the field of biosensing or bioimaging. Therefore, to shed light in the sensing of bioanalytes, in this contribution, we have developed new perylene diimide (PDI) based small fluorescent probe, benzoannulated PDI that selectively detect diamines and biogenic amines in solution *via* 'AIE switching' phenomenon. The synthesized probe containing *bay*-annulated anhydride moiety exhibit strong cyan coloured emission in solution. Mechanistically, it can be proposed that terminal free -NH_2 group of BAs readily reacts with highly reactive anhydride moiety, that open the cyclic anhydride moiety. In the opened conformation, free amine groups along with carboxylate ion increase the polarity of the system strikingly. Because of the induced polarity, the monomer of dye-BAs complex aggregated in solution, exhibited significant change of emission property in solution. Noteworthy to say, the fluorescence colour change was so spontaneous in solution that led the detection of BAs as ultrasensitive. The process also may be called as a very simple and straightforward 'naked eye' detection of BAs in solution,with limit of detection (LOD) value as low as 0.2 μM. The existence of aggregated state was evinced by emission and excitation spectra, fluorescence lifetime measurement and SEM studies. As the dye fluoresced strongly in solid state (yellowish-orange), it has driven to conduct the vapour phase detection of BAs by the sensor easily with LOD as low as 4.3 ppm. Finally, we applied the vapor phase detection in determination of spoilage of raw fish very effectively.

Keywords: AIE switching, Perylenedimide dyes, ratiometric detection, biogenic diamines, vapour phase detection



- AIE-switching
- Ratiometric Response
- Nanomolar LOD
- Vapor-phase Detection

Synthesis and Characterization of Silver-Graphene Nanocomposites for New Class of Plasmonic Photo Electric Conversion Device

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Plasmonics is an evolving research area of optics and nanoelectronics in today's world by confining light of relatively large wavelengths to nanoscale. Graphene's optics and photonics have been reviewed several times and it is seen to have tunable and adjustable inherent plasmons. However, graphene with noble metal nanostructure enhances its plasmonic properties and offers a variety of applications such as efficient photodetectors, ultrasensitive chemical sensors, surface enhanced Raman scattering (SERS) or biosensors. In the current work, silver (Ag) nanoparticles were deposited on graphene (G) sheets to develop Ag/G nanocomposites via a simple process of thermal reduction wherein graphite oxide (GO) is used as a precursor to graphene, silver nitrate ($AgNO_3$) as a precursor to Ag nanoparticles, and sodium citrate as an environmentally-friendly reduction and stabilizer. Through enhanced modified Hummer process, GO is synthesized from graphite powder. The produced Ag/G nanocomposites were characterized by X-ray diffraction (XRD), field scanning electron microscopy (FESEM), UV visible spectra, and Raman spectra (RS). For developing a new plasmonic energy harvesting system, the plasmonic properties of Ag/G nanocomposites coupled with TiO2 thin film will be used. Simulation of the nanomaterial, the impact of the material's dimensions, geometry and dielectric properties, and optimization of the unit's architecture will be carried out and analyzed. Further an optimized framework will be presented for the fabricated device along with the inherent plasmonic physics.

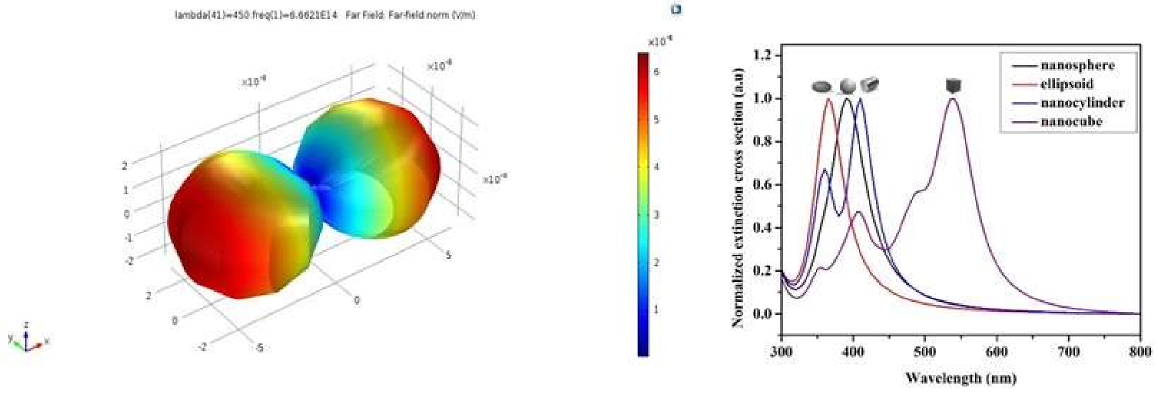

Figure. (a) 3D image of electric field distribution (b)Extinction spectra of various shapes of Ag nanoparticle

Encapsulation of Pertechnetate Inside the Framework of Keplerate-Type Polyoxometalate {Mo132}

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Pertechnetate (TcO_4^-) which is frequently used as diagnostics in nuclear medicine is considered as one of the most radio-active perilous pollutant owing to its elongated half-life period, strong ecological mobility. To remove Pertechnetate (TcO_4^-) by trapping it with a suitable anionic receptor is most facile way to minimize hazard contaminant. Till now trapping of pertechnetate has got little attention as it is very difficult to choose suitable receptors as it has bulky size and small charge-surface ratio. Recently "Inorganic Superfullerenes", the $\{Mo_{132}\}$ capsule has received considerable attention as promising anionic receptor to entrap Pertechnetate (TcO_4^-). Mo_{132} is considered as one of the latest branch of Polyoxometalate (POM) cluster having symmetrical ring kind structure/spherical shapes. Mo_{132} capsule generally possesses following structure as: $\{Mo_{11}\}_{12} \equiv \{(Mo^{VI})(Mo^{VI}_5)(Mo^{V}_5)\}_{12}$. Owing to their symmetrical porosity it can easily entrap Pertechnetate (TcO_4^-) through molecular recognition.

Keywords: Pertechnetate, Keplerate-type polyoxometalate, encapsulation, molecular recognition.

Nano-Porous Keplerate Capsule: A Leading Edge Biological Ion Transporter

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The Keplerate $[\{Mo^{VI}(Mo^{VI})_5O_{21}(H_2O)_6\}_{12}\{Mo^{V}_2O_4(RCO_2)\}_{30}]^{42-}$ is molybdenum oxide-based highly charged water soluble inimitable nucleophilic nano-porous capsule which can act as "molecular lock gates" by trapping hydrated ions $\{[M(H_2O)_6]^{3+}$ ($M = Al^{3+}$ and Cr^{3+})]. This nano-porous cluster had been synthesized by "self-assemble" method by using pentagonal shaped $\{Mo^{VI}(Mo^{VI})_5O_{21}(H_2O)_6\}^{6-}$ and dumbbell-type dinuclear cluster $\{Mo^{V}_2O_4(H_2O)_2\}^{2+}$ in presence of the carboxylate buffer medium. This Keplerate containing numerous receptor sites in which hydrated cations of hard acids such as Cr^{3+}, Al^{3+} are trapped very readily *via* hydrogen bonds and formed unique supramolecular complex. When spherical nano-porous capsule of $[\{Mo^{VI}(Mo^{VI})_5O_{21}(H_2O)_6\}_{12}\{Mo^{V}_2O_4(RCO_2)\}_{30}]^{42-}$ snatches Al^{3+}/ Cr^{3+} by releasing pentagonal (Mo)Mo_5 unit by reversible fashion which may consider important factor to uptake metal ions.

The encapsulation of hydrated cations inside the cavity mainly depends on pore size of Keplerate and electrochemical gradient of above metal hydrate. Both Cr^{3+}, Al^{3+} are hard acids and having strong polarising power and high charge to radius ratio value like alkali or alkaline earth metal ions. So, such type of modelling study denotes that the nano-porous Keplerate can be used as biological cation transport.

Keywords: Keplerate, self-assemble, encapsulation, cation transport.

Nano Catalyst from Waste Material

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Today the environmental problems increase worldwide due to the large amount of industries established and demand for everything by the increase in the population. By the increase in the industries of chemicals worldwide large amounts of chemical waste are generated. So by utilizing waste for the preparation of various chemical synthesis many environment problems are solved such as if we use nano catalyst from waste for the transesterification of waste cooking oil. There are many benefits of using nano catalyst that lower the reaction temperature, have high selectivity for the reactant, not affected by the fatty acid, ease of separation and water content present in the oil in case of transesterification reaction. Due to high selectivity, it gives the higher yield of the product. In this way there are many reactions in which nano-catalysts can replace other chemicals which reduces the use of chemicals that pollute the environment.

Nano Catalyst Obtained from Plants Extract

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Nowadays the use of nano catalyst increases in every research program and also in the industries. There are various kinds of nano catalyst that are used that are obtained from plant extract. Various advantages of the nano catalyst include that biomolecules present in the nano catalyst obtained from plant extract replaces metal ions. By using nano catalyst reactions occur in a short period of time and also at room temperature. Therefore the synthesis done by nano catalyst from plant abstract is green synthesis due to replacement of toxic metal ions, inexpensive, easily used, recovery of the catalyst. The major advantage of the plant based nano catalyst is controllable size and morphology. The use of these nano catalysts in various fields such as in the preparation of drugs, antimicrobial agents, water purification, energy storage cells, application of carbon nanotubes and many more other fields.

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Green Synthesis of Full-Color Fluorescent Carbon Nanoparticles from Eucalyptus Twigs for Sensing the Synthetic Food Colorant and Bioimaging

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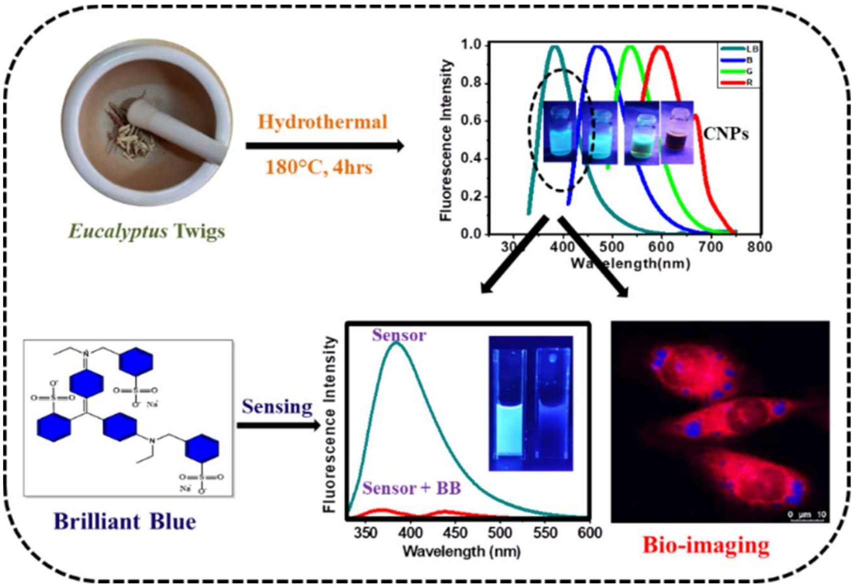
Full-color fluorescent carbon nanoparticles (CNPs) are produced by a facile and green hydrothermal method followed by the differential washing technique. *Eucalyptus* twigs are used as a precursor to synthesize multiemissive light blue, blue, green, and red CNPs. Brilliant Blue FCF (BB) is a widely used synthetic food colorant, which is toxic for the human body, when consumed beyond the permitted limit. Herein, we demonstrate light blue CNPs as a sensor for selective and sensitive detection of BB *via* a fluorescence quenching mechanism with a limit of detection of 200 nM. Temperature-dependent fluorescence and ^{1}H NMR studies confirmed the mechanism as combined dynamic and static quenching. To demonstrate the practical efficacy of the sensor, BB is effectively detected and estimated in selected food samples procured from the market. Moreover, the biocompatibility of light blue and blue CNPs is examined and confirmed by performing a cytotoxicity assay on MDA-MB-231 cell lines. Subsequently, the cellular imaging study is also carried out to explore the internalization process of the CNPs as a function of concentration. To the best of our knowledge, this is the first time that *Eucalyptus* twigs, a natural source of high abundance, are used as raw materials and valorized for sensing artificial food color and bioimaging purposes.

Keywords: *Eucalyptus* twigs, carbon nanoparticles, sensing, brilliant blue, Bioimaging



Telluride versus Selenide: Diffusion Induced Tuning Epitaxial Orientation Angles of Disk-on-Rod Nano-Heterostructures for Boosting Charge Transfer

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Controlling the diffusion of anion channels of Se (VI) and Te (VI) on 1D structure of Sb (V) chalcogenides, disk-on-rod heterostructures having three different epitaxial angles with different surface facets is reported for the first time. Different orientations resulted due to thermally induced anion migration; where injection temperature of anion determined the extent of ion migration, ensuing heterostructure formation with trigonal $Sb_2Se_xTe_{3-x}$ disks on orthorhombic Sb_2Se_3 rods having orientation angles 180º, 135º and 90º (Figure 1). Manipulation of the growth kinetics of disks connected at one head and two heads of parent rods is achieved by using Se (VI) precursor as a limiting reagent. These materials have the same constituents but different composition, singularizing it from all nanomaterials reported till date. These are supported with theoretical calculations to establish the energy minimization of different orientations, their possible formation and suitability in energy transfer applications. Further, amperometric I-t and electrochemical impedance spectroscopic measurements were performed which are found to be in consonance with the findings of DFT calculations. Hence, this is a case study of advanced modular synthesis of 2D on 1D material with different shaped disk-on-rod nanostructures that would lead a step further in nanocrystal engineering for more desirable complex structures.

Keywords: Heterostructure, Diffusion, Disk-on-rod, Epitaxy, Energy Transfer

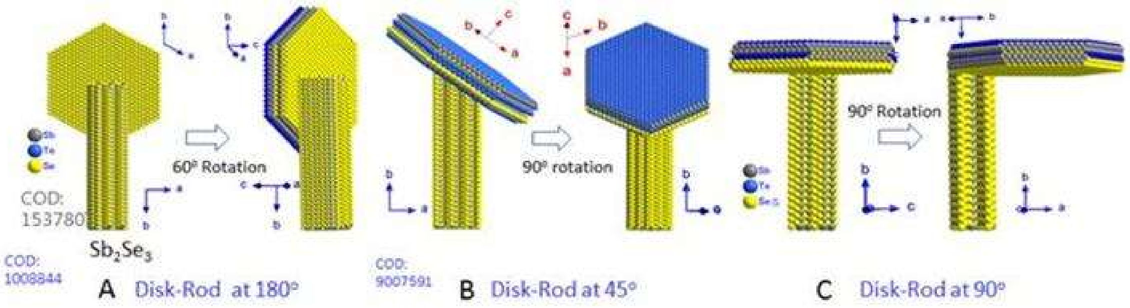

Figure . Orientations of Sb_2Se_2Te, Sb_2SeTe_2 and $Sb_2S_xSe_{1-x}Te_2$ disks on Sb_2Se_3 rods at A) 180°, B) 135° and C) 90° respectively.

Mechanism of Peroxidase-Like Activity of Carbon Dots Synthesized from L-Glutamic Acid

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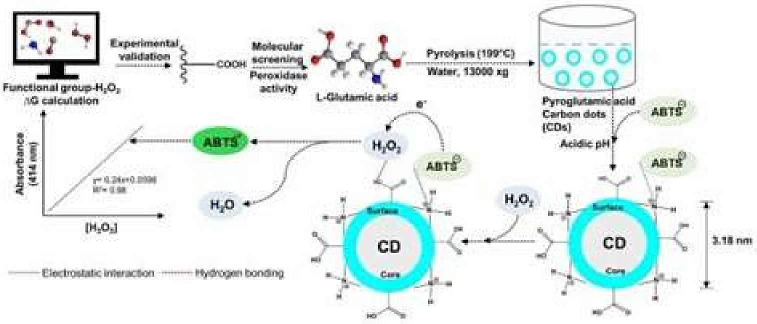
The recent interest in carbon dots (CDs) as efficient peroxidase-mimics has urged to understand the mechanism for this reaction because of its utmost commercial importance. Firstly, using a theoretical-cum-experimental approach, the -COOH group was identified as an active moiety for strongly binding and degrading H_2O_2 in the presence of a reducing equivalent. Next, the stringency of different compounds containing the -COOH group was examined and identified L-glutamic acid with higher peroxidase-like activity. The $-NH_2$ group present in the vicinity of the -COOH group increased the activity of L-glutamic acid. Following a pyrolysis method, L-glutamic acid was transformed into CDs having a diameter of 3.18±0.53 nm with its core made of pyroglutamic acid. The CD exhibited thermostability (~90°C) and higher peroxidase-like activity than the L-glutamic acid. The higher activity of the CD was attributed to its binding affinity with ABTS and H_2O_2. The K_m and K_{cat} of the CD for H_2O_2 were 5.85 mM and 0.011 s^{-1}, respectively. Based on spectroscopic investigations, we confirmed the peroxidase-like activity is a surface phenomenon that did not have a significant link to the photophysical property of the CD and proposed a mechanism for the reaction. The colorimetric reaction could be reproduced on a paper platform, confirming the application potential of the CD for developing a low-cost peroxide sensor.

Keywords: Carbon dots, L-glutamic acid, Peroxidase, Hydrogen peroxide, Carboxylic acid group



Fabrication, Characterization of Fibroin Based Nanomaterials Derived from Eri and Muga Silk

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Silk fibroin derived from Eri *(Philosamia ricini),* Muga (*Antheraea assamensis)* and B. Mori *(Bombyx mori)* distinguishes for their unique mechanical performances, excellent thermal properties, specific optical properties and controllable degradation rates strongly attract researcher for tuneable material fabrication. Moreover, being biodegradable and biocompatible along with cost effective features make them attractive materials for a variety of biomaterial design. The unique behaviour of fibroin originated from the structural composition of silk proteins through their self-assembly strategies offers divers applications. This paper reports the fabrication and characterisation of fibroin-based nanomaterial derived from Eri and Muga silk and compared with B. Mori silk. The prepared sample were characterised by XRD, FTIR and UV-vis spectroscopy. The absorption coefficient ($\acute{a}$), and extinction coefficient (κ) of silk fibroin are directly obtained from U-V visible spectra. Using $\acute{a}$ and $\hat{e}$, the refractive index(μ)is calculated and the real and imaginary parts of dielectric constant ($\mathring{a}_r$ and $\mathring{a}_i$) for the studied sample have been investigated and analysed. The optical band gap calculated from Tauc's equation found to be 3.8eV, 4.1eV and 4.3eV for Eri, Muga and B. Mori respectively. These results shows that fibroin derived nanomaterial could be used as wide bandgap semiconductor material.

Keywords: Silk Fibroin, Optical Band Gap, Refractive Index, Dielectric Constant

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CeO_2@rGO Nanocomposite Incorporated within Tragacanth Hydrogel for Photocatalytic Applications

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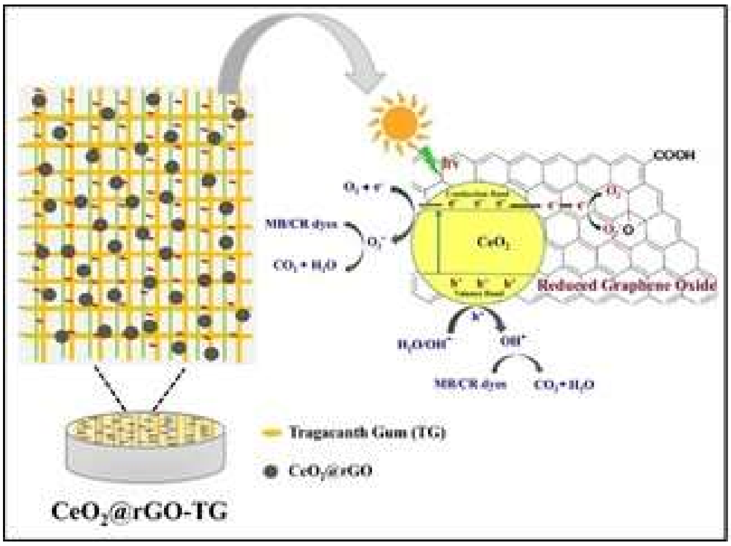
Photocatalytic degradation utilizing sunlight has emerged as a facile approach to tackle the issue of water contaminating organic dyes. Herein, we investigate the efficiency of reduced graphene oxide (rGO) decorated with nanoceria (CeO_2) to degrade pollutant dyes namely methylene blue (MB) and congo red (CR), after sunlight irradiation. The as-synthesized nanocomposite (CeO_2@rGO) was monitored using UV-Visible, Field Emission Scanning Electronic Microscopy (FESEM), Fourier transfer infrared (FTIR) and RAMAN spectroscopy, X-ray diffraction (XRD), and Photoluminescence (PL). Time-dependent degradation studies were conducted for 5 h and found to follow Langmuir-Hinshelwood first-order kinetics. At equivalent concentrations, CeO_2@rGO demonstrated improved degradation of MB and CR when compared to bare CeO_2. Further, the photocatalytic efficiency of CeO_2@rGO was augmented by incorporating in a tragacanth (TG, a natural polymer) based hydrogel. The hydrogel photocatalyst (CeO_2@rGO-TG) exhibited enhanced degradation, at lower amount of CeO_2@rGO in free form. Nonetheless, CeO_2@rGO-TG could be easily segregated from the dye solution and re-used for multiple cycles of degradation.



Understanding the Effect of Magnetic Spin Impurity using Spin Flipper in Finite Width Quantum Transistors

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Metal halide perovskites have emerged as an interesting alternative semiconducting material in the field of optoelectronics, however the performance of these devices is majorly limited by the presence of defects which originate from a number of factors. Here we present a detailed analysis of presence of magnetic spin impurity in finite width 4-terminal quantum transistor which is one of the defect present in these perovskite materials. The magnetic impurity is introduced using a spin flipper where the incoming electron interacts with the flipper through spin-exchange interaction whose strength is given by a factor G. To make these results consistent with practical devices finite width is introduced in 3-terminal and 4-terminal quantum transistors using the modified Griffith's scheme. Electron transmission probability which is analogous to quantum conductance is calculated to have a direct correlation with the width of the quantum wire, spin exchange interaction of the magnetic defect and the energy of the incident electron. Furthermore, the rate of change of spin transmission with the spin exchange strength bears an analogy with the experimentally obtained FMR plot for characterizing paramagnetic Pb^{3+} magnetic impurity prevalent in $MAPbI_3$ devices.

Keywords: Quantum transistor, Magnetic-spin impurity, Spin flipper, Spin-exchange interaction, Electron transmission probability.

Enhanced Solid-State Plasmon Catalyzed Oxidation and SERS Signal in the Presence of Transition Metal Cations at the Surface of Gold Nanostructures

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The effect of several metal cations (Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+} and Zn^{2+}) on the photochemical conversion of 4-aminothiophenol (4-ATP) into 4,4´-dimercaptoazobenzene (DMAB) is probed using surface enhanced Raman scattering (SERS). The coupling reaction is carried out on the surface of Au nanoparticles and Au nanorods using 532 nm and 632.8 nm laser excitations, respectively, in the absence and presence of metal cations. Here, we report that DMAB formation on the surface of Au nanostructures – when carried out in the solid state – is augmented significantly (by a factor of 1.98 to 4.07 and 3.34 to 5.74 for Au nanoparticle and Au nanorod substrates, respectively, and depending on the metal). Furthermore, the SERS signal is also markedly enhanced. Thus, the results underpin a new way of carrying out a photochemical reaction with a higher yield along with a higher SERS signal.

Keywords: Nanoparticles, Nanorods, Plasmons, Catalysis, SERS

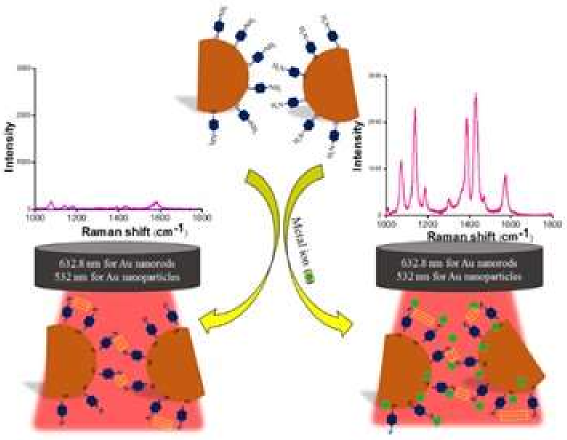

Figure: Cartoon depiction of photochemical conversion of 4-ATP into DMAB in the presence and in absence of metal cations on the surface of Au nanostructures

Synthesis, Characterization and Ferroelectric Properties of Linbo$_3$- Type (LN-Type) Polar Zinc Titanate (ZnTio$_3$) Nanocrystals

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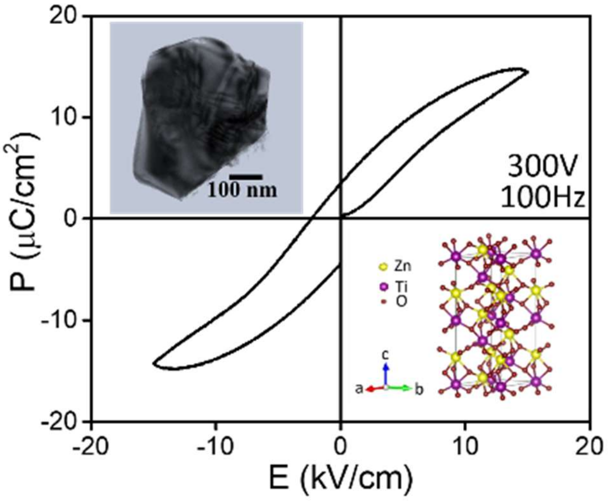
$LiNbO_3$(LN)-type $ZnTiO_3$ belongs to the class of non-centrosymmetric (NCS) polar structure which can form as a metastable quenched phase for a restricted range of tolerance factors and ionic radii. [1-3] Hexagonal LN-type $ZnTiO_3$ was first synthesized by Inaguma et.al by high temperature and high-pressure method. [1] Although, they only explained by theoretical calculations that novel Pb free LN-type polar $ZnTiO_3$ had a possibility of displaying high saturation polarisation (saturation polarization P_s~ 80 μC/cm^2) compared to other LN-type polar $ZnMO_3$ (M= Sn, Ge, Zr), [4] and $LiNbO_3$, [1-4] experimentally the material is rarely studied. We report on facile synthesis of LN-type $ZnTiO_3$ nanocrystals (~100-150 nm in size) by a tuned hydrothermal method. X-ray diffraction pattern match with hexagonal LN-type $ZnTiO_3$, the crystal structure of which was refined furthermore by Rietveld method. Systematic characterisation of the phase and the nanostructure were carried out by high resolution transmission electron microscopy (HR-TEM), X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy. Dense pressed pellets of LN-type $ZnTiO_3$ was tested by Radiant Premier LC II ferroelectric measurement system and well-formed ferroelectric hysteresis graphs were obtained at room temperature upto 300 V with a P_s ~13 μC/cm^2. To our knowledge this is the first evidenced ferroelectricity in LN-type $ZnTiO_3$ and will add to the class of stable perovskite materials for further properties exploration

.**Keywords:** $LiNbO_3$(LN)-type, Ferroelectric, Metastable phase



Bimetallic Ag-Cu Alloy Microflowers as SERS Substrates with Single Molecule Detection Limit

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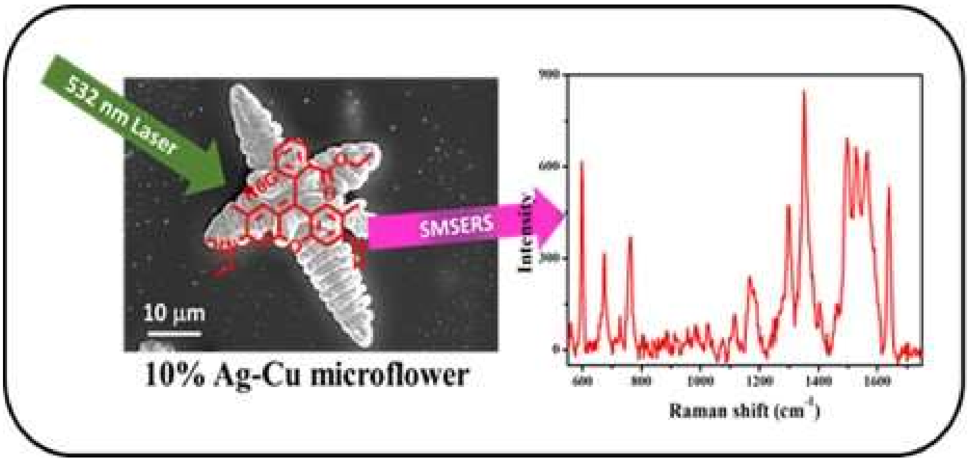
Bimetallic Ag-Cu alloy microflowers with tunable surface compositions were fabricated as SERS substrates with a limit of detection in the zeptomolar range for the analyte molecule Rhodamine 6G (R6G). The substrates were prepared on a glass coverslip through a bottom-up strategy by simple thermolysis of metal-alkyl ammonium halide precursors. The reaction temperature and composition of the alloy were varied sequentially to find out the maximum SERS efficiency from the substrates. While, UV-Vis spectroscopy were employed to characterize the optical properties of the substrates, the bulk and surface composition of the microflowers were determined using ED-XRF and XPS techniques, respectively. Also, the structural and morphological characterization of the substrates were performed by X-ray diffraction and SEM, respectively. For alloys, the ED-XRF studies confirmed that the bulk compositions matched with the feed ratio, while the surface compositions were found to be rich in copper in form of both elementary copper and copper oxide, as revealed by XPS studies. From the efficiency studies for different compositions prepared, it was found that 10% Ag-Cu alloy microflowers produced maximum SERS intensity for resonant R6G molecule as probe. In fact, R6G evidence 50-fold enhancement in SERS spectra with 10% alloy microflowers as against pure Ag microflower. Using 1, 2, 3-benzotriazole as a non-resonant Raman probe, uniform enhancement factors in the order of $\approx 10^8$ were achieved from different parts of the 10% Ag-Cu alloy microflower. The same substrate showed excellent Raman response for detecting R6G at very low concentrations such as 10 zM, leading to detection and analysis of SERS spectra from a single R6G molecule.

Keywords: SERS, Ag-Cu, bimetallic, alloy, Rhodamine 6G, single molecule.



Rational Control of Hole Transport Layer for High Performance Perovskite Light Emitting Diodes

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Charge balance in the emissive layer through well-match energy levels and reduced barrier of the transport layers can attain maximum radiative recombination. In this work, four hole transporting layers (HTLs) has been used to regulate the hole injection in the emissive layer. The HTLs have varying HOMO level in between the work function of FTO and HOMO of the emissive layer. Among the four HTLs, NPD-based perovskite LED device demonstrated the best performance with highest brightness of 24343 cd m^{-2}, current efficiency of 16.2 cd A^{-1}, and turn-on voltage of 4.7 V. The main reason for such improved results was well-match HOMO of NPD to both the anode and emissive layer supporting enhanced hole injection. Both the photo-luminescent and electro-luminescent studies confirm pure green emission with CIE coordinates around (0.22, 0.75). Morphology show best quality film for NPD-based perovskite film supporting smooth transport of the charges. The crystallinity of the NPD-based perovskite film was also found to be optimum. Finally, stability of the working PLEDs is tested and superior stability with 79% of the retention of initial brightness is observed for NPD-based device.

Keyword: Charge balance, energy barrier, perovskite LED, luminance, and stability.

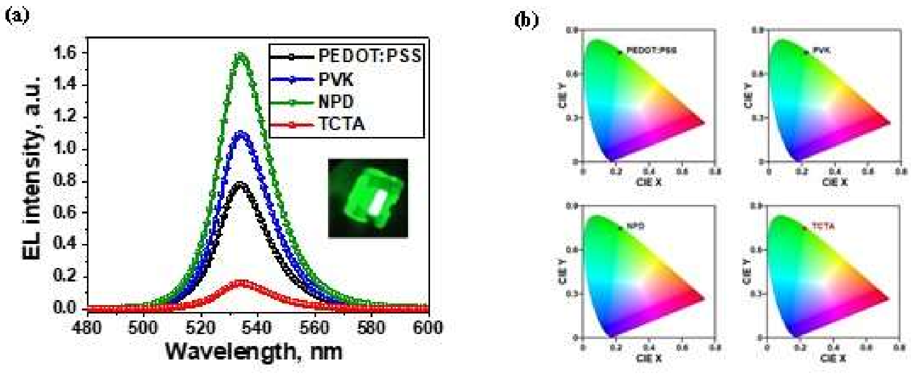

Figure: (a) EL spectra for different HTLs and (b) CIE diagrams for all individual HTL devices

Temperature Dependent Carrier Hopping Characteristics of White Light Emitting Quantum Dot Complex in Ambipolar Transistor

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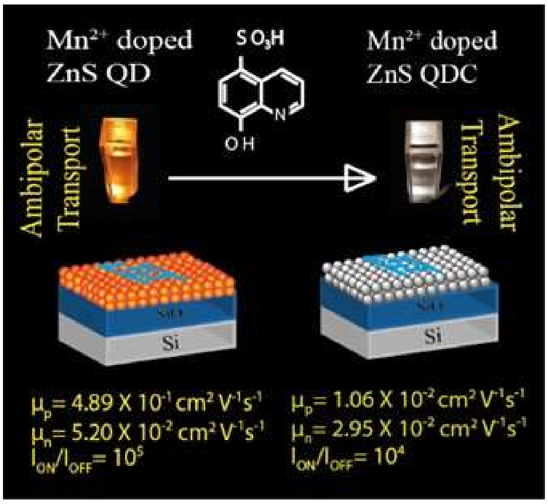
Ligand interactions at quantum dot surface not only help passivate the surface but also can modulate the photo-physical properties and thus bringing in diverse applicability. Herein, thin film transistors were fabricated from surface complexed Mn^{2+} doped ZnS Quantum dot (QDC) which exhibits dual emission at 480 nm and 590 nm having overall white photoluminescence. Room temperature ligand interactions with 8-hydroxyquinoline 5-sulfonic acid resulted in complexation of Qdot surface with luminescent $Zn(QS)_2$ complex. Ambipolar characteristics with hole mobility of 1.06×10^{-02} cm^2 V^{-1} s^{-1}, electron mobility of 2.95×10^{-02} cm^2 V^{-1} s^{-1} and I_{ON}/I_{OFF} ratio of 10^4 were observed in the QDC-transistor. Carrier mobilities of QDC exhibited nearest-neighbour hopping characteristics between 257-357K, whereas at temperatures between 77-217 K it exhibited variable range hopping characteristics. Excited state carrier lifetimes of QDC were also studied through time-resolved photoluminescence analyses.[1] The dual emitting nature of QDC and its transport characteristics indicates that it can be used as an efficient light emitter in optoelectronic device.

Keywords: Quantum dot complex, ambipolar, thin film transistor.



Defect Induced Trion in Monolayer WS2 at Room Temperature

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Unusually high exciton binding energies (BEs), as much as ~1 eV in monolayer transition-metal dichalcogenides, provide opportunities for exploring exotic and stable excitonic many-body effects. These include many-body neutral excitons, trions, biexcitons, and defect-induced excitons at room temperature, rarely realized in bulk materials. Nevertheless, the defect-induced trions correlated with charge screening have never been observed, and the corresponding BEs remain unknown. Here we report defect-induced A-trions and B-trions in monolayer tungsten disulfide (WS_2) via carrier screening engineering with photogenerated carrier modulation, external doping, and substrate scattering. Defect-induced trions strongly couple with inherent SiO2 hole traps under high photocarrier densities and become more prominent in rhenium-doped WS2. The absence of defect-induced trion peaks was confirmed using a trap-free hexagonal boron nitride substrate, regardless of power density. Moreover, many-body excitonic charge states and their BEs were compared via carrier screening engineering at room temperature. The highest BE was observed in the defect-induced A-trion state (~214 meV), comparably higher than the trion (209 meV) and neutral exciton (174 meV), and further tuned by external photoinduced carrier density control. This investigation allows us to demonstrate defect-induced trion BE localization via spatial BE mapping in the monolayer WS_2 midflake regions distinctive from the flake edges.

Keywords: exciton binding energy defect-induced B-trion scanning tunneling spectroscopy spatial binding energy distribution neutral-to-trion conversion

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Regulating the 'Locally excited states'to facilitate spin-flip processes in efficient 'acceptor free' TADF emitters

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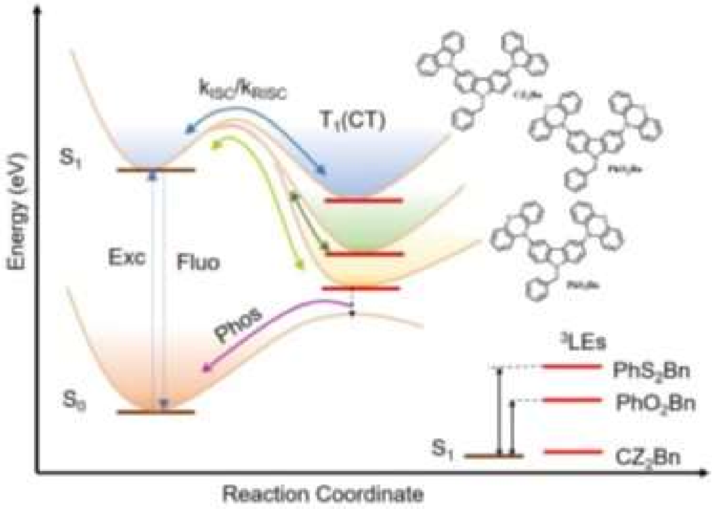
Thermally activated delayed fluorescent materials are emerging as promising emissive layer materials for the next generation organ ic light emitting diodes (OLEDs) due to their high internal quantum efficiency. This would assist the development of low power operational devices with high luminescence efficiency and device durability. The overall efficiency of the process is known to be limited on the triplet to singlet up conversion mechanism and the rate constant (k RISC) of this process. The conventional TADF emitters consists of Donor Acceptor (D A) units in the chemical structure to facilitate the k RISC , by reducing the singlet trip let energy offset. At the same time the geometrical distortion reduces the oscillator strength considerably thereby reducing the rate of singlet radiative processes. Our strategy to improve the k RISC without compromising on the singlet radiative processes was achieved by introducing tailor designed locally excited state (LE) which is isoenergetic with the charge transfer states (CT) energy levels. This approach provides an effective strategy for designing effective TADF emitters without the conventional Don or acceptor (D A) structural backbone by managing LE and CT energy level alignments to facilitate the up conversion process enhancing reverse intersystem crossing rate. In the present poster, three TADF emitters are considered for comparison that consistin g carbazole as the core unit with different peripheral donor groups covalently connected to it, in particular CZ 2 Bn having almost similar LE and CT energy levels exhibited efficient TADF feature and exciton utilization.

Keywords: Secondary donor moiety, Reverse intersystem crossing, Singlet triplet energy gap, Charge transfer state and locally excited state alignment, Radiative rate constant



SPICE Simulation of Hybrid Organic Inorganic Perovskite Memristive Devices

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This work presents anovel strategy to mimic memristive characteristics using experimental data fitting andSPICE simulation. The simulation of memristor characteristics is essential to incorporate these memristors in circuitsand system design tools. However, as of now, noneof thesimulation tools have anymemristorsmodels that are available out of the package for the circuit designers. We propose an algorithm for the simulation of memristor current-voltage characteristics which is inspired by standard SPICE based Yakopcic model of memristor. The proposed model fits the high resistancestate (HRS) and low resistance state (LRS) separately to the standard current conduction models from which the fitting parameters are being extracted. Using these extracted fitting parameters, the complete simulation of memristor hysteresis loop is done in SPICE. The validity of the modeldemonstrate is demonstratedby fitting characteristics of a hybrid organic inorganic perovskite (HOIP)memristorwhich yield per-cycle mean errors of <6.67%.The piecewise fitting of experimental data shows that the current during its HRSin our HOIP memristors,is dominated by tunnelling process, and whiletheLRScurrent shows ohmic conduction.

Keywords: Memristor, SPICE simulation, Hybrid organic inorganic perovskite,resistance switching

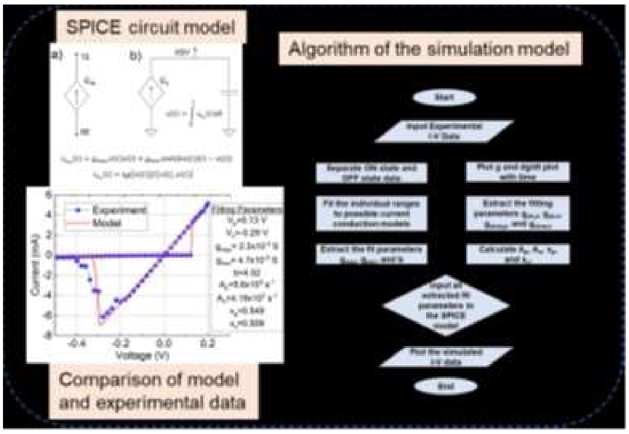

Figure: Schematic of the SPICE circuit model (top-left figure), comparison of the model experimental data for HOIP memristor (bottom-left figure), and algorithm for the simulation model (right side figure).

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The Potential Applications of Nano Enzyme and Their Future Perspective

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Nano enzymes are nanoparticles that mimic and exhibit similar properties to natural enzymes. Enzymes such as peroxidase, catalase, superoxide dismutase, oxidase, and oxygenase are widely employed in the degradation of persistent organic and inorganic pollutants but they are less susceptible to environmental changes. Nano enzymes have a variety of advantages, including simple synthesis method, low cost, high stability, smooth catalysis surface and offer high catalytic efficiency even in harsh environmental conditions. In addition, nano enzymes have applications in the degradation of hazardous organic and inorganic pollutants, biosensing, immunoassays, disease diagnostics, theranostic, tissue culture, and protection against oxidative stress in living organisms. The present communication specifically emphasizes potential applications of nanoparticles mimicking peroxidase-like activity and their future scope for large-scale industrial utility.

Keywords: Nano enzymes, Peroxidase, Organic transformations, Catalyst

ICANN2021 **ID: D1074**

Synthesis of Biocompatible Carbon Dots as Label Free Fluorescent Probe for Sensing and Preparation of 5-Fluorouracil-CD Nanoconjugate for *In Vitro* Antiproliferative Activity

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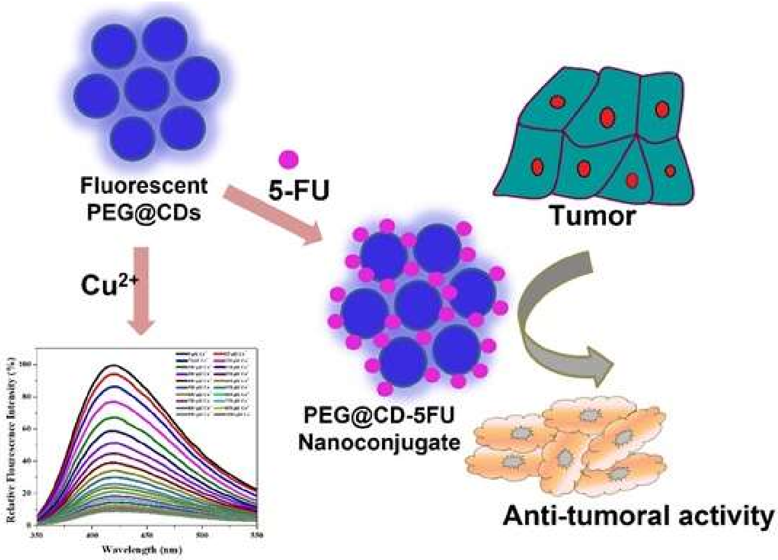
In this work we report one step eco-friendly route for the synthesis of biocompatible carbon dots (PEG@CDs). The as synthesised carbon dots were used successfully for loading and release of 5- Fluorouracil (5-FU). The photophysical and morphological characterization has been done using HR-TEM, XPS, XRD, FT-IR and UV-Vis spectroscopy. The results are indicative of improved photostability of the drug after conjugation with the carbon dots. The enhanced release of 5-FU in acidic environment makes it a selective antiproliferative drug carrier. The effective antiproliferative action of nanoconjugate has been explored using scratch assay, ROS generation assay and Hoechst staining. The reduced cytotoxicity of the carbon dot conjugated drug in comparison to free drug towards normal cells opens doors to explore the possibilities to design next generation antiproliferative drug delivery vehicle. The as synthesised PEG@CDs were further employed for assaying cobalt. The highly stable nature of PEG@CDs under various conditions such as different pH, high ionic strength, UV light irradiation, wide temperature range and prolonged storage time indicating their capabilities for expanding approach towards other applications.

Keywords: Carbon dots; Antiproliferative; Sensing; fluorescence; nanoconjugate



Sustained Generation of Peroxide from Air by Carbon Nano Onion Under Visible Light to Combat RNA Virus

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Carbon nano onion (CNO) from dried grass has been synthesized by its carbonization in the size range, 20 to 100 nm. A concept has been developed to show that this CNO even inside room light generate hydrogen peroxide which inhibits WSN influenza virus (H1N1). With high degree of surface charge (Zeta potential, ~ –70 mV), the hydrodynamic size range of CNO cover the size of SARS-CoV-2. This will readily allow macromolecular collisions between CNO and virus involving electrostatic and hydrogen bonding interactions. Before invoking any such collision, CNO initially form adduct with aerial oxygen: $\{CNO+{}^3O_2= CNO\|{}^3O_2\}$, which under visible light excitation activate the CNO to generate singlet oxygen followed by electron transfer: $\{CNO^+\|{}^1O_2^-\}$, producing superoxide radical. The superoxide radical anion disproportionate to peroxide or hydro peroxide ion and oxygen and finally to hydroxyl radical leading to the generation of all reactive oxygen species (ROS). The advantage of introducing CNO, synthesized from the cheapest source to cater global need, is to sterilize infected hospitals indoor and outdoor, public auditorium, aircraft carriers, air conditioner vents due to its sustained conversion of air to ROS for a long time. This CNO is benign to plants, animal kingdoms including human. Its solubility around pH 7.5 in water helps it for spraying and under slow exposure with acidic carbon dioxide present in air it gets deposited as insoluble on the building walls around pH 6.5. Thus its use could prevent not only frequent evacuation as used by toxic hypochlorite or strong radiation to sterilize infected places from the present RNA virus, SARS-CoV-2, but also permanently against many hospital pathogens.

Keywords: Water soluble CNO; Peroxide generator; RNA virus; COVID-19

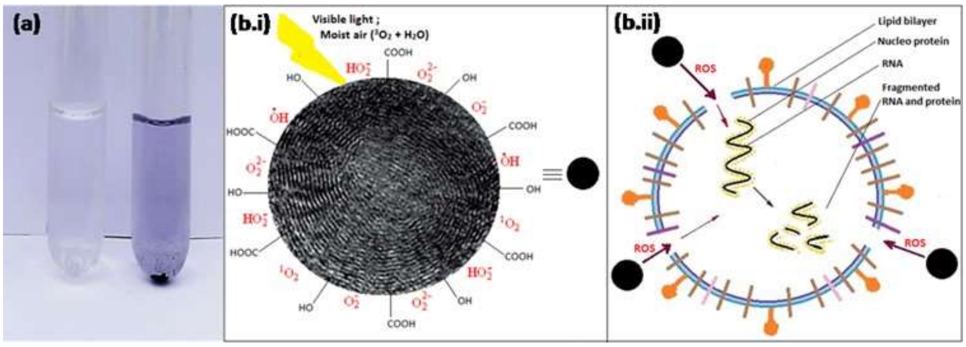

Figure: a) Starch iodide solution with CNO shows ROS generation. (b.i) a cartoon depicting ROS generation on the surface of CNO (b.ii) Collision of CNO with SARS-CoV-2 to rupture lipid layer and disintegrate virus RNA.

Pharmacoengineered Lipid Core-Shell Nanoarchitectonics to Influence Macrophage Uptake for Mitigating Tuberculosis Burden

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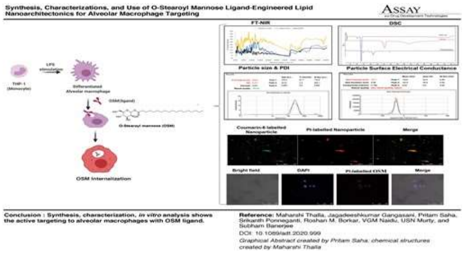
Tuberculosis is a devastating disease caused by *Mycobacterium tuberculosis*, which clock and thrive within the macrophages. Despite being exposed to the *Mycobacterium tuberculosis* by macrophage leads to overexpression of membrane receptors like CD206, mannose receptor. The mannose-mediated receptor will sensitize and internalization of the pathogen by detection of glycan present on antigens. Based on the thorough investigation on internalization, favourable conditions of macrophage, drug delivery has been constructed in such a way that would easily be engulfed. Therefore, we have explored the pathway with a mannosylated ligand tethered lipid core-shell nanoarchitectonics (LCSNAs) as a potential translational drug delivery system. LCSNAs were fabricated through the modified double emulsification method and surface engineered with the ligand systematically. Detailed i*n vitro* physico-chemical characterization was done by means of several sophisticated analytical tools such as Zetasizer, SEM, AFM, FTIR, DSC, XRD, and *in vitro* drug release profile were evaluated using dialysis sac method including through *in vitro* cell-line studies on human alveolar macrophages (THP-1). LCSNAs were found to be in the range between 200-300nm with a negative charge around -30mV. Surface morphology revealed irregular shape particles but with a smooth surface as evident from FE-SEM and AFM analysis. FTIR, DSC, and XRD data revealed that the loaded drug was accommodated in an amorphous form. *In vitro* drug release was persisted for 48 hours with a biphasic release pattern. To assess the macrophage internalization process, where ligand tethered LCSNAs showed a superior uptake in comparison to the non-ligand tethered LCSNAs. Thus, we had continued our further studies with the ligand tethered LCSNAs for intracellular compartmental analysis study to reveal the colocalization pattern with different antibodies which overexpresses during diseased conditions such as pH-rodo Red Dextran, Lyso Tracker Red, ER Tracker Red along with ligand tethered LCSNAs. In addition. a comparative efficacy analysis of different formulations in *Mycobacterium smegmatis* incubated THP-1 cells were examined. Ligand tethered LCSNAs were shown comparatively lower CFU/ml than the LCSNAs, and pristine drug. Therefore, it can be concluded that this pharmacoengineered lipid core-shell nanoarchitectonics having significant influence in macrophage uptake for mitigating tuberculosis burden

Keywords: Pharmacoengineering, Lipid core-shell nanoarchitectonics, Mannose receptor, Cellular uptake, Efficacy



Synthesis, Characterizations, and Use of O-Stearoyl Mannose Ligand-Engineered Lipid Nanoarchitectonics for Alveolar Macrophage Targeting

Conclusion : Synthesis, characterization, *in vitro* analysis shows the active targeting to alveolar macrophages with OSM ligand.

Reference: Maharshi Thalla, Jagadeeshkumar Gangasani, Pritam Saha, Srikanth Ponneganti, Roshan M. Borkar, VGM Naidu, USN Murty, and Subham Banerjee

DOI: 10.1089/adt.2020.999

Graphical Abstract created by Pritam Saha, chemical structures created by Maharshi Thalla

ICANN2021 **ID: D1116**

Non-invasive Point-of-Care Nanobiosensing of Cervical Cancer as an Auxiliary to Pap-Smear Test

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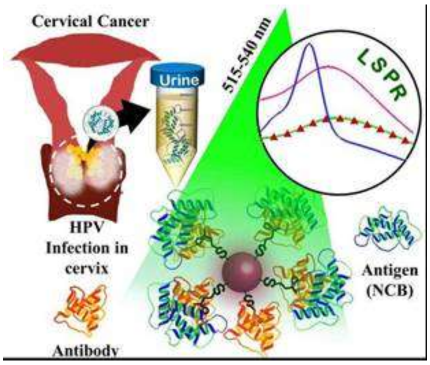
A potential cancer antigen (Ag), Protein-Phosphatase-1-gamma-2 (PP1ϒ2) with a restricted expression in testis and sperms has been identified as a biomarker specific to cervical cancer (CaCx). Detection of this novel cancer biomarker antigen (NCB-Ag) in human urine opens up the possibility of non-invasive detection of CaCx to supplement the dreaded and invasive Pap-smear test. A colorimetric response of an assembly of gold nanoparticles (Au NPs) has been employed for the quantitative, non-invasive, and point-of-care-testing (POCT) of CaCx in the urine. In order to fabricate the immunosensor, Au NPs of sizes ~5–20 nm have been chemically modified with a linker, 3,3'-di-thio-di-propionic-acid-di(n-hydroxy-succinimide-ester) (DTSP) to attach the antibody (Ab) specific to the NCB-Ag. Interestingly, the addition of Ag to the composite of Ab-DTSP-Au NPs leads to a significant hypsochromic shift due to localized surface plasmon resonance (LSPR) phenomenon, which originates from the specific epitope-paratope interaction between the NCB-Ag and Ab-DTSP-Au NPs. The variations in the absorbance and wavelength shift during such attachments of different concentrations of NCB-Ag on the Ab-DTSP-Au NPs composite have been employed as a calibration to identify NCB-Ag in human urine. An in-house prototype has been assembled by integrating a light emitting diode (LED) of a narrow range wavelength in one side of a cuvette in which the reaction has been performed while a sensitive photodetector to the other side to transduce the transmitted signal associated with the loading of NCB-Ag in the Ab-DTSP-Au NPs composite. The proposed immunosensing platform has been tested against other standard proteins to ensure non-interference alongside proving the proof-for-specificity of the NCB detection.

Keywords: Cervical cancer, novel cancer biomarker, non-invasive; urine; sensor; LSPR; nanoparticle.



ICANN2021 **ID: D1144**

Developing Membrane-Derived Nanocarriers for Ex Vivo Therapy of Homologous Breast Cancer Cells

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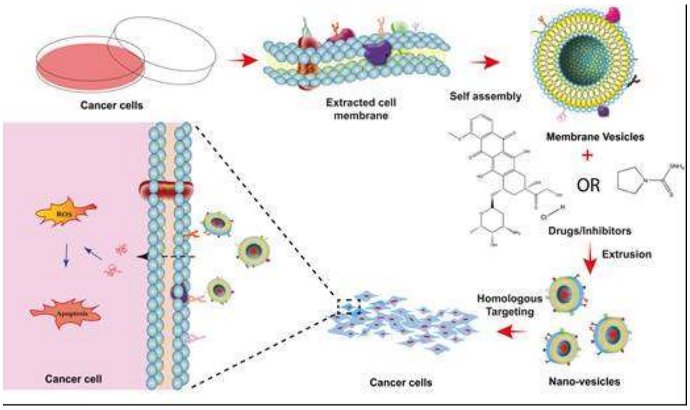
Biocompatible nanocarriers are quite intriguing delivery systems for effective and sustained delivery, drug release, long-time survival in circulation, immune evasion and target specific recognition. The primary aim of our study was to develop biomimetic nanocarriers for specific homologous targeting of anticancer drugs. Membranous nano-vesicles were synthesized from breast cancer cell lines (MCF-7) by syringe extrusion process and loaded with ammonium pyrrolidinedithiocarbamate (PDTC) and doxorubicin (Dox), respectively. Besides their abilities for self-homing, the drug loaded nano-vesicles showed anti-cell proliferative effect via generation of reactive oxygen species (ROS). Delivery of the anti-cancer drugs showed better drug efficacy in both monolayer and spheroids as compared to the other cell types (heterologous systems) mainly due to self-homing, recognition and internalization. Experimental results demonstrated increased anti-proliferative potency of ammonium PDTC against MCF-7 cells by inducing apoptosis via generation of reactive oxygen species, while retaining its biphasic activity and minimal effect on non-cancerous HEK 293 cells. Thus, the membrane-derived nanocarrier is an attractive biocompatible system for *ex vivo* drug delivery for homologous targeting

Keywords: biomimetic, cell membrane, nano-vesicles, homologous targeting, reactive oxygen species, apoptosis



Schematic: Ammonium PDTC or doxorubicin-loaded nanovesicles for homologous targeting. Targeted delivery results in increased generation of reactive oxygen species in the cancer cells, thereby leading to apoptosis.

D-Penicillamine Templated Au-Cu Bimetallic Nanocluster Containing Nanocomposite Inhibits Metastatic Property of Triple Negative Breast Cancer

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Triple-negative breast cancer (TNBC), the most aggressive subtype of breast cancer, lacks effective targeted therapies due to negative expression of the targetable bioreceptors [1]. Additionally, hypoxic condition in solid tumors contributes to the epithelial to mesenchymal transition (EMT), which aggravates cancer progression, multidrug resistance (MDR), migration, and stemness of the TNBC. Earlier, our team reported combination of drugs to alter signaling pathways and effectively block the EMT and thus metastasis of TNBC [2]. However, to integrate the system into a single platform, a novel therapeutic module has been fabricated by coating a nontoxic, biodegradable PLGA nanoparticle core with D-penicillamine templated Au-Cu bimetallic nanoclusters [3, 4]. Further, the resultant nanomaterials were coated with recombinant transferrin protein to specifically. target transferrin receptor overexpressing TNBC [5]. Experimental results demonstrated efficient cellular internalization and significant anti-cell proliferative potential of the nanocomposites. The EMT-induced TNBC cells exhibited reactive oxygen species (ROS) generation, depolarization of mitochondrial membrane potential, and apoptosis upon treatment with nanocomposites. Gene expression by real-time PCR indicated that treatment of EMT-induced TNBC cells with nanocomposites promoted mesenchymal to epithelial transition (MET). The nanocomposites treatment led to increase in epithelial marker E-cadherin and decrease in mesenchymal marker vimentin in MDA-MB-468 cells. Similarly, decrease in stemness markers such as ALDH1A3 and EpCAM were observed in MDA-MB-231. Downregulation of EMT with concomitant alteration of STAT-3 and β-catenin signaling pathways led to reduced migration ability of the TNBC cells. Thus, the synthesized nanocomposites portray biomedical application potential for cellular imaging and targeting TNBC.

Keywords: Nanocomposites, TNBC, EMT, MDR, Hypoxia.

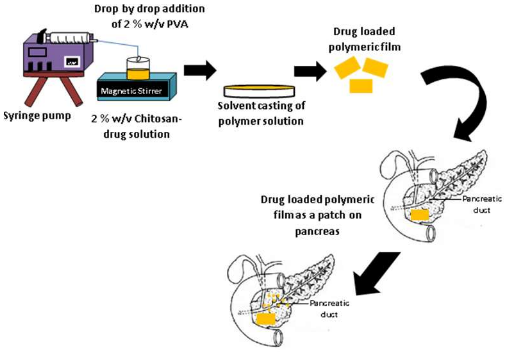

Figure : Drug loaded chitosan-PVA composite filmfor local drug delivery

Development and Characterization of Nanocluster Studded Luminescent Bacteria

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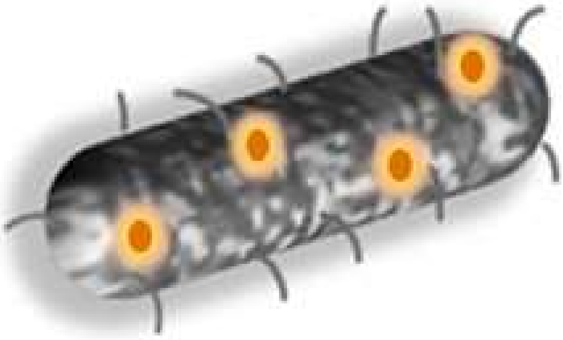
The bacteria as a payload delivery system are self-driven and target specific due to their inherent properties. The attenuated strains are developed and channelized to work as delivery vehicles to microenvironments of tumours by gene regulation, genetic engineering, surface modifications etc. The current study focuses on developing and characterisation of such a delivery system, which is luminescent and self-propelling without using genetic modifications. Thus, creating a luminescent system that could be traced and imaged while working as a vehicle to reach the core of tumours. Such systems can be used for drug delivery to hypoxic tumour areas

Keywords: attenuated strains, gene regulation, self-propelling, luminescent



Surface Modified Nanoparticle Impregnated Activated Carbon for Disinfection of Water

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Availability of safe drinking water is one of the current global challenges affecting millions of people and the situation is projected to worsen in coming decades. Conventional disinfection techniques used in the urbanized world has limitations, such as generation of toxic by-products or they require high capital investments. One of the most promising solutions to this problem is through the use of cheap, autonomous point-of-use water disinfection systems. In our work we have aimed to develop a nanoparticle (NP) conjugated activated carbon (AC) hybrid that can be used in column-based water decontamination.

We have prepared copper nanoparticles (CuNP) with a mean diameter of 4.37 nm using green synthesis protocol and deposited them on the surface of acid functionalized AC to prepare the AC-NP hybrid. The exact chemistry behind the acid functionalization of AC was investigated using FTIR and XPS, while the impregnation of CuNP was characterized, both qualitatively using SEM and EDX, and quantitatively though ICP-AES. A maximum loading of 0.8 ± 0.08 wt% of CuNP is obtained in case of 48-hour acid treated AC hybrid. Further, batch killing studies performed with the hybrid shows complete inactivation of *E. coli* in contaminated water within 35 minutes of residence time, thus demonstrating good antibacterial performance of the hybrid and its potential for use in column-based systems for water disinfection.

Keywords: nanoparticle, synthesis, bacteria, water, disinfection

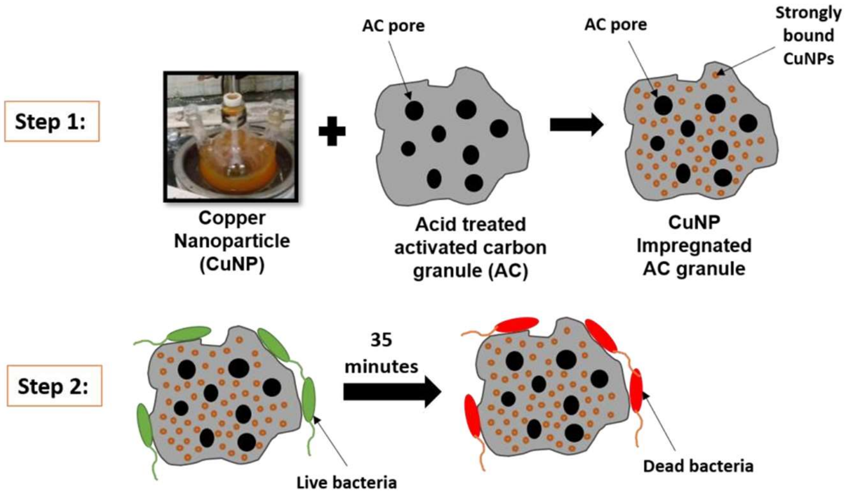

Figure Schematic illustration of the proposed methodology for decontamination of drinking water by nanoparticle conjugated activated carbon hybrid

Photo-Responsive Azobenzene Clay Nanocomposite Doped with Carbon Dots with Tunable Electrical Properties

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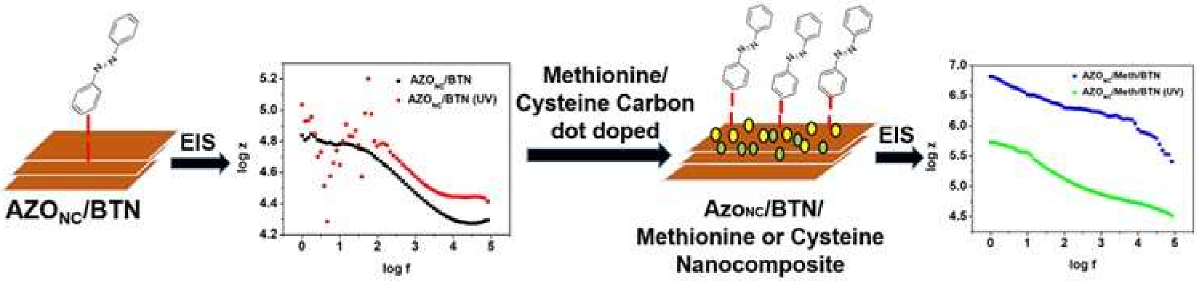
The development of photo-responsive nanocomposite materials plays an important role in the fabrication of optoelectronic devices. Here, we have synthesized an Azobenzene-clay nanocomposite doped with carbon dots. This nanocomposite possesses different ac conductivity under different conditions of visible and UV light. Initially, Azobenzene nanoclusters were synthesized from commercially available Azobenzene, and then a composite was made of this Azobenzene nanocluster and clay. The photo-responsive behaviour of Azobenzene was also observed in its nanocluster form. The Azobenzene-clay nanocomposite showed small changes in ac conductivity in the presence and absence of UV light. However, by doping this nanocomposite system with electron-rich methionine and cysteine carbon dots, the ac conductivity of the modified systems can be enhanced and also tuned in the presence and the absence of UV light. Using Electrochemical Impedance Spectroscopy, the ac conductivity properties of carbon-doped Azobenzene-clay nanocomposite were determined and studied. Thus, fabrication of such tunable doped photo-responsive nanocomposites will lead to its use in photoswitchable optoelectronic devices.

Keywords: Photo-responsive, carbon dots, nanocomposite, conductivity, doping



Stimuli-Responsive Hybrid Jute Carbon Dot-Cotton Patch Nanocomposite System

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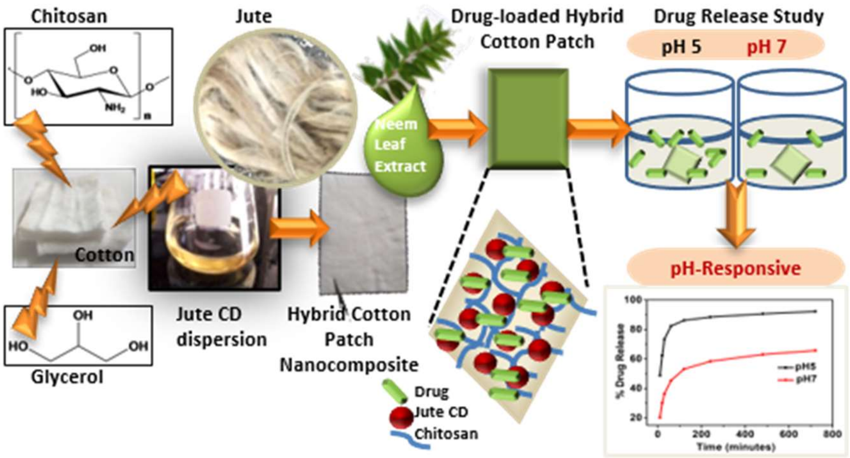
This work exhibits the fabrication of a bio-polymeric hydrogel laden-hybrid cotton patch nanocomposite, immobilized with carbon dots (CDs) that acted as a stimuli-responsive smart drug delivery system. Jute was taken as the carbon source to synthesize fluorescent CDs. A herbal formulation in terms of neem leaf (*Azadirachta indica*) extract was used as the model drug to exemplify the release study. Two different pH environments (pH 5 and 7) were chosen for this aspect. The jute CDs incorporated-cotton patch responded differently under two different pH environments, where the release was shown to be higher at pH 5 than at pH 7. In certain cases, due to the growth of pathogenic bacterial infection around the cut/wound region, the pH gets lowered – therefore, this enhanced release of the drug from the fabricated patch at pH 5 is desirable. Different characterization techniques such as FTIR spectroscopy, thermogravimetric analysis, tensile measurement etc. were taken to study the physicochemical properties of the patch. Besides, the drug release study under pH 5 and 7 were also performed by fabricating different hybrid cotton patch nanocomposites by incorporating nanomaterials/CDs derived from other sources viz. Graphene oxide, tea, ascorbic acid, *Aloe vera*. All of them were non-responsive at both pH 5 and 7. Mechanistic interpretation provides the underlying drug release behaviour of the cotton patch. Such stimuli-responsive behaviour of hybrid cotton patch would pave the way for utilizing systems as smart wound-dressing material using sustainable materials.

Keywords: Carbon dot, Nanocomposite, Stimuli-responsive, Drug delivery



Amine doped UIO-66 nanocomposite as a high-performance filler for CO_2/N gas separation

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In the present scenario, the requirement for an efficient and reliable CO_2 capture nanocomposite material is of prime importance. Even though several materials have been explored as a nanocomposite filler like graphene oxide, ionic liquids, porous organic frameworks, covalent organic frameworks etc. metal organic frameworks (MOF) are more prioritized. From the commercialization, researchers are focusing on the enhancement of CO_2 capture capacity, rate capability, chemical and thermal stability, cost-effectiveness, safety and eco-friendly materials. UIO-66 nanomaterial has been extensively studied in CO_2 capture technologies ever since the discovery, owing to the flexibility, thermal stability, high surface area etc. In this research a comprehensive study has been accomplished to examine the physicochemical properties of the fabricated UIO-66 and membrane by using FTIR, XRD, TGA, AFM, FESEM, FETEM, etc.

This three-dimensional MOF when doped with amino acid showed a better separation performance.

Keywords: UIO-66, Amine doped nanocomposite, CO_2 capture, mixed matrix membrane

Impact of Surface Treatment of Halloysite Nanotubes (Hnts) for Improvement of Mechanical Properties of The Epoxy Based Nanocomposites

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In this study, halloysite nanotubes (HNTs)/epoxy composites were fabricated using sulfuric acid-treated HNTs and epoxy resin. Halloysite Nanotubes (HNTs) are found naturally and has unique physical, chemical and electrochemical properties.It has many attractive advantages such as unique micro-space structure, large aspect ratio, high lumen volume, non-toxicity, and wide availability, and is widely used in various scientific fields. The chemical formula of halloysite nanotubes is $Al_2Si_2O_5(OH)_4.2H_2O$. Halloysite nanotubes (HNTs) were treated with sulfuric acid, the physical and chemical properties of HNTs when exposed to sulfuric acid under different treatment times and different temperatures were studied. The halloysite is treated with sulfuric acid to increase its BET surface area, thereby improving the interfacial adhesion with the polymer matrix. The significantly increased properties of the hybrid are attributed to the covalent bonding between the nanotubes and the matrix. HNTs/epoxy resin nanocomposites are prepared by mixing different proportions of HNTs with pure epoxy resin. Ultrasonic and mechanical stirrers are used for better dispersion. When HNTs are modified to the surface, the tensile strength, flexural strength and impact strength of these composite materials will increase. The conclusion is that the modification of HNTs helps to enhance the dispersion and cross linking in the epoxy resin matrix.

Keywords: Composite, Halloysite Nanotubes (HNTs), Dispersion, Acid-Treatment, Mechanical Properties.

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Effect of Hnts Modification with H_2SO_4 on the Thermo-Mechanical Properties of PEEK/PEI Nanocomposites

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Halloysite nanotubes (HNTs) modified with sulfuric acid to expose the tubular morphology by increasing silicone content and removing a significant amount of iron and carbon elements from the surface of HNTs. The unmodified and modified HNTs were incorporated into the blend comprising of polyether ether ketone (PEEK) and polyetherimide (PEI) (50:50) ratio using melt mixing process by co-rotating twin-screw extruder followed by injection molding. Mechanical properties such as tensile strength, tensile modulus, and elongation at break had been tested by a Universal testing machine (UTM) and show a significant improvement at modified HNTs loadings. Thermogravimetric analyzer (TGA) results demonstrated the incorporation of inorganic modified HNTs nanofiller into the PEEK/PEI matrix, which obstructs the time to reach the degradation point, and hence improved thermal stability. Dynamic mechanical analyzer (DMA) results revealed that the significant increment in glass transition temperature (T_g) of the developed PEEK/PEI blends with modified HNTs has been improved as compared to the pure blend matrix attributed to the creation of a nano-particles network that exhibits the polymer chain mobility. The microscopic analysis of tensile fracture surface was analyzed by SEM & TEM which reveals that there are excellent interfacial adhesion and uniform dispersion of modified HNTs into the PEEK/PEI matrix. The enhancement in the properties is due to better interfacial adhesion between modified HNTs and blend matrix.

Keywords: HNTs, PEI, PEEK, TEM, TGA, and DMA.

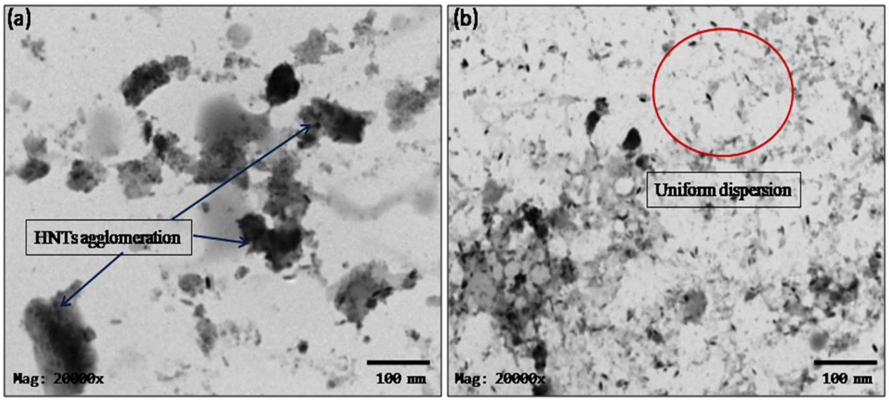

Figure 1. TEM images of PEEK/PEI blend matrix with (a) unmodified and (b) modified HNTs.

An Efficient Visible Active ZnO/rGO Nanocomposites for Removal of Cationic and Anionic Dyes

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Graphene is widely used as a photocatalyst for solar energy conversions, while its photosensitizer role to transform wide band gap semiconductor to efficient visible active photocatalyst enriches the demand of graphene-based composite photocatalyst. Herein, we have designed a graphene based visible active photocatalyst with wide band gap semiconductor of desired nanostructures via hard integration technique. The prepared materials were characterized by X-ray diffraction spectroscopy (XRD), UV-vis diffuse reflectance spectroscopy (DRS), Fourier transform infrared (FTIR), X-ray photoelectron spectroscopy (XPS), field emission scanning electrons microscope (FE-SEM) and transmission electrons microscope (TEM). The prepared materials have shown excellent degradation efficiency against both cationic and anionic dyes under visible irradiations. The excellent efficiency is proposed for the photosensitization and enhanced adsorption of graphene. Further, the radical scavenger test confirms the generated electrons which transfer to conduction band of wide band gap semiconductor for the reduction reactions. The well encapsulated rGO over semiconductor provide large surface contact for better electrons transfer process. The obtained results would provide complete information regarding the development of graphene-based composite materials with desired pre-selected nanostructure for solar energy conversion.

Keywords: Zinc Oxide, Reduced Graphene oxide, Composite, Photocatalyst, Interfacial contact.

Modeling of Surface Roughness of Abrasive Jet Machined Nanocomposite using Artificial Intelligence Approach

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Processing of polymer based nanocomposite using advanced machining processes like abrasive jet machining is very challenging. Though these materials possess unique properties and developed for specific applications. Therefore analysis of material processing performance of a particular machining process is become essential. Performance of a process can be understood by establish a mathematical relationship between input and output parameters. This empirical relationship can be useful for election of significant variable factors. Once these factors elected then better quality characteristics can be obtained at economical cost. In present study a mathematical model for surface roughness is developed using artificial neural network. To check the accuracy of developed mathematical model the predicted values of consider quality characteristic is compared with previous published experimental values. Input parameters jet pressure, traverse rate, weight percentage of multi-walled carbon nanotubes and stand of distance for abrasive jet machining of carbon fiber reinforced polymer composite are considered. Average percentage prediction error found less than10% that shows predicted values from developed model is well coped with experimental values.

Keywords: Carbon fiber reinforced polymer composite, abrasive jet machining, surface roughness and artificial neural network.

ICANN2021 **ID: F1045**

Negative Magnetization and Sign Reversal Exchange Bias Behavior in Nanocrystalline Ho2CoMn1-xNixO6 (x = 0 - 0.4) Double Perovskite

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Single phase nanocrystalline samples of $Ho_2CoMn_{1-x}Ni_xO_6$ (x = 0-0.4) double perovskite were successfully prepared by a gel combustion method. The present work associated with their structural and some novel magnetic properties. Structural studies reveal a formation of nanocrystalline samples, which crystallizes into monoclinic structure (space group P21/n). Magnetization versus temperature (M-T) analysis shows a single FM transition for x = 0.0 at 83 K (TC1) and it is attributed to the super exchange interaction of Co^{2+} - O^{2-} - Mn^{4+} networks. However, two FM transitions (TC1, TC2) has been noticed after Ni substitution, where TC2 is arises due to super exchange interaction of Co^{2+} - O^{2-} - Ni^{4+} networks. The transition temperature TC1, is decreasing from 83 K for x = 0.0 to 76 K for x = 0.4. Whereas TC2 is increasing from 84 K for x = 0.1 to 88 K for x = 0.4. A magnetization reversal has been observed in the field cooled state for x = 0.4 sample with a compensation temperature (Tcomp) at 10 K and is attributed to the negative exchange interaction between transition metal (TM) and rare-earth (RE) ions. The hysteresis (M-H) loops recorded at 5 K show a drop-in saturation magnetization (MS) and coercivity (Hc) value after Ni substitution. However, the observed large value of MS of the order of 11.6 µB/f.u. at 5 K is attributed to the FM interaction of RE ions with net magnetic moment of TM ions. A sign reversal exchange bias behaviour has been observed by the samples after Ni substitution with a maximum value of exchange bias field up to 230 Oe at 5 K and is attributed to the competition between spin canted magnetic moment of RE ions and FM moment of TM ions. Keywords: Double Perovskite, gel combustion, nanocrystalline, negative magnetization, sign reversal exchange bias behavior.

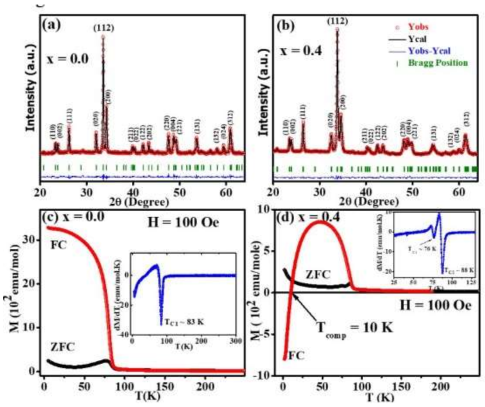

Figure (a, b) Rietveld refinement of room temperature XRD patterns and (c, d) ZFC and FC, M - T plots at an applied field of H = 100 Oe, inset show dM /dT versus T plots for x = 0.0 and 0.4 respectively

Exchange Bias and Dynamic Magnetic Properties of Mg Substituted $NiCr_2O_4$ Nanoparticles

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Single phase Mg substituted nanoparticles of $NiCr_2O_4$were synthesized by hydrothermal route. X –ray diffractometer and Rietveld refinement confirmed cubic (Fd-3m) crystal structure with lattice constant 8.3471(5)Å. Temperature dependent magnetization(M-T)measurements suggested a ferrimagnetic transition around 100K followed by a cluster spin glass like phase around at 10K. The observed cluster glass phase is assigned to the result of interaction between ferrimagnetic core and surface spins of nanoparticles. Temperature dependent exchange bias field has been studied above and below the glassy transition temperature. The core spin structure of the present system is showing tendency towards collinearity with considerably small frustration index. Memory and relaxation protocols were followed to confirm the metastability of glassy phase. Hierarchical model has been used to successfully explain the memory effect in positive and negative temperature cycle of relaxation. Strong inter cluster interaction has confirmed between these highly dense nanoparticles at low temperature.

Keywords: Nanomaterials; Cluster spin glass; Exchange bias; Memory effect.

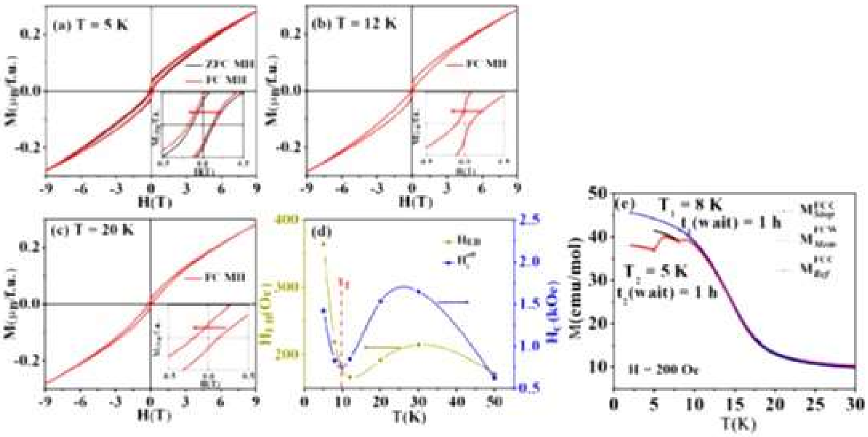

Figure 1: M-H loops recorded under zero field cooled(ZFC)and field cooled condition(FC)at (a)T = 5 K (b)T = 12 K & (c)20 K. (d)Temperature dependence of coercivity and exchange bias field. (e)Memory effect in M-T under FC protocol.

ICANN2021 **ID: G1008**

In Vitro Biomineralized Vaterite Derived Efficient Solid-State Synthesis of Pure $CaMnO_3$ Perovskite as an Effective Photocatalyst

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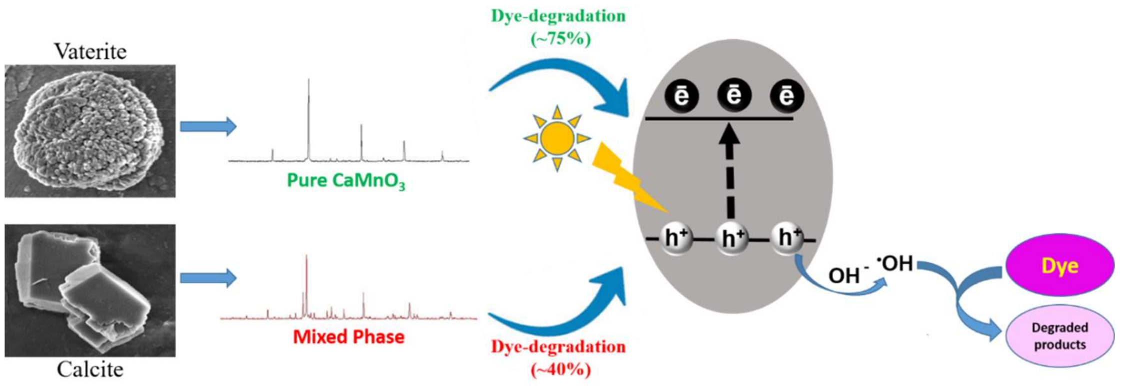
In recent years, perovskite materials have attracted immense popularity due to their role in energy-based applications. Calcium manganese oxides are analogous to the systems that perform water-splitting in the natural photosynthesis process. In this work, we report a convenient method to synthesize the perovskite $CaMnO_3$. *In vitro* biomineralized vaterite was used as the calcium source to synthesize pure $CaMnO_3$ efficiently. In contrast, commercial $CaCO_3$ comprising of the calcite phase led to the formation of a mixture of calcium manganese oxides. The low bandgap energy of pure $CaMnO_3$ (1.21 eV) enables it to absorb visible light, to be subjected as a photocatalyst to catalyze the photolytic degradation of the toxic dyes *viz.* Rhodamine 6G, Rhodamine B, Methylene blue and Methyl orange. The photocatalytic degradation of Rhodamine 6G was studied in detail including the mechanistic pathway. 72% of dye degradation was observed within 2 hrs. in the presence of pure $CaMnO_3$ in contrast to 46% in the presence of the mixed-phase calcium manganese oxide.

Keywords: *In vitro* biomineralized vaterite; perovskite; calcium manganese oxide; photocatalysis; dye degradation.



ICANN2021 **ID: G1024**

FeO(OH)/CoCeV (Oxy)Hydroxide as a Water Cleavage Promoter

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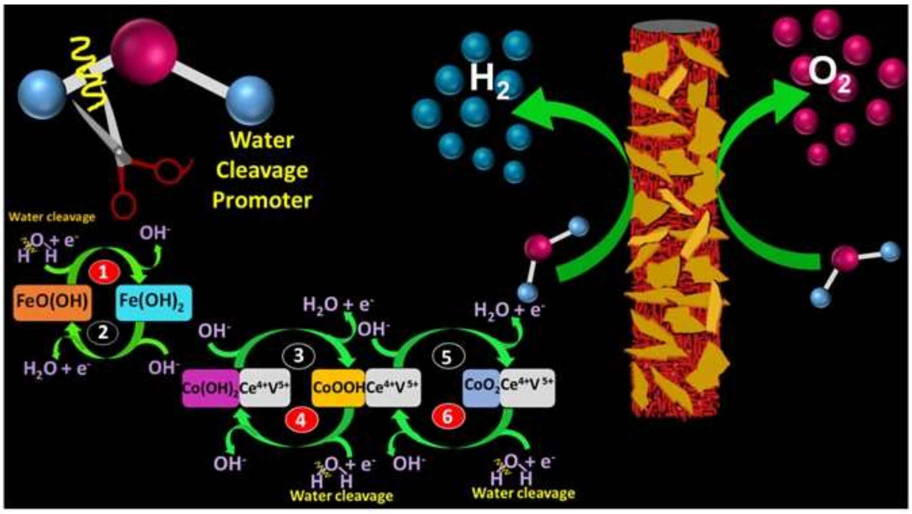
Search for a bifunctional electrocatalyst having water cleavage promoting ability along with the operational stability to efficiently generate oxygen and hydrogen could lead to robust systems for applications. These fundamental ideas can be achieved by designing the morphology, tuning the electronic structure, and using dopants in their higher oxidation states. Herein, we have fabricated a binder-free FeO(OH)-CoCeV-layered triple hydroxide (LTH) bifunctional catalyst by a two-step hydrothermal method, in which the nanograin shaped FeO(OH) coupled with CoCeV-LTH nanoflakes provide more electro catalytically active sites and enhanced the charge transfer kinetics for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). The composition optimized electrocatalyst (FeO(OH)-$\text{Co}_{0.5}\text{Ce}_{0.05}\text{V}_{0.15}$-LTH) acts as an efficient water cleavage composite by virtue of its favorable oxidation states leading to cyclic redox couples which yields an overpotential of 53 mV for HER, and 227 mV for OER to drive 10 mA/cm^2 current density in 1M KOH, with a corresponding Tafel slope of 70 mV/dec for HER and 52 mV/dec for OER. Furthermore, for the overall water splitting reaction, the heterostructure FeO(OH)-$\text{Co}_{0.5}\text{Ce}_{0.05}\text{V}_{0.15}$-LTH, acts as a dual-functional electrocatalyst, which requires a cell voltage of 1.52 V vs RHE to drive 10 mA/cm^2 current density.

Keywords: Overall water splitting; Iron oxide hydroxide; Layered Triple Hydroxides; Oxygen Evolution Reaction; Hydrogen Evolution Reaction



Transcription Methodology for Rationally Designed Morphological Complex Metal Oxides: a Versatile Strategy for Improved Electrocatalysis

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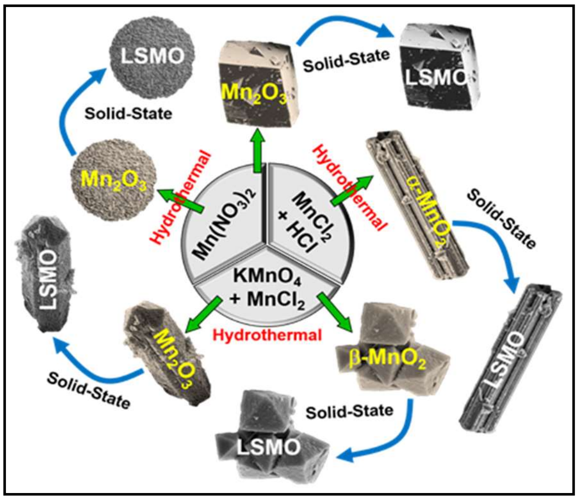
Complex metal oxides such as 3D perovskites, known for their high activity and stability, are traditionally synthesized at high temperatures leaving little scope for morphological tuning using structure-directing and high temperature unstable reagents. Present approach utilizes rationally designed hard-template precursors with desired morphology and adopting transcription of the same to achieve morphologies of complex metal oxides. In present work, we chose strontium doped lanthanum manganite (**LSMO**) as model system to demonstrate our transcription methodology. The improved electrochemical active sites of **LSMO** are achieved by tuning unique morphologies of manganese oxide (Mn_xO_y). Diffusion controlled solid-state route enables transcription of the pre-defined morphologies of Mn_xO_y into corresponding **LSMO**. Our champion morphological **LSMO** achieved ~4-fold increment in overall electrocatalytic OER performance compared to its solid-state synthesized counterpart. This approach offers unique way to realize highly efficient OER catalysts of high temperature synthesized complex metal oxides and can be extended to any general system.

Keywords: Morphology transcription, Electrochemical active surface area, Oxygen evolution reaction, Turnover frequency, Water oxidation kinetics.



Scheme 1. Synthetic protocol for the formation of morphological Mn_xO_y synthesized via hydrothermal route which are used as template during the solid-state reaction for transcription of its morphology into the corresponding **LSMO**

ICANN2021 **ID: G1028**

Two-Step Deposition Approach for Lead Free (NH4)3Sb2I9 Perovskite Solar Cells with Enhanced Open Circuit Voltage and Performance

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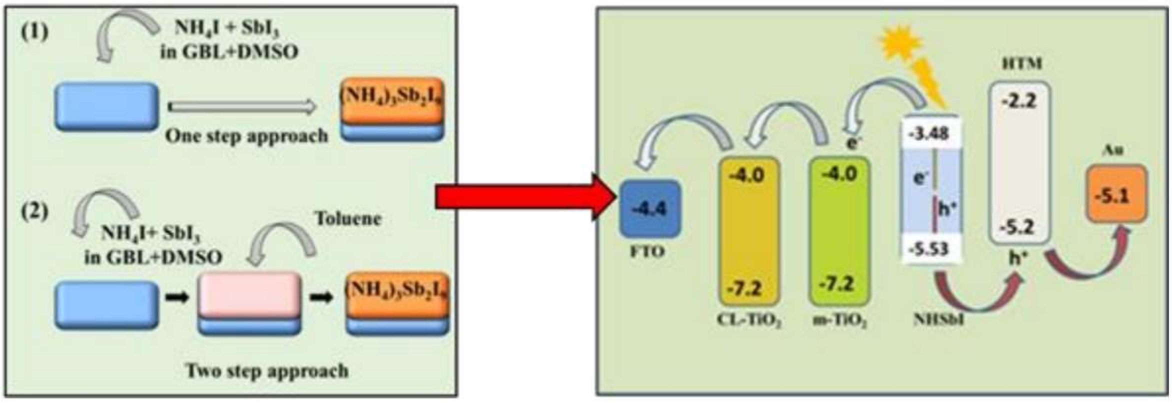
In recent years, development of lead (Pb) free perovskite solar cells (PSCs) has attracted scientific community because of their stability in air and less toxic nature. Antimony (Sb) based perovskite like-materials such as $(CH_3NH_3)_3Sb_2I_9$ and $(NH_4)_3Sb_2I_9$ have been employed as light absorbers and showed promising features for photovoltaic applications. Herein, we have utilized $(NH_4)_3Sb_2I_9$ as light absorber for the construction of Pb free PSCs. Moreover, we have employed modified two step procedure for the preparation of $(NH_4)_3Sb_2I_9$. The developed Pb free PSCs device (FTO/CL-TiO_2/m-TiO_2/$(NH_4)_3Sb_2I_9$/HTM/Au) exhibited enhanced power conversion efficiency (PCE) of 0.42% with open circuit voltage (Voc) of 945 mV.

Keywords: Pb free perovskite • $(NH_4)_3Sb_2I_9$• perovskite solar cells• photovoltaics • open circuit voltage

Figure/Scheme:



Entropy Driven Catalytic Activity for Low Cost OER Electrocatalysts

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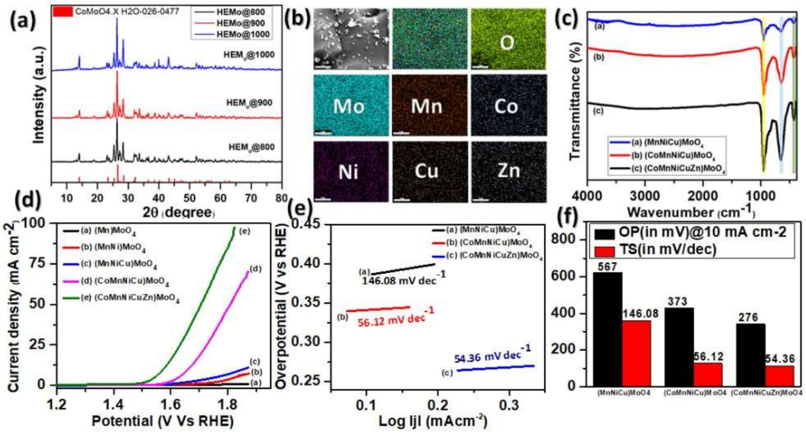
Oxygen Evolution Reaction (OER) is an important process coupled with four electrons in water splitting and metal-air batteries. But it is suffered from sluggish kinetics. So electrocatalyst plays an important role in the OER process to catalyzing the reaction kinetics. Noble metals such as Pt, Ir, and Ru have been state-of-the-art electrocatalysts so far; however, their practical application is limited due to their scarcity and high cost. Besides noble metals and their composites, their intrinsic properties like low electrical conductivity, sluggish kinetics, and stability restrict electrocatalysts' performances. In this respect, high entropy materials have aroused severe interest recently, thanks to their modified electronic structure via tailorable chemical composition and structural stability even in harsh conditions. Here we synthesized high entropy molybdates via coprecipitation followed by an annealing approach. This electrocatalyst showed good OER catalytic performance with a low overpotential of 276 mV to delivering 10 mA cm^{-2} current density and less Tafel slope of 54.36 mV dec^{-1} . Due to incorporation of more number of metals ensuing the high entropy effect, synergistic effect and modified electronic structure, which beneficial to enhanced active sites, fast electron and mass transport. So this work will be helpful in designing new kind of catalyst materials with enhanced catalytic performance

Keywords: High Entropy Materials, Electrocatalyst, Oxygen Evolution Reaction, and High entropy molybdates



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Excited State Relaxation Mechanism of Red-Emitting Carbon Dots: The Effect of Boron Doping

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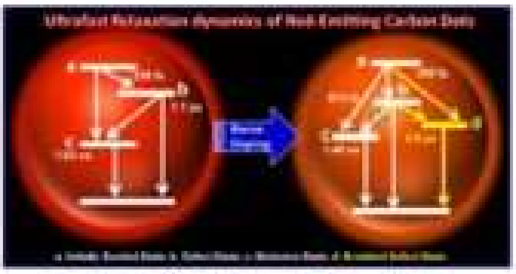
Beginning from their discovery in 2004, the research on carbon dots (C-dots) has stimulated a lot of interest for biomedical and optoelectronic applications for their novel properties. Redemitting C-dots have potential interest for cell labeling and optical imaging due to their higher tissue penetration with minor damage, photostability, and high solubility in aqueous medium. Additionally, they possess high absorption in visible region which is potentially important for photocatalytic applications. Heteroatom doping, especially boron doping modifies the optical properties of C-dots, which are advantageous for electrochemical oxygen reduction, non-linear optics, and sensing. Despite the considerable effort that has been given on understanding the photophysical properties of C-dots, ultrafast excited state dynamics is still unclear and such studies are mostly limited to the blue-emitting carbon dots. Herein, we have adapted a straightforward approach to synthesize red-emitting C dots with and without boron doping and elucidated the excited state relaxation processes using transient absorption spectroscopy (TAS) and global target analysis. XPS study reveals that the relative percentage of pyrridinic nitrogen is increased at the expense of amino nitrogen and graphitic nitrogen after boron doping. For both C-dots, excitation wavelength independent photoluminescence (PL) and mono-exponential PL decay indicates a single emissive state but blue-shifted PL maxima and increased PL lifetime is evident after boron doping. Our detailed analysis of TAS data reveals the presence of three excited state species for the undoped C-dots: initially excited state, defect state and emissive state; whereas, an additional excited state assigned as B-related defect state is formed due to boron doping. This newly emerged state withdraws a significant amount of excited state population and blocks a supply channel for the emissive state. Emissive state's energy is higher after boron doping that accounts for the blue-shifted PL. The initial relaxation process towards the emissive state is slowed down from 317 fs to 750 fs which eventually increases the overall lifetime from 1.03 ns to 1.45 ns in B-doped C-dots. This deep understanding will help to design better artificial light-harvesting systems based on red-emitting C-dots.

Keywords: Carbon dots, Boron doping, Ultrafast Excited State Dynamics.



Carrier Relaxation Dynamics of 2D $CsPbBr_3$ Nanoplatelets: Effect of Monolayer Thickness

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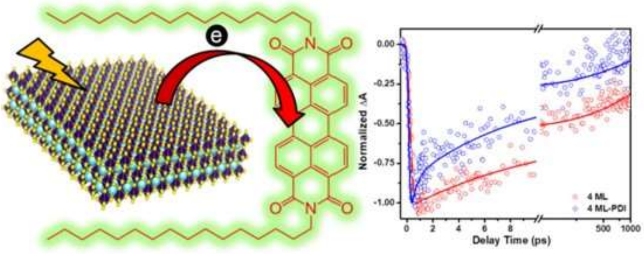
The recent emergence of the quantum confined nanostructures such as two dimensional (2D) colloidal perovskite nanoplatelets (NPLs) has stimulated a lot of interest in developing light harvesting systems because of their engrossing photo-induced properties. However, understanding the exciton dynamics of 2D perovskite NPLs remains largely unexplored as compared to three dimensional (3D) perovskite nanocrystals (NCs). Notably, charge separation and charge extraction are extremely challenging in 2D nanostructures due to strong exciton binding energy. Herein, we investigated the impact of monolayer (ML) thickness on the carrier relaxation dynamics of 2D $CsPbBr_3$ NPLs by employing femtosecond transient absorption spectroscopy. We found that the intra-band cooling time increases from 140 fs to 210 fs with an increase of monolayer thickness from 2 ML to 4 ML, which is a manifestation of the reduced screening of the Coulomb-mediated carrier−longitudinal optical (LO) phonon interaction in the low-dielectric surrounding. In addition, we monitored thickness dependent charge and energy transfer processes from 2D $CsPbBr_3$ NPLs to organic molecular acceptor, namely N,N'-Bis(hexadecyl)-perylene-3,4,9,10-tetracarboxylic acid diimide (PDI) molecule, which follows the order: 4 ML > 3 ML > 2 ML. We unequivocally confirm the dissociation of strongly bound exciton of 2D CsPbBr3 NPLs by the signature of long lived charge separated state (PDI•−). Our analysis shows that the thickness of the NPLs, as a consequence of the quantum confinement and dielectric screening effect, plays a vital role in the charge carrier separation in 2D CsPbBr3 NPLs. This fundamental understanding of the excitonic behaviour of the 2D CsPbBr3 NPLs will pave the way to develop 2D perovskite-based photovoltaic devices.

Keywords: Perovskite, Nanoplatelet, Carrier Dynamics, Transient Absorption Spectroscopy



ICANN2021 **ID: G1047**

Co-decorated Tellurium Nanotubes for Pseudocapacitors

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Metal chalcogenide have been extensively used and proven to be most promising in storage devices since it provides good electrical conductivity, affluent electrochemical redox reaction, better cyclic stability with easier diffusion of both electron and electrolyte ions.[1,2] Transition metal oxides, sulphides and selenides have been well investigated and reported to show high specific capacitance.[3] However, transition metal tellurides are still new to this field and been recently studied for supercapacitor applications. Tellurium (Te) is a p type semiconducting material with a narrow bandgap of 0.35 eV. Te has a highly anisotropic growth tendency with unique helical chains providing its growth along one direction.[4] Tellurium can act as a self sacrificing template to grow one dimensional metal telluride which can show promising application in the field of energy storage providing high conductivity developed from synergistic effect. We followed simple efficient and wet chemical strategies for the synthesis of cobalt (Co) decorated over Te nanotubes (NTs), and fundamental investigations of the material in the performance of supercapacitor applications. The synthesized one dimensional Te NTs were in-depth characterized by spectroscopic and microscopic tools such as UV-visible, XRD, XPS, FESEM, HRTEM and EDX analyses. The assemble of CoTe-2//AC achieved excellent energy density of 51.1 Wh Kg^{-1} at power density of 2294 W Kg^{-1} confirmed that the as synthesized Co-decorated Te NTs to be an excellent electrode material.

Keywords: Supercapacitor, Tellurium, Cobalt, Nanotubes, Template

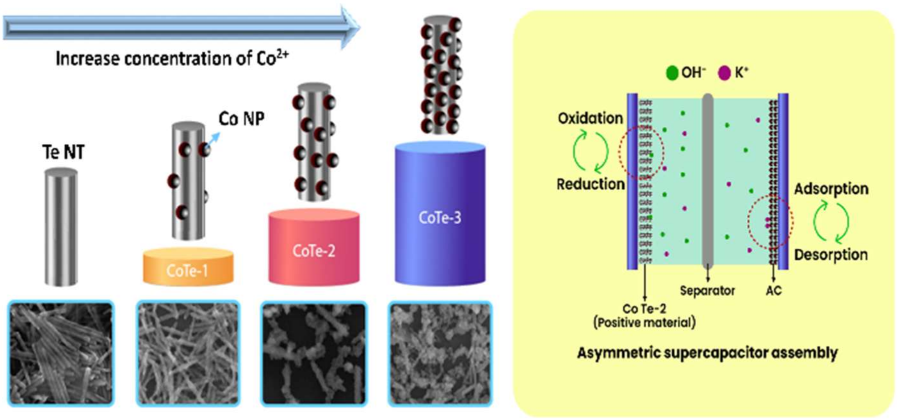

Figure . Schematic illustration of growth of Co-Decorated Te NTs for Assymetric supercapacitor.

Fabrication of Pressure-Responsive Energy Device from Nanofluidic Vanadium Pentoxide and Polymeric Hydrogel

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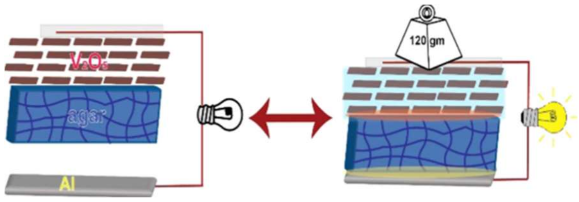
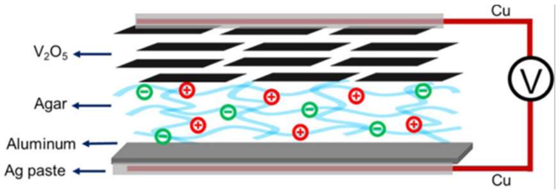
Owing to their unique advantages like environmental compatibility, low cost, and high energy density, metal− water batteries are gaining a great deal of attention. The principles of metal−water batteries were applied here to develop a sustainable pressure-responsive energy delivery system. Application of a gentle pressure of 56 kPa on agar and a glycerol-based hydrogel membrane sandwiched between the aluminum foil and the nanofluidic V_2O_5 membrane (Al-gel-VO device) generates open circuit voltage up to 1.3 V accompanied by an output current of 85 μA (power density = 0.45 W m^{-2}). The output power of Al-gel-VO can be further improved by tuning parameters like lateral dimensions of the layers, applied pressure, and ionic conductivity of the gel membrane. Remarkably, under ambient conditions, the hydrogel and V_2O_5-based devices can provide a constant potential difference up to five consecutive days. Unlike typical humidity powered energy systems, the energy output of the current device is resistant to the diurnal variations in environmental conditions. Remarkably, both gel and V_2O_5 membranes can be completely regenerated after damage caused by prolonged use or accidents without any deterioration in the energy efficiencies. Moreover, the Al-gel-VO devices can also be connected in series (or parallel) to add up the voltage (or current) values of the individual devices

Keywords: energy harvesting, pressure-responsive, vanadium pentoxide, agar gel, self-heal





Copper Sulfide Nanostructures: Synthesis and Photocatalytic Activities

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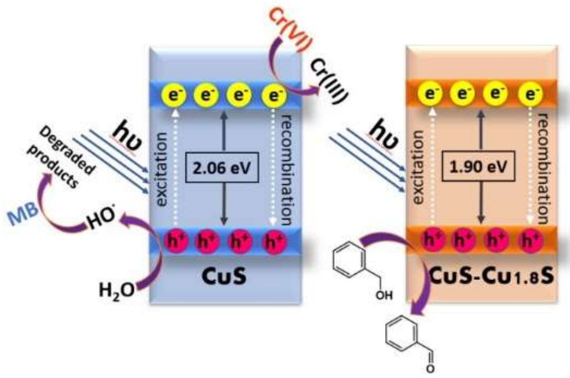
Multifunctional and eco-friendly photocatalyst is the demand of 21st century for a sustainable living without compromising its efficiency and activity. A low cost, greener and versatile nanomaterial was developed as a bifunctional catalyst for the synthesis of industrially concerned benzaldehydes and removal of water pollutant. Pure (CuS) and mixed phase copper sulfide (CuS-Cu1.8S) nanostructures were designed through a simple and green protocol through hydrothermal route. Sodium dodecyl sulfate in the synthesis is employed as the growth directing reagent to obtain hexagonal nanoplates and broken nanosheets. The optical study revealed the UV-visible absorption in the near UV and visible region with band gap of 2.06 and 1.90 eV for pure and mixed phase copper sulfide respectively. The synthesized pure hexagonal covellite CuS turned out to be highly efficient in the removal of water pollutant (MB degradation and Cr(VI) reduction) while the mixed phase exhibited photocatalytic conversion of benzyl alcohols to corresponding benzaldehydes with ~99% selectivity.

Keywords: Bifunctional, copper sulfide, photocatalyst, benzaldehyde



Ultrafast Carrier Relaxation Dynamics in 2D CdSe Nanoplatelets for Photodetector Applications

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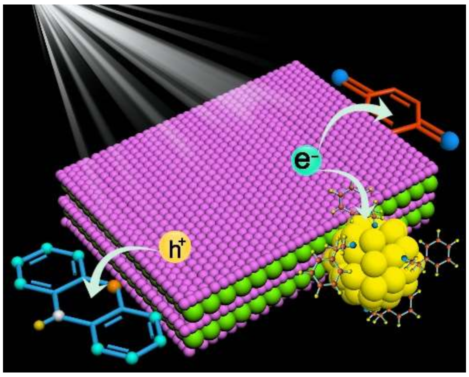
Two-dimensional (2D) atomically thin colloidal semiconductor nanoplatelets (NPLs) have recently emerged as a novel nanostructure exhibiting several unique photophysical properties such as large absorption cross-section and high exciton binding energy, very narrow emission line-width, tunable emission, high molar extinction coefficient, and high photo-stability. Designing of hybrids or heterostructures and understanding the ultrafast carrier dynamics is essential for optoelectronic and photocatalytic applications. We have designed heterostructure/hybrids based on 2D CdSe NPLs with metal nanoclusters and molecular acceptors. Transient absorption spectroscopy depicts ultrafast electron/hole transfer and the presence of radical ion in the transient absorption signal, confirming the efficient charge separation between CdSe NPLs and metal nanoclusters/molecular acceptors. The devices exhibit more considerable photocurrent enhancement, higher responsivity, detectivity than pure NPLs based devices. It holds promise for the future design of 2D NPLs-based materials for optoelectronic applications.

Keywords: 2D nanoplatelets, CdSe NPLs, Ultrafast charge transfer, Photodetectors.



Remarkable Rate of Water Evaporation through Naked Veins of Natural Tree Leaves

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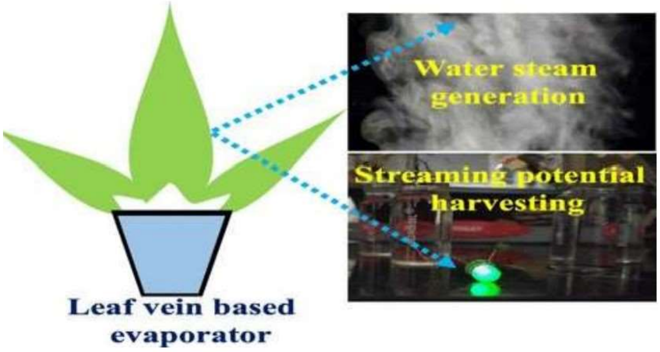
In the form of leaves, nature designs the finest photothermal evaporators, and the tremendous evaporation efficiency of leaves is supported by a precisely designed network of veins. Here, we have demonstrated that the vein network of a natural leaf can be extracted through a simple water-assisted digestion process and exploited for low-energy steam generation. The naked leaf veins exhibit a remarkable flux (evaporation rate, 1.5 kg·m–2·h^{-1}) of capillary evaporation under ambient conditions (25 °C and 30% RH), close to the photothermal material-based evaporators reported in the recent literature. Even inside a dark box, naked veins exhibit an evaporation rate up to 4.5 kg·m–2·h^{-1} (at 30% relative humidity (RH) and a wind speed of 22 km·h^{-1}). The mechanistic studies performed with variable atmospheric conditions (temperature, humidity, and wind speed) suggest the evaporation process through the naked veins to be a kinetic-limited process. Naked veins with remarkable evaporation efficiency are found to be suitable for applications like water desalination and streaming potential harvesting. Experiments with the naked veins also unveiled that the biofluidic channels in leaves not only exhibit the characteristics of surface charge-governed ionic transport but also support an exceptional water transport velocity of 1444 μm·s^{-1} .

Keywords: Biochannels, water stream generation, salt desalination, streaming potential harvesting.



Light Assisted Bond Activation by “Hot Electrons” at Room Temperature

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Plasmonic nanomaterials can couple their electron density with electromagnetic radiation by localized surface plasmon resonance (LSPR) which results in absorption of light energy by these nanomaterials[1,2]. The relaxation of LSPR, generates hot charge carriers, which drives chemical reactions on the nanoparticle's surface. Chemists have used this property of nanoparticles to discover new and selective reaction pathways. However, the number of metals that exhibit LSPR in visible light is restricted, limiting the types of reactions that can be catalyzed

The multicomponent catalyst idea, known as the "antenna-reactor" system[3], in which a plasmonic metal "antenna" is kept near a non-plasmonic catalytic metal "reactor," can be utilized to overcome this problem. The light energy is harvested by the LSPR active “antenna”, which results in polarization of the “reactor” due to an intense electric field around it. This causes plasmon to form on the non-plasmonic metal, resulting in the generation of hot charge carriers. Charge transfer from the “antenna” to the “reactor” is also a possibility.

For optimal light energy utilization, the "antenna" should absorb the whole broadband solar spectrum. A recently reported novel material from our group known as dendritic plasmonic colloidosomes (DPCs), also known as “black gold” (DPC-C4)[4], can be an ideal candidate for an antenna. The Au nanoparticles supported on the nanosilica (DFNS)[5-9] have heterogeneous particle size distribution and varying interparticle distances, which results in its broadband light absorption property from the visible region to the near-infrared region.

In this work, we deposited Ni nanoparticles on black gold to get DPC-C4-Ni, in which Au nanoparticles will act as “antenna” and Ni nanoparticles will serve as “reactor”. The hot electron transfers from Au to Ni nanoparticles under light irradiation and the intense electric field around the Ni nanoparticles resulted in the activation of molecules adsorbed at Ni sites. We then explored DPC-C4-Ni for several challenging reactions like H_2 dissociation, C-Cl bond activation, and hydrogenation of propene and acetylene at room temperature. DPC-C4-Ni under light irradiation showed exceptional activity demonstrating the "antenna-reactor” concept. The reaction mechanism was explored by i) one-electron reduction of Fe^{3+} to Fe^{2+}, ii) competitive C-Cl bond activation and Fe^{3+} reduction, iii) finite-difference time-domain simulations (FDTD), and iv) ultrafast transient absorption spectroscopy.

Miniaturization of Transition Metal Hydroxides to Hydroxide Dots: A Direction to Realize Giant Cyclic Stability and Electrochemical Performance

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Binary metal hydroxides have tailored to quantum size in situ by manipulating the solvent medium in the co-precipitation process. Bimetallic cobalt-nickel hydroxide dots reveal hydrotalcite structure, and the mean hydrodynamic diameter is restricted to 2.5 nm when Co:Ni molar ratio 1:1. The bandgap values obtain around 2.64 eV using Tauc relation, which is within the quantum confinement region. The fitting results of X-ray photoelectron spectroscopy suggested the presence of redox couple Co^{2+}, Co^{3+}, Ni^{2+}, and Ni^{3+} in the hydroxides dots, which facilitates more electroactive sites. Again, excellent stability of hydroxide dots in solvent medium obtained by measuring T2 relaxation time. The binary dots electrode exhibits excellent pseudocapacitance performance with specific capacitance of 1926 F g^{-1} (221 mAh g^{-1}) at 1 A g^{-1} with outstanding cycling retention of ~96% up to 20 000 cycles. Parallelly, an asymmetric supercapacitor device has been assembled by monitoring different mass loading of active material as +Ve and carbon black as -Ve electrode cells. The ASC device utilizes to brighten a commercial LED to validate the electrode. Also, the specific capacitance of the ASC device has been calculated about 250 F g^{-1} (353 mAh g^{-1}) with a holding energy density of 85 W h kg^{-1}.

Keywords: cyclic stability, dots, electrochemical, metal hydroxides, supercapacitor

Gelatin-Assisted Co-Exfoliation of Graphene Nanoplatelets/MoS_2 via Temperature Control and Its Application in High-Performance Supercapacitors

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Herein, we demonstrate, one step efficient method to prepare low-cost, sustainable, bio-based co-exfoliation of GNP/MoS_2 by using gelatin as a stabilizer and exfoliant. The preparation parameters were influenced by elevate the temperature of the sonication bath, sonication time. The temperature elevation was achieved by the dissipation of the sonic wave and achieved high yield (~2.34 mg ml^{-1}) under the conditions of 12 h sonication at (~60 ° C). Stronger stability achieved greater than 45 days through the maintenance of high temperature. Raman spectroscopy, transmission electron microscopy indicates that co-existence of Graphene and MoS_2. Raman spectra suggest 3-4 layer of graphene and few layer of MoS_2 flakes with lower defects. The as prepared GNP/MoS_2 heterostructure nanosheets via co-exfoliation were further investigated for electrochemical energy storage applications and achieve highest specific capacitance of 311.14 Fg^{-1} at 1Ag^{-1} and the cyclic performance with 95 % initially capacitance maintained after 2000 cycles and the properties is superior to MoS_2 and GNP electrode. Moreover, an asymmetric supercapacitor device (ASC) was fabricated and could powered commercial LED (1.8 V) for 25 min.

Key words: Gelatin, Co-exfoliation GNP/MoS_2, binder free, Cyclic, voltammetry, Supercapacitor

Sputtered Grown Nanostructure Transparent Thin Film Oxide for Energy Storage Application

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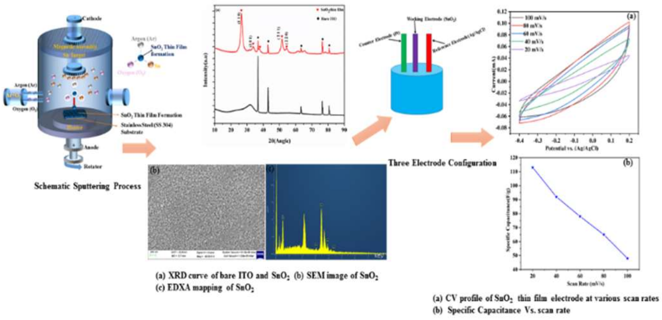
Recently, oxide-based nanostructured materials are extensively used in numerous energy storage applications such as supercapacitor, batteries etc. because of their fascinating electrical and chemical properties. Here, in the present work we have deposited a transparent nanostructured thin film of SnO_2 using reactive DC magnetron sputtering by maintaining high vacuum level for the enhancement of energy storage application. The SnO_2 thin film was grown on ITO substrate at temperature of 200°C for 30 minutes using gas ratio 1:2 of Ar and O_2. The SnO2 thin film was characterized by XRD (X-ray diffraction), SEM (Scanning electron microscopy), EDXA and its electrochemical properties. XRD help to reveal the crystal structure of deposited thin film of SnO_2 (JCPDS No.00-005-0467). SEM study showed the thickness and confirmed the nanosphere like morphology of transparent SnO_2 thin film. The composition of transparent SnO_2 thin film was confirmed by EDXA which is attached with SEM. Further, the electrochemical analysis was done for transparent Sno_2 thin film electrode using three electrode configuration. Here, in Ag/AgCl taken as reference electrode, thin film electrode material taken as working electrode and Pt (platinum wire) as counter electrode respectively. The CV (cyclic Voltammetry) test was done using 1 M aqueous KOH electrolyte solution at various scan rate of 20 to 100 mV/s with voltage window of -0.2 to 0.4 V. There is no oxidation and reduction peaks found in CV profile which indicates the pseudo- capacitive behaviour of transparent thin film electrode. It could be found that at low scan rates specific capacitance (Cs) of active electrode increase with integral area of CV curves. The specific capacitance of SnO_2 transparent thin film electrode was found to be 113 F/g at scan rate of 20 mV/s.

Keywords: Metal oxide, sputtering, cyclic voltammetry, SEM, XRD



Nanotechnology for Bioenergy

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Today's urbanization and industrial demands of energy is growing to greater eights. It's not possible to meet both the ends of the supply and need. Biofuel is the solution which can solve this ever growing thirst. Various types of biodiesel are in the market satisfying the demands of the stakeholders. Blends of biodiesel are always preferred. Sustainable long term production of biodiesel is essential. Nanoparticles can increase the efficiency of fuel. At the same time, use of NP in biodiesel production can make the process cost effective. It is helpful in reducing the harmful emission from diesel engines. Application of np in biofuel production is reviewed in this paper. Such np based biofuel reduces the brake specific fuel consumption, increases the brake power with enhancement in the combustion process. HC, CO and PM in the diesel engine get reduced considerably. It can be concluded that addition of NP with biodiesel blend is always useful for better performance and emissions control.

Key words: Nanoparticles, biofuel, emissions, biodiesel blend.

Simulation of Bifacial Heterojunction Solar Cells with Gradient Doping Using Afors-Het

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Since the discovery of solar photovoltaic effect in 18th century, at present, this technology has reached to an output efficiency of 24.7% out of 29.43% of its theoretical limit using the heterojunction solar cell structure. The main focus is to improve the solar cell efficiency and reduce the production cost. This work on solar cells focuses on the heterojunction structure with bifacial model to obtain the optimum efficiency. The role of different layers of the heterojunction solar cell and the effect of various parameter variation on the output is studied by simulation model using AFORS-HET.

The simulation tool, AFORS-HET offers the numerical simulation of homojunction as well as heterojunction devices by solving the one-dimensional semiconductor equations in steady-state and also the small sinusoidal ac-perturbations. In this study we have simulated a bifacial solar cell (TCO/a-Si:H(p)/a-Si:H(i)/c-Si(n)/ a-Si:H(i)/a-Si:H(n+)/TCO/Ag).[2] The parameter variations such as emitter layer thickness, uniform vs gradient doping of emitter layer and back surface field layer, and the introduction of texture in the front transparent conducting oxide (TCO) layer were studied and their effect on open circuit voltage, short circuit current density, fill factor and efficiency were observed.

It is observed that with the increase in the emitter layer thickness, the efficiency of the solar cell decreases. The best results were obtained with emitter layer thickness of 3nm with gradient doping. However, the gradient doping of the back surface layer has not affected the performance of the solar cell. Furthermore, the texturization of the front TCO layer has also contributed a significant increase in the solar cell performance. The best outcome of output efficiency of 16.37% is obtained with the fill factor of 81.93%. At this efficiency the open circuit voltage of 613.7 mV and short circuit current density of 32.56 A/cm^2 is observed. The best model parameters are given in the table below:

Fabrication of solar cell is a very expensive and resource consuming process due to which we cannot use hit and trial methods to obtain best output results. This simulation work can provide the optimum values of various parameters like layer thickness, doping levels, etc. in the solar cell for the best possible output results in terms of open circuit voltage, short circuit current, fill factor and efficiency. therefore, the cost of redundant fabrication of solar cells can be saved.

Scalable Drop-to-Film Condensation on a Nanostructured Hierarchical Surface for Enhanced Humidity Harvesting

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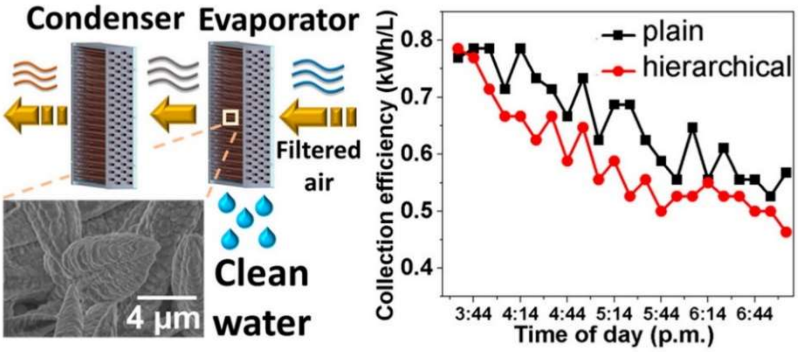
Active cooling-based atmospheric water generators, despite their growing demand, continue to be energy intensive and offer poor collection efficiencies (energy consumption per liter of water production). Despite progress in micro-/ nanofabrication techniques and functional coatings, advanced surfaces have not been successfully scaled onto such harvesters to accelerate condensation and improve their efficiencies. Here, we present a scalable dual-nanostructured hierarchical surface that comprises sporadically distributed bundles of randomly oriented faceted microcones having facets composed of nanostructures, which are either bumps or ridges. Condensate removal on this surface occurs via drop-to-film coalescence, followed by film shedding in the form of macrodrops. Compared to a conventional plain metal surface used for condensation, the improvement in latent heat transfer coefficient using a hierarchically textured surface ranged from 19.9% at a subcooling of ~8 °C to 1048.4% at a subcooling of ~1 °C in laboratory scale experiments, subcooling being defined with respect to the dew point. To demonstrate utility at industrial scale and to ensure scalability of the modified surfaces, we create a prototype assembly comprising a tube-fin heat exchanger with hierarchically textured fins, cooled using a standard refrigeration cycle, producing ~25 L of water per day. The prototype containing hierarchically textured fins provides ~10.8% enhanced water collection at ~10.4% improved average collection efficiency compared to the traditional water generator when tested in outdoor conditions.

Keywords: condensation, heat transfer, hierarchical nanostructures, water harvesting, drinking water



Development of Biotin Conjugated Carbon Dots from Chitosan and Silk Fibroin Blend for Target-Specific Delivery of Antitumor Agents

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In this study, we have developed a highly fluorescent, tunable, primary amine-functionalized Carbon dots (CDs) using LMWC and SF blend. CDs have been a promising theranostic tool with high biocompatibility and a tailorable fluorescence profile. The size of the synthesized CDs was obtained to be quasi-spherical in shape with a size of 3 ± 1.5 nm, thus capable of penetrating cells. It was observed that the CDs formulated using the blend possess high fluorescence intensity and quantum yield compared to the CDs prepared from blank LMWC and SF. The live-cell imaging on MCF-7 cell lines showed bright blue fluorescence with increased internalization of the conjugated CDs compared to normal cell lines, also investigation in two different human carcinoma cell lines, MCF-7 and HeLa showed potent cytotoxicity for 5-FU loaded conjugated CD as compared to normal HEK-296 cell lines due to biotin receptor-mediated endocytosis. The drug encapsulating efficiency, fluorescence properties, and target specificity proves the efficiency of the synthesized biotin-conjugated CDs to act as an effective nanotheranostics tool.

Keywords: Chitosan; Carbon dots; 5-fluorouracil; Silk fibroin; Low molecular weight chitosan

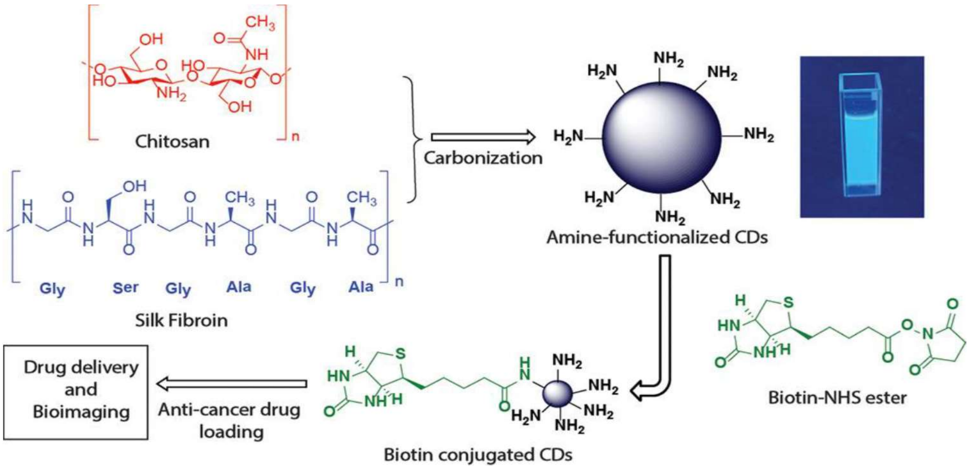

Figure : Synthesis process of 5-FU loaded biotin-conjugated CDs.

Control of Glucose-Induced Degradation and Cargo Release in Multi-Responsive Polymer Hydrogels

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Drug release from hydrogel under physiological conditions is challenging for the state-of-the-art in therapeutics. Specifically, splendid hydrogels fit for glucose-responsive arrival of hostile to diabetic medications are of tremendous continuous interest. Despite the new turns of events, there is a requirement for more glucose-detecting hydrogel that holds the properties in a wide extent of pH environment. In our hydrogel system, we report an easy and summarized production of hydrogel system responsive to different stimuli (pH, glucose, and hydrogen peroxide)- responsive hydrogels. Here, a Poly(vinyl alcohol) is crosslinked with three bis-boronic acids benzene-1,4-diboronic acid (1,4-BDBA), 4,4′-biphenyldiboronic acid (4,4′-BPDBA), tetrahydroxydiboron(THDB). These hydrogels containing water are also incorporate macromolecular cargo/drugs participate in the structure. Wide logical assessments recommend that hydrogels produced from 1,4-BDBA, 4,4′-BPDBA show degradaion under all stimuli. However, THDB crosslinked hydrogel doesn't degrade under pH or glucose environment. This unusual property allows the fuse of glucose oxidase(GOx) in the hydrogel network that concedes the glucose responsiveness for THDB crosslinked hydrogel. Finally, the glucose-specific appearance of macromolecular cargo/drugs is displayed in a glucose oxidase containing Polymer/THDB hydrogel in the physiological condition. The hydrogel developed in this will open better approaches to foster a glucose-specific material for the on-request release of drugs.

Keywords: Stimuli-responsive hydrogel, glucose-responsive material, smart insulin release

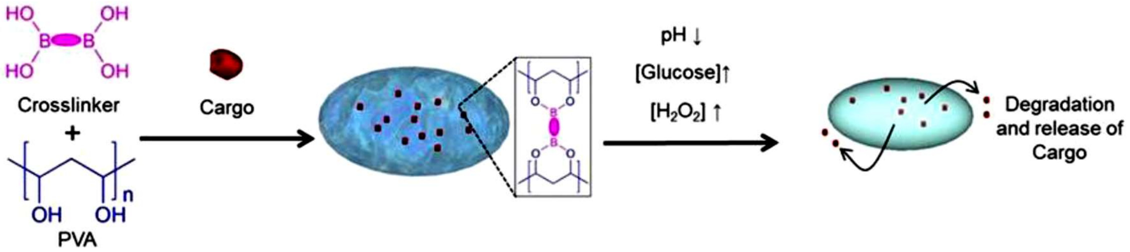

Figure: Schematic representation of the multi-stimuli responsive hydrogel. PVA chains are crosslinked with bis-boronic acid molecules to create a matrix for drugs encapsulation. The hydrogel undergoes degradation and releases cargo as chemical stimuli (low pH, glucose, and hydrogen peroxide) selectively break bis-boronate linkages.

Designing BF_2 complexed Smaragdyrin Dye Loaded Liposomes for NIR Triggered Photothermal Therapy Towards a Nanotheranostic Agent for Cancer Treatment

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Understanding the characteristics and unique features of a therapy helps to develop a better insight of the treatment required to deal with any disease. With the increasing stats of death tolls and number of cases being reported each year for cancer, affordable treatment and diagnosis options have to be devised to cover the larger section of population. Multifunctional modalities that can simultaneously provide therapy and diagnosis for cancer seems to be an assurance with more personalized, precise, effective and affordable treatment.

Photothermal therapy (PTT) has gained significant interest along with Near Infrared based non-invasive imaging and has come up as a promising area lately to provide real time imaging along with thermal ablation for cancer tumour. Using the fluorescent dyes encapsulated in nanomaterials for anti-cancer therapy is currently a hot topic for cancer theranostic research. Nanomaterials that can act as both the tracker and the photosensitive agent, can serve the dual purpose for cancer nanotheranostics. Also, functionalisation of the nanomaterials will aid in actively targeting the tumour site in the body and increasing the percentage accumulation of the formulation at the desired location thereby. This capability of nanotheranostic platforms that products can be developed to exploit the therapeutic potential of the active compound, and also improve the safety and efficacy of that multifunctional composition are proving to be more promising for locally guided imaging and hyperthermia based clinical applications.

Herein, we report the detailed study of synthesis, optimization, characterization and *in-vitro* evaluation of liposomes loaded with novel organic BF_2 complexed smaragdyrin dye nanoformulation. This lipid based nanoformulation has shown high biocompatibility and hemocompatibility with high photothermal conversion and transduction efficiency that is efficient in killing the cancer cells. Photostability of dye enables us to provide the laser therapy multiple times, if needed for providing higher therapeutic efficiency. Also giving an edge to use this as a combinational therapy with conventional chemotherapy, surgery and radiation therapy. Furthermore, these results have opened doors to explore the efficacy in the animal models. The talk will be focusing various detailed aspects of this works along with the potential of translating this treatment approach with minimalistic requirements towards the final nanotheranostic product.

Keywords: Photothermal therapy, non-invasive imaging, photosensitive agent, nanotheranostic.

Gold Nanoparticles Capped DHPMs for Meliorate Detection of Antiretroviral Drug: Azidothymidine

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3’-Azido-3-deoxythymidine (AZT) commonly known as Zidovudine is majorly used as a drug to delay the development of HIV virus causing AIDS. Its side effects include the blockage of certain human polymerase enzyme, including mitochondrial DNA polymerase, So AZT treatment can lead to destroy muscle cells and heart cells also. AZT also suppresses the production of red blood cells, neutrophils, and other cells in the bone marrow, causing symptoms such as fatigue, malaise, and anaemia. Because of the various side effects of AZT which are life threating, an economic and ready to use sensor was prepared for the selective detection of AZT. We found a way in multicomponent reaction to selectively sense the concentration of AZT by preparing organic nanoparticles. Further these organic nanoparticles were coated with gold to improve the limit of detection by 14 nM. The sensing system was prepared and performed in aqueous medium to reduce the use of organic solvent in detection. The sensing ability of the developed probes was checked by using UV-visible spectrometer, cyclic voltammetry and circular dichroism. Quantification in AZT capsules supplied to HIV patients was performed which gives the recovery percentage of 97%

.**Keywords:** Azidothymidine, Dihydropyrimidinedione, Biginelli reaction, gold nanoparticles, Chemosensor.

Benzimidazolium-Calix Coated ZnO Nanoparticles: Sensor for Selective Recognition and Abasement of Azinphos-methyl

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Nowadays, organophosphorus pesticides in agriculture field remains a life-threatening problem on the health of living beings. These organophosphorus pesticides show toxicity by inhibiting the activity of Acetylcholinesterase enzyme (AChE), that helps in hydrolysing acetylcholine neurotransmitter into choline and acetic acid. As due to increasing mandate of hazardous pesticides for harmful, there is rapid increase in these toxic substance in the environment, and thus we need to develop an effective method to detect the level of these toxic substance with high selectivity. In the present context, we fabricate the ZnO nanoparticles with benzimidazolium group of R1 have high affinity towards phosphordithioate group, enhance the detection affinity of present sensor R1@ZnO. The surface modification of hybrid nanomaterial was confirmed by SEM, TEM, FTIR, PXRD. The R1@ZnO was further utilized for the selective detection and degradation of Azinphos methyl (AZM) in H_2O : DMSO medium. This sensor needs only 2 µL of analyte for the detection and the limit of detection was 69 nM calculated by 3 sigma methods. The AZM is further degraded into non-toxic products which was analysed by mass spectroscopy. Real time application of R1@ZnO was carried out by selecting field water, citrus fruits and vegetable as real sample, displays that the prepared solution was up to the task in the estimation of AZM in the collected samples

.**Keywords:** Azinphos-methyl, Benzimidazolium-calix, ZnO nanoparticles, Fluorometric sensor.

A Biginelli-Azophenol Based Robust Sensor for Rapid Diagnosis of Cyanide in Real Samples

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The self-aggregation of multifunctional Biginelli-azophenol (**Ligand1**) in water (**ONPs**) led to sensitive and selective detection of toxic pollutant cyanide in an aqueous medium and solid matrix. The origin behind the excellent sensing performance of **Ligand1** is assessed by ^{1}H NMR spectroscopy which confirmed the deprotonation of OH and simultaneous H-bond formation by cyanide with NH of **Ligand1**. Furthermore, the UV–Visible absorption titration studies resulted in two isosbestic points at λ_{max} 399 nm and 314 nm, which also confirmed the complex formation between **Ligand1** and CN^- with the detection of the lowest concentration of cyanide at 14.5 nM. Additionally, the colorimetric detection was supported by RGB color quantification as well as a thin column impregnated with **Ligand1**, which gives high-performance on-site cyanide detection in real water samples. Remarkably, such a cost-effective, robust colorimetric sensor having several key features, offered novel opportunities for real-time cyanide monitoring in polluted water and hence, this makes it unique among the other reported sensors for the same

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In-situ Polymerized Electrospun Nanofibers for Breath Humidity Sensing

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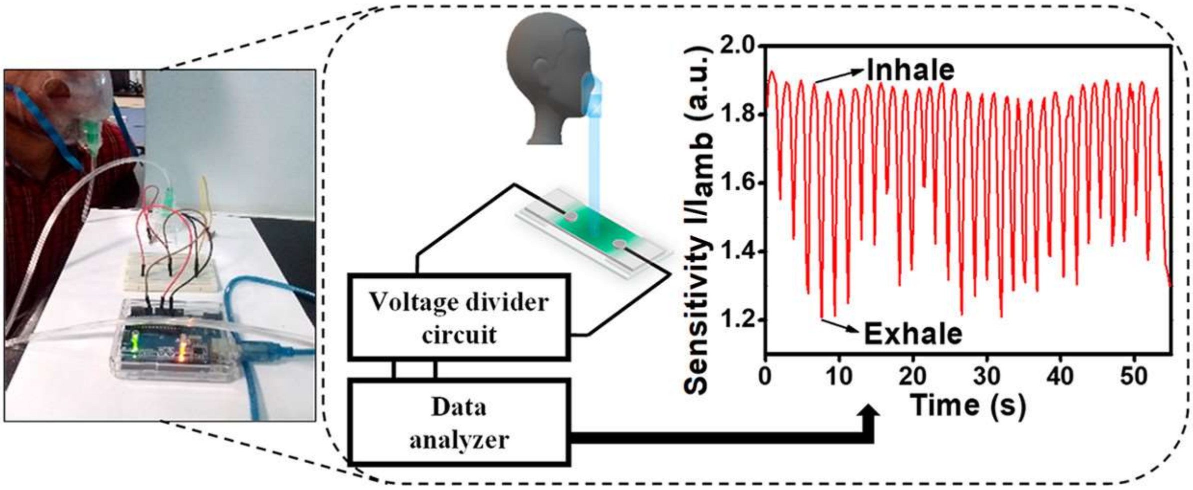
As wearable electronics have gained momentum in the past few years, there is a dire need for smart, responsive, and, most importantly, affordable sensors for biological monitoring. One such noninvasive method to gauge body metabolism is via breath analysis. In a successful attempt to sense and record relative humidity levels (%RH) in nasal and oral breath, this work presents an economical route to fabricate a wearable humidity sensor with high sensitivity and a response time of ~1 s. The sensor consists of a flexible backbone of electrospun poly(vinylidene fluoride)/reduced graphene oxide (PVDF/rGO) nanofibers which have been selectively sensitized to humidity via surface polymerization of aniline using the inexpensive successive ionic layer adsorption and reaction (SILAR) technique. We report a high sensitivity and a full response range (0 − 95% RH) supported by a low working voltage and minimalistic circuitry as an attractive feature for integration into wearable electronics. Moreover, as the device sensitivity is adequate even up to 95% RH, it is conducive to detect nasal breath and saturated humidity conditions accurately. Apart from humidity the sensor was also sensitive to acetone and ethanol.

Keywords: Humidity sensor, reduced graphene oxide, nanofibers, polyaniline, SILAR



Highly-Sensitive As^{3+} Detection using Electrodeposited Nanostructured MnO_x and Phase Evolution of the Active Material During Sensing

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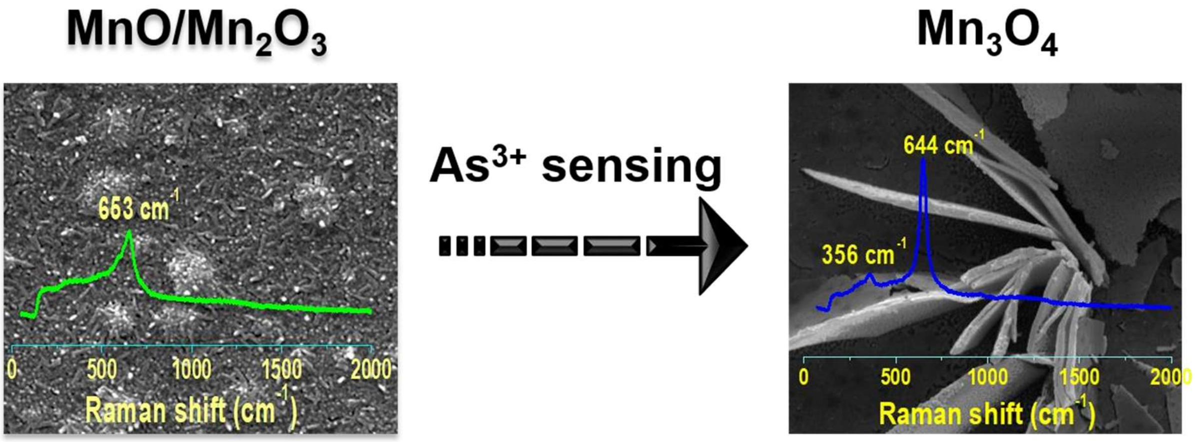
A simple, one-step electrodeposition approach has been used to fabricate MnO_x on indium doped tin oxide (ITO) substrate for highly sensitive arsenic (As^{3+}) detection. We report an experimental limit of detection of 1 ppb through anodic stripping voltammetry (ASV) with selectivity to As^{3+} in the presence of 10 times higher concentrations of several metal ions. Additionally, we report the simultaneous phase evolution of active material occurring through multiple stripping cycles, wherein MnO/Mn_2O_3 eventually converts to Mn_3O_4; as a result of change in the oxidation states of manganese. This occurs with concomitant changes in morphology. Change in the electronic property (increased charge transfer resistance) of the material due to sensing results in eventual decrease in sensitivity after multiple stripping cycles. In a nutshell, this paper reports stripping voltammetry-induced change in morphology and phase of as-prepared Mn-based electrodes during arsenic sensing.

Keywords: arsenic, nanostructured electrode, manganese oxide, electrochemical sensor



Understanding the Mechanism of Sensing in a Conducting Polymer Based Chrono-Amperometry Sensor for Non-Invasive Disease Detection

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Development of ultra-sensitive bio-sensors from bio-compatible materials has been a matter of extensive research for developing non-invasive quick diagnostic tools for health care monitoring. Diabetes mellitus, one of the most common lifestyle related diseases, requires continuous monitoring of the glucose level in the blood. We have designed a poly-pyrrole based biosensor which works on the principle of acetone detection in the breath of the patient as acetone is the biomarker of Type-I diabetes. Poly-pyrrole is used as a bio-receptor to detect extremely low levels of acetone in the range of 1 ppm to 50 ppm. From a range of spectroscopic and RC circuit analysis it was possible to develop an understanding of the electrochemical reaction. On the basis of the analysis we conclude that reaction between acetone and poly-pyrrole proceeds as a typical oxidation-reduction type wherein upon reduction the resistance of the conducting biosensor increases.

Keywords: Bio-sensors, Diabetes, Non-invasive, Chorno-amperommetry, FTIR.

Strategic Shuffling of Clay Layers to Imbue Them with Responsiveness

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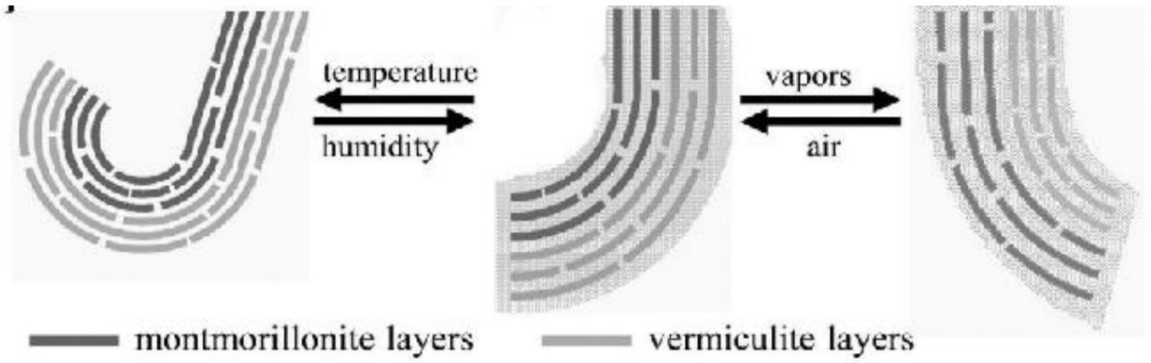
Naturally occurring clays, one of the most abundant minerals on earth, are possibly the most widely used materials. Layers of naturally occurring clay minerals are rearranged to prepare highly sensitive multiresponsive clay–clay bilayer membrane (CCBM). The CCBM introduced here responds to the minuscule changes in the surrounding environments including temperature, humidity, and presence of solvent vapours by morphing in specific manners. Strips cut from CCBM exhibit up to 588 Nkg−1 force output when exposed to temperature fluctuations. Inheriting the natural stability of clay minerals, CCBM demonstrates extreme robustness, heating up to 500 °C, cooling with liquid N2 and exposure to corrosive chemical vapours did not deteriorate its bending performance. Mechanistic studies suggest that shape transformations of CCBM are driven by the unequal response of its components to external stimuli.

Keywords: Soft actuators, Stimuli- Responsive materials, 2D nanosheets, Clay-Clay bilayer, Vermiculite layer.



Application of Reduced Graphene Oxide-Based Actuators for Real-Time Chemical Sensing of Liquid and Vapour Phase Contaminants

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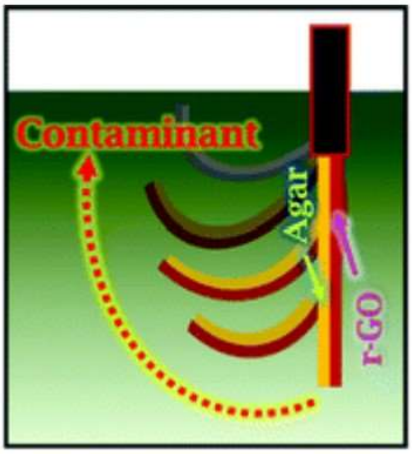
Real-time detection of contaminants dissolved in a liquid medium is critical for various technological and industrial operations. Here, we have demonstrated the possibility of employing reconstructed layered material-based responsive membranes for the in situ detection of chemical contaminants in the liquid phase. A bilayer membrane prepared by sequential vacuum filtration of reduced graphene oxide (r-GO) and agar (r-GO/agar) displayed remarkable responsiveness towards the presence of solvent vapours in their surrounding atmosphere. The shape-morphing property of the r-GO/agar membrane is attributed to unequal changes in the mechanical properties of the individual components. Rectangular strips of the bilayer membrane also displayed shapetransforming properties inside the liquid medium. Depending upon the chemical nature of the molecules, inside the liquid medium, the strips of r-GO/agar membrane bend at a definite speed to adopt a coil-like shape. The original shape of the strip is easily recovered after dipping in water or drying in air. The bending angle and the response time of the r-GO/agar strips were found to be sensitive towards trace amounts of impurities present in the solvent system, which can be exploited for the detection of contaminants in the liquid phase, like trace amounts of water molecules dissolved in acetone or different alcohol molecules dissolved in toluene.

Keywords: Soft actuators, Stimuli-Responsive materials, rGO-agar bilayer membrane, Chemical sensing.



ICANN2021 **ID: K1063**

Detection of Nuclear Hydrogen Peroxide in Living Cells by Carbon Dot-Based Nucleus Targeted Fluorescent Imaging

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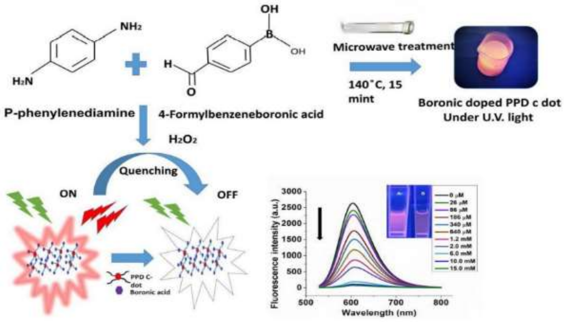
Among various reactive oxygen species (ROS), H_2O_2 is one of the major ROS produced by living cells. Under oxidative stress conditions, intracellular generation of H_2O_2 becomes high which indicates the beginning of inflammation-related various diseases. However, investigation of intracellular generation of H_2O_2 is crucial for preventing various diseases since it is closely linked with different physiological and complex cell signaling pathways. Despite the development of various fluorescent probes, the drawback of the majority of the fluorescent probes is that they cannot move across the nuclear membrane. However, detection of the nuclear level of H_2O_2 is very important since it can directly cause oxidative DNA damage which ultimately leads to various diseases. Therefore, in this study, *p*-phenylenediamine based carbon quantum dots (B-PPD CDs) have been synthesized and integrated with 4-formyl benzene boronic acid as a doping agent for the detection of H_2O_2. The detection mechanism showed that, upon exposure to H_2O_2, the fluorescence of the B-PPD CDs was immediately quenched. Further investigation has been done in the *in vitro* RAW 264.7 cell line by both exogenous and endogenous exposure of H_2O_2 to demonstrate the feasibility of the method. It is shown successfully that the exogenous presence and endogenous generation of H_2O_2 in RAW 264.7 cells can be detected using B-PPD CDs. The limit of detection (LOD) was determined to be 0.242 μM. Thus the synthesis of such fluorescent probes using carbon quantum dots will lead to the practical application in live-cell imaging as well as ROS detection in the nucleus of the cell.

Keywords: ROS, Exogenous, Endogenous, B-PPD CD, Fluorescence, H_2O_2 detection



Scheme: Schematic representation of the synthesis of B-PPD CDs and fluorescent switch on-off sensor for H_2O_2 detection.

ICANN2021 **ID: K1065**

Multifunctional N-Doped Carbon Dots for Bimodal Detection of Bilirubin and Vitamin B12, Living Cell Imaging, and Fluorescent Ink

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A N-doped carbon dot (NCD) has been synthesized via a simplistic one-step hydrothermal technique using L-aspartic acid and 3,6-diaminoacridine hydrochloride. The NCDs exhibit a high quantum yield (22.7%) and excellent optical stability in aqueous media. Additionally, NCDs display good solid-state yellowish-green emission and are suitable for security ink applications. The remarkable fluorescence (FL) properties of NCDs are further applied to develop a multifunctional sensor for bilirubin (BR) and vitamin B12 (VB12) via fluorescence quenching. We have systematically studied the FL quenching mechanisms of the two analytes. The primary quenching mechanism of BR is via the Förster resonant energy transfer (FRET) pathway facilitated by the H-bonding network between the hydrophilic moieties existing at the surface of BR and NCDs. In contrast, the inner filter effect (IFE) is mainly responsible for the recognition of VB12. The practicability of the nanoprobe NCDs is further tested in real-sample analysis for BR (human serum and urine samples) and VB12 (VB12 tablets, human serum, and energy drink) with a satisfactory outcome. The in vitro competency is also verified in the human cervical cancer cell line (HeLa cell) with negligible cytotoxicity and significant biocompatibility. This result facilitates the application of NCDs for bioimaging and recognition of VB12 in a living organism.

Keywords: N-doped carbon dots, bilirubin detection, vitamin B12 sensing, cell imaging, fluorescent ink

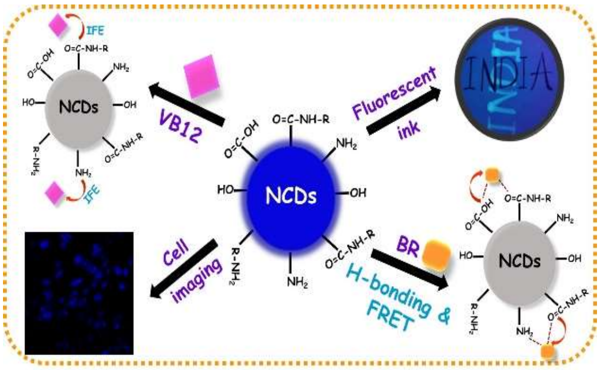

Figure: Blue emitting N-doped carbon dot for highly selective and sensitive detection of bilirubin, vitamin-B12, living cell imaging and fluorescence ink.

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Synthesis of Surface Modified Carbon Nanotube Composite for Environmental Pollutant Sensing Application

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A great deal of research is directed towards real-time monitoring of environmental pollutants as their excessive presence has a negative impact on environmental and human health. With rapid urbanization and industrialization, the need for an affordable, rapid, reliable, and portable gas sensor is of paramount importance. This study reports the fabrication of a room temperature carbon monoxide (CO) sensor based on multiwalled carbon nanotube (MWCNT)-poly(diallyldimethylammonium chloride) solution (PDDA) composite. The surface of MWCNT is functionalized with PDDA, and confirmed with appropriate characterizations. Interdigitated electrodes of silver are patterned on glass substrates, and MWCNT-PDDA composite is used as a sensing material. The electrical conductivity of the sensor changes due to charge transfer from CO to the positively charged quaternary ammonium group present on PDDA. The developed sensors can detect very low concentrations of CO gas ranging from 1 to 20 ppm with high sensitivity and limit of detection (LOD) of 127 ppb. The influence of other interfering gases and volatile organic compounds on the sensor has been investigated. The stability and repeatability of the sensor are examined, and the sensor shows almost stable performance for two months with excellent reproducibility. The sensors have shown excellent potential for rapid CO gas sensing, and they can be used in wearable electronics applications.

Keywords: Carbon nanotubes; Carbon monoxide; Nanomaterial; Sensor

A Banana Peel Derived Heteroatom Doped Green Carbon Dots and Its Reduced Form as an Efficient Fluorescence Sensor for Heavy Metal Ions

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Carbon dots with inherent optical property have diverging application in the fields such as catalysis, bioimaging, therapeutics, photovoltaics, electronics and sensing. Due to their facile synthesis method and tremendous fluorescent property, they have been utilized as a FL probe since last two decades. In the present work, a Co-doped (fluorine, boron and nitrogen) carbon dots (CBP) have been prepared from banana peel and further its reduced counterpart was prepared using $NaBH_4$ as a reducing agent (rCBP). After a thorough and systematic study of various optoelectronic and photophysical properties of two carbon dots they were utilized as an efficient nanosensor. Cobalt, mercury and Monocrotophos are among the wide range of contaminants present in the environment and food products which affects the human health as well as the eco-system. The fabrication of a cost effective and easy to use sensor for various contaminants is the need of the hour to solve our present environment predicaments. Therefore, to solve the present problem a fluorescence turn-off-on model was created. The FL turn-off system for Cobalt ion and mercury ion were static in nature. Importantly, CBP and rCBP have shown a highly sensitive and selective behaviour towards Co^{2+} and Hg^{2+} ions respectively by responsive fluorescence turn off behaviour. Monocrotophos, a pesticide was found to be responsible for the turn-on mechanism for both the system. The limit of detection was calculated to be 75.11nM and 190 nM for Co^{2+} and Hg^{2+}. The developed sensor was designed for Co^{2+} and Hg^{2+} and Monocrotophos sensing.

Keywords: Carbon dots, fluorescence, Metal ions, pesticides.

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White-light-emitting Quantum-dot Complex for Ratiometric Sensing of Long-chain Unsaturated Fatty acids in Commercial Vegetable Oil

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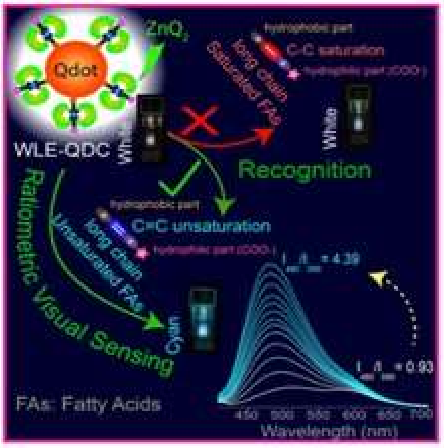
Herein we report a white-light-emitting quantum-dot complex (WLE-QDC) made of orange-emitting Mn^{2+}-doped ZnS quantum dots (Qdots) and a green-emitting zinc quinolato (ZnQ_2) complex to detect long-chain unsaturated fatty acids (LCUFAs; e.g., Na-salt of oleic acid) with a visual color change from white to cyan. Importantly, the WLE-QDC is capable of recognizing LCUFAs from their corresponding saturated forms that make the nanoprobe a suitable tool to determine the quality of commercially available vegetable oils. The WLE-QDC provided a selective, sensitive, and ratiometric visual detection of LCUFAs within the linear range of 4.2-16.6 μM with a limit of detection of 0.127 μM (for example Na-salt of oleic acid). The concurrent hydrophobic and π–π interactions between the ZnQ_2 complex (present in WLE-QDC) and LCUFAs might help in turn-on ratiometric sensing. Extraordinarily, the high selectivity of WLE-QDC towards LCUFAs headed towards their practical application in the quantification of LCUFAs in commercial vegetable oils.

Keywords: Quantum Dots; Quantum Dot-Complex; Ratiometric Sensing; Long Chain Unsaturated Fatty Acids; Vegetable Oils.



ICANN2021 **ID: A1142**

Halide Engineering for Mitigating Ion Migration and Defect States in Hot-Cast Perovskite Solar Cells

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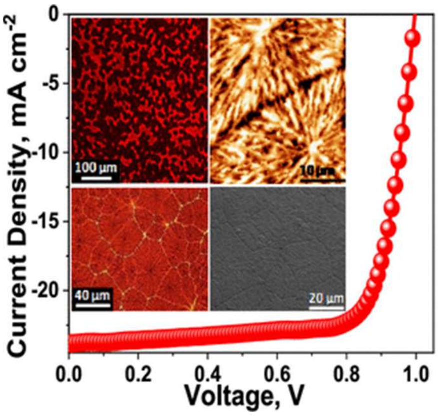
Precise control of perovskite morphology to achieve large-sized grains with small-width grain boundaries is challenging and a pre-requisite for realizing high photovoltaic performance. Ion migration is another problem with perovskites, which hinders the device results. Herein, the incorporation of MABr into the mixed halide perovskite $MAPbCl_xI_{3-x}$ has been carried out to minimize ion migration by replacing the mobile I– ions in the perovskite with Br^-. Moreover, the introduction of MABr results in high-quality and smooth films with large grains of average size ~45 μm. An increasing ratio of MABr was added in the perovskite precursor solution, and devices with the architecture FTO/PEDOT:PSS/Perovskite/PCBM/Rhodamine-101/Ag were fabricated using the hot-casting technique. The device with an MABr ratio of 0.1 (0.1MABr) showed a superior power conversion efficiency of >18% compared to ~14% of the control without any MABr. For higher ratios, the performance deteriorated due to the increase in band gap of the perovskite, which resulted in the reduction of short-circuit current density. For 0.1MABr, minimum defect states and trap density were obtained using various experimental techniques, supporting its optimum device performance. Furthermore, minimum recombination loss took place in the 0.1MABr device. Similarly, the applicability of this technique in large-area devices was studied, and an efficiency of ~17% was obtained, which is the highest in the literature for devices with 2.5 cm^2 dimensions. These innovative concepts and approaches are vital tools to achieve large-area grains for increasing the solar cell performance for commercial applications.

Keywords: Morphology, ion migration, perovskite solar cells, hot-casting, defect states.



➢ Micrometer-size grain, nanometer-size width of grain boundary

➢ Reduced ion migration and hysteresis

➢ Lowered defect states and trap density

ICANN2021 **ID: A1162**

Highly Efficient Purely Organic Triplet Harvesting AIE Photosensitizer for Image-guided Photodynamic Therapy

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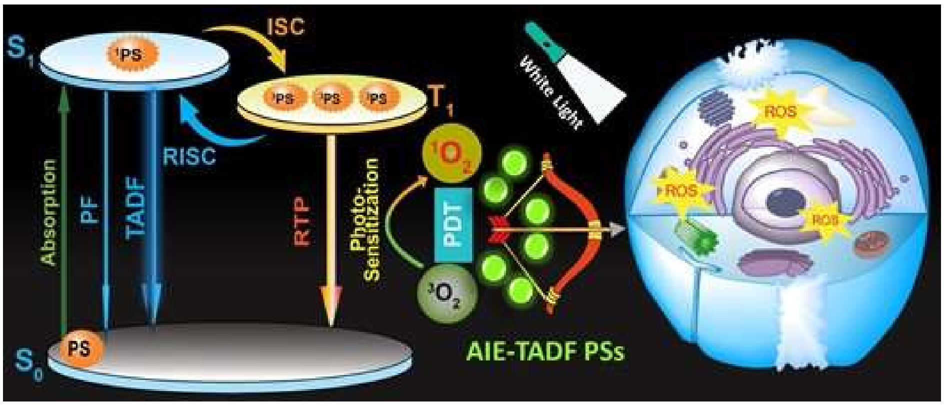
Triplet harvesting image-guided photodynamic therapy (PDT) has been acknowledged as one of the most representative strategies for cancer and other diseases, owing to its precision, non-invasiveness and improved imaging. Unlike, conventional fluorescence molecules with lower sensitivity and hinder high-resolution imaging with cytotoxic heavy metal ion containing metal complexes based photosensitizer for PDT study, here, we formulate purely organic triplet harvesting photosensitizer (PS) BTMCZ, BTMPTZ and BTMPXZ exhibiting thermally activated delayed fluorescence (TADF) and room temperature phosphorescence (RTP) with aggregation induced emission (AIE) characteristics. Remarkably, integrated PSs could generate reactive oxygen species (ROS), singlet oxygen ($^1O_2$) under white-light irradiation to kill the cancer cells efficiently. In addition, the molecules are self-assemble into nanoparticles/ nano-ribbons and accumulate homogeneously in the cancer cells thereby a high-resolution imaging was recorded. This novel photosensitizer could be a good candidate for cancer treatment in clinical practice.

Keywords: Aggregation Induced Emission; Delayed Fluorescence; Phosphorescence; Photodynamic Therapy.



ICANN2021 ID: G1141

Surface Recrystallized Stable 2D–3D Graded Perovskite Solar Cells for Efficiency Beyond 21%

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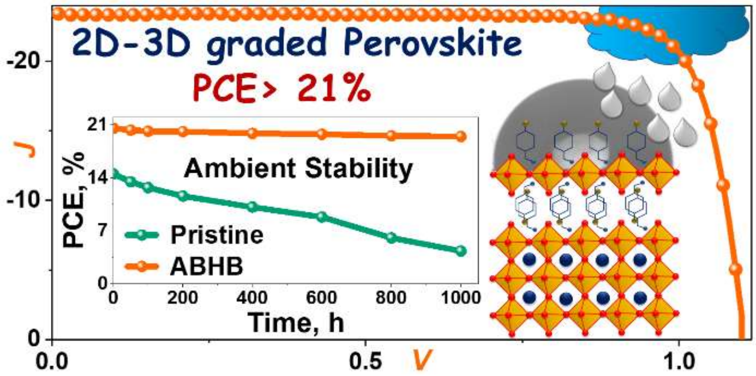
Recently, organic–inorganic hybrid perovskite solar cells (PSCs) have experienced a rapid growth in terms of efficiency. However, the instability of hybrid perovskite materials towards ambient conditions restricts their commercialization. Formation of a thin layer of 2D perovskite over a 3D structure has now boosted the strategy to improve the perovskite stability. This 2D–3D heterostructure enables improved light harvesting properties and enhanced carrier transport of the 3D perovskite along with augmented ambient stability due to the capped 2D layer. Herein, we demonstrate the untapped potential of the surface recrystallized 2D–3D graded perovskite fabricated with the surface treatment of the strategically synthesized multifunctional 4-(aminomethyl)benzoic acid hydrogen bromide (ABHB) molecule. In particular, the bromide ions fill the halide vacancies in the perovskite lattice, while the amine groups and the carboxylic acid functionality significantly minimize the defect states and reduce ion migration. Consequently, ABHB treatment delivers outstanding efficiencies of 21.18% (for a small-area device – 0.12 cm^2) and 18.81% (for a large-area device – 2 cm^2) as well as negligible hysteresis. Furthermore, the capped 2D layer restricts moisture penetration into the perovskite layer because of improved hydrophobicity and significantly enhances the ambient stability of PSCs.

Keywords: Perovskite solar cells, 2D–3D heterostructure, surface recrystallization, outstanding efficiency, high stability



ICANN2021 ID: K1108

Conjugated Polymer-Based Electrical Sensor for Ultra-trace Vapor Phase Detection of Nerve Agent Mimics

Nehal Zehra[a], Anamika Kalita[b], Akhtar Hussain Malik[a], Ujjwol Barman[b], Mohammad Adil Afroz[a] and Parameswar Krishnan Iyer[a,b*]

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Considering the need to strengthen the national security from chemical threat, we presented a low-cost electrical sensor for monitoring the ultra-trace level of nerve gas agent in a realistic conditions. A conjugated polymer, Poly(3-(9,9-dioctyl-9H-fluoren-2-yl)benzene-1,2-diamine) PFPDA was synthesized via Suzuki cross-coupling polymerization and has been used as a sensory layer to fabricate the two terminal gas sensor device. The gas sensor shows excellent sensitivity towards Diethyl chlorophosphate, a nerve gas mimic with a limit of detection limit 5.88 ppb. The sensor device is very rapid in detecting the DCP vapor as it shows a fast response within 3 sec. The amine moiety of PFPDA CP plays a vital role in redox interaction between the semiconductor CP and organophosphates, which ultimately leads to the amplified current signal. Furthermore, PFPDA fabricated device is incorporated with an electronic prototype using a combinational circuit of Operational Amplifier (OPAMP) and logic AND gate for onsite detection of DCP vapor with the visual alerts from LED and alarm sound signal. The designed electronic model produces rapid, precise and decisive output independent of human error and thus offers fast onsite detection of nerve agent with high degrees of accuracy in milliseconds.

Keywords: Conjugated Polymer, Electrical Sensor**,** Nerve Agent, Portable, Onsite-Detection

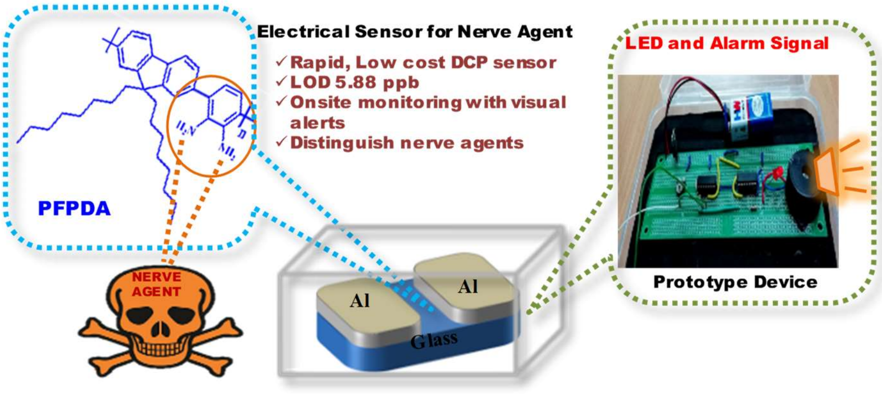

Figure 1: Table of Content (ToC) for Conjugated Polymer-Based Electrical Sensor for Ultra-trace Vapor Phase Detection of Nerve Agent Mimics

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