Group as on December 27, 2022

# Annual Report 2022

INDIAN INSTITUTE OF TECHNOLOGY MADRAS · सिद्धिर्भवति कर्मजा ·

pradeep RESEARCH GROUP

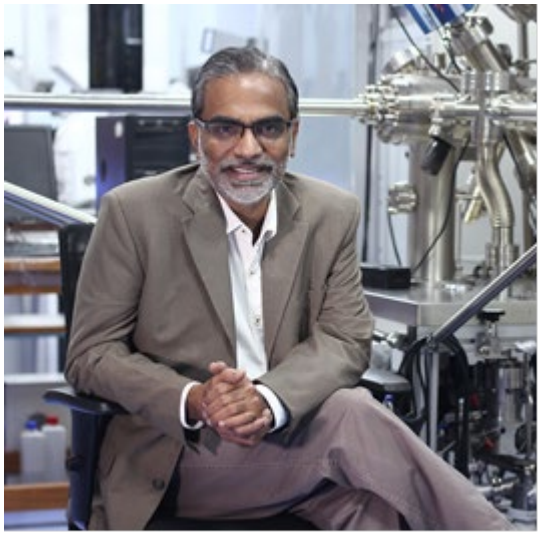
THEMATIC UNIT OF EXCELLENCE

Please visit the links for annual reports of 2014, 2015, 2016, 2017, 2018, 2019, 2020 and 2021.

# Our Team

## Thalappil Pradeep

Institute Professor
Deepak Parekh Institute Chair Professor and
Professor of Chemistry
Department of Chemistry
Indian Institute of Technology Madras
Chennai 600036 INDIA
Phone: +91-44-22574208
Fax: +91-44-22570545/0509
Email: pradeep@iitm.ac.in
Laboratories: DST Unit of Nanoscience and
Thematic Unit of Excellence
Web: https://pradeepresearch.org/



## Ph.D. Students

- Anil Kumar
- A. Suganya
- Amoghavarsha R. Kini
- Anagha Jose
- Ankit Nagar*
- Arijit Jana
- Bijesh K. Malla
- B. K. Spoorthi
- B. S. Sooraj
- Deepak Kumar Patel*
- Gaurav Vishwakarma
- Harshita Nagar
- Jayoti Roy
- Keerthana Unni
- Paulami Bose
- S. Jenifer*
- Sinchan Mukhhopadhyay
- Samapti Mondal
- Sonali Seth
- Soham Chowdhury
- Srikrishnarka Pillalamarri*
- Subrata Duary
- Sujan Manna
- Swetashree Acharya
- Tanmayaa Nayak
- Vishal Kumar*
- Vivek Yadav

* Jointly advised students

## Postdoctoral students/Project associates

- Dr. Sourav Kanti Jana
- Dr. Anish R Nath
- Dr. Tanvi Gupte
- Ms. Anshu Priya
- Dr. Anupriya Nyayban
- Mr. Vikash Khokhar
- Ms. Asmitha Shri
- Ms. Karthika Kalyansundar

## Administrative Officer

- Ms. K. Priya

## M.S. /M.Sc. /Visiting Students

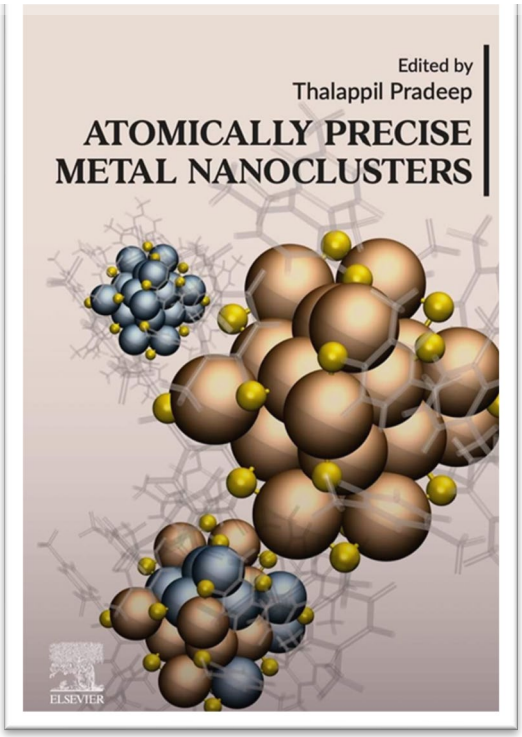
- Ramesh Kumar*
- Mansi Prajapati
- Mahima Dutta
- Muhammad Ijas
- Rima Chandra
- Mohammed Shafeeullah
- Manish Mukherjee
- Sakshi Khandare
- Shreelakshmi. J
- Akshyata Kirtania

## Project Technicians

- Mr. S. Balamurugan
- Ms. K. Banupriya

# What's Inside

# Glimpses of 2022




New book

Molecular Materials and Functions: An IIT Madras Conference, December 5-7, 2022

Water for Life: An IIT Madras Conference, December 15-17, 2022


Prof. T. Pradeep delivers his acceptance speech after winning the VinFuture Prize at the Hanoi Opera House, Hanoi, Vietnam on December 20, 2022.


Poster of the pCOE lecture series

# Publications

## Journal Publications

1. Carborane-thiol protected copper nanoclusters: Stimuli-responsive materials with tunable phosphorescence, Arijit Jana, Madhuri Jash, Wakeel Ahmed Dar, Jayoti Roy, Papri Chakraborty, Ganesan Paramasivam, Sergei Lebedkin, Kaplan Kirakci, Sujan Manna, Sudhadevi Antharjanam, Jan Machacek, Monika Kucerakova, Sundargopal Ghosh, Kamil Lang, Manfred M. Kappes, Tomas Base and Thalappil Pradeep, Chem. Sci., 2022. (DOI:10.1039/D2SC06578A).
2. Phosphine protected atomically precise silver-gold alloy nanoclusters and their luminescent superstructures, Madhuri Jash, Arijit Jana, Ajay K. Poonia, Esma Khatun, Papri Chakraborty, Ankit Nagar, Tripti Ahuja, K. V. Adarsh, and Thalappil Pradeep, Chem. Mater., 2022. (DOI.10.1021/acs.chemmater.2c03222).
3. Human skin-cell-based sensor for environmental arsenic detection and for creating social awareness, Tanvi Gupte, Suryalakshmi Pandurangan, Md Rabiul Islam, Pillalamarri Srikrishnarka, Ankit Nagar, Niraikulam Ayyadurai, Tiju Thomas, and Thalappil Pradeep, ACS Sustain. Chem. Eng., 10 (2022) 17124 - 17133. (DOI:0.1021/acssuschemeng.2c04586).
4. Ion-exchanging graphenic nanochannels for macroscopic osmotic energy harvesting, Ankit Nagar, Md Rabiul Islam, Kartheek Joshua, Tanvi Gupte, Sourav Jana, Sujan Manna, Tiju Thomas, and Thalappil Pradeep, ACS Sustain. Chem. Eng., 10 (2022) 15082-15093. (DOI: 10.1021/acssuschemeng.2c04138 ).
5. Rapid crystallization of amorphous solid water by porosity induction, Gaurav Vishwakarma, Bijesh K. Malla, Rabin Rajan Methikalam, and Thalappil Pradeep, Phys. Chem. Chem. Phys., 24 (2022) 26200-26210. (DOI: 10.1039/D2CP02640F).
6. Spatial reorganization of analytes in charged aqueous microdroplets, Pallab Basuri, Amrita Chakraborty, Tripti Ahuja, Biswajit Mondal, Jenifer Shantha Kumar, and Thalappil Pradeep, Chem. Sci., 13 (2022) 13321-13329. (DOI: 10.1039/D2SC04589C).
7. Formation of ethane clathrate hydrate in ultrahigh vacuum by thermal annealing, Bijesh K. Malla, Gaurav Vishwakarma, Soham Chowdhury, Premkumar Selvarajan, and Thalappil Pradeep, J. Phys. Chem. C, 126 (2022) 17983–17989. (DOI: 10.1021/acs.jpcc.2c06264).
8. Aggregation of molecules is controlled in microdroplets, Pallab Basuri, Jenifer Shantha Kumar, Keerthana Unni, Sujan Manna, and Thalappil Pradeep, Chem. Comm., 58 (2022) 12657-12660. (DOI: 10.1039/D2CC04587G).
9. Toward continuous breath monitoring on a mobile phone using a frugal conducting cloth-based smart mask, Pillalamarri Srikrishnarka, Raaga Madhuri Dasi, Sourav Jana, Tripti Ahuja, Jenifer Shantha Kumar,

Ankit Nagar, Amoghavarsha Kini, Boby George, and Thalappil Pradeep, ACS Omega, 2022. (DOI: 10.1021/acsomega.2c05017).

10. A selective and practical graphene-based arsenite sensor at 10 ppb, Sourav Jana, Kamalesh Chaudhari, Md Rabiul Islam, Ganapati Natarajan, Tripti Ahuja, Anirban Som, Ganesan Paramasivam, Addanki Raghavendra, Chennu Sudhakar, and Thalappil Pradeep, ACS Appl. Nano Mater., 5 (2022) 11876–11888. (DOI: 10.1021/acsanm.2c02860).
11. Strong and elastic membranes via hydrogen bonding directed self-assembly of atomically precise nanoparticles, Anirban Som, Alessandra Griffo, Indranath Chakraborty, Hendrik Hähl, Biswajit Mondal, Amrita Chakraborty, Karin Jacobs, Päivi Laaksonen, Olli Ikkala, Thalappil Pradeep, and Nonappa, Small, (2022) 2201707. (DOI: 10.1002/smll.202201707).
12. Accelerated non-enzymatic fatty acid esterification during microdroplet collision: A method for enhanced sustainability, Pallab Basuri, Jenifer Shantha Kumar, Subhashree Das, and Thalappil Pradeep, ACS Sustainable Chem. Eng., 10 (2022) 8577–8587. (DOI: 10.1021/acssuschemeng.2c02070).
13. Carborane-thiol protected propeller-shaped photoresponsive silver nanomolecule, Arijit Jana, Parvathy Unnikrishnan, Ajay Poonia, Jayoti Roy, Madhuri Jash, Ganesan Paramasivam, Jan Machacek, Kumaran Nair Valsala Devi Adarsh, Tomas Base, and Thalappil Pradeep, Inorganic Chemistry, 61 (2022) 8593–8603. (DOI: 10.1021/acs.inorgchem.2c00186).
14. Molecular engineering of atomically precise silver clusters into 2D and 3D framework solids, Wakeel Ahmed Dar, Arijit Jana, Korath Sugi, Ganesan Paramasivam, Mohammad Bodiuzzaman, Esma Khatun, Anirban Som, Ananthu Mahendranath, Amrita Chakraborty, and Thalappil Pradeep, Chemistry of Materials, 34 (2022) 4703–4711. (DOI: 10.1021/acs.chemmater.2c00647).
15. Role of zinc oxide in the compounding formulation on the growth of non-stoichiometric copper sulfide nanostructures at brass-rubber interface, Kannan Murugesan Paulthangam, Anirban Som, Tripti Ahuja, Pillalamarri Srikrishnarka, Appukuttan Sreekumaran Nair, and Thalappil Pradeep, ACS Omega, 7 (2022) 9573–9581. (DOI: 10.1021/acsomega.1c06207).
16. Shell-isolated assembly of atomically precise nanoclusters on gold nanorods for integrated plasmonic-luminescent nanocomposites, Amrita Chakraborty, Harsh Dave, Biswajit Mondal, Nonappa, Esma Khatun, and Thalappil Pradeep, J. Phys. Chem. B, 126 (2022) 1842–1851. (DOI: 10.1021/acs.jpcb.1c10207).
17. Industrial Utilization of Capacitive Deionization Technology for the Removal of Fluoride and Toxic Metal Ions ($As^{3+/5+}$ and $Pb^{2+}$), Md Rabiul Islam, Soujit Sen Gupta, Sourav Kanti Jana, and Thalappil Pradeep, Global challenges, 6 (2022) 2100129. (DOI: 10.1002/gch2.202100129).

## Editorials of 2022

1. Building pathways to a sustainable planet, David T. Allen, Peter Licence, Bala Subramaniam, Paul T. Anastas, D. Julie Carrier, Jingwen Chen Nicholas Gathergood, Jeannette M. Garcia, Jinlong Gong, Hongxian Han, King Kuok (Mimi) Hii, Bing-Joe Hwang, Andrew Marr, Michael Meier, Audrey Moores, Ryuhei Nakamura, Thalappil Pradeep, Liane Rossi, Bert Sels, Michael K. C. Tam, Lin Zhuang, and Julio F. Serrano, ACS Sustainable Chem. Eng., 10 (2022) 1-2.

## Books/Book chapters

1. Atomically precise metal nanoclusters, edited by Thalappil Pradeep, Elsevier, Amsterdam, 2023.
2. Concepts of sustainability in clean water technologies, Sritama Mukherjee, Jenifer Shantha Kumar, Ankit Nagar, and Thalappil Pradeep in Peter Boul (Ed.), Energy Transition: Climate Action and Circularity, ACS Symposium Series; American Chemical Society: Washington, DC, 2022.

# Patents

## Indian Patents (Granted)

1. Synthesis of highly anisotropic metallic mesostructures, T. Pradeep, Chandramouli Subramaniam, application no. 2262/CHE/2008, dated February 19, 2008, issued as patent no. 392320, dated March 18, 2022.
2. A method for the preparation of immobilized graphene-based composite from asphalt and its application in water purification, T. Pradeep, Theruvakkattil Sreenivasan Sreeprasad, Soujit Sengupta, Mundampra Maliyekkal Shihabudheen, application no. 3863/CHE/2012, dated September 17, 2012, issued as patent no. 393415, dated March 29, 2022.
3. Method for generating different phases of copper sulphide nanostructures using electrospray deposition (ESD) under ambient conditions, T. Pradeep, Arijit Jana, Sourav Kanti Jana, Depanjan Sarkar application no. 201941032379, dated August 9, 2019, issued as patent no. 396273, dated May 5, 2022.
4. Visible detection of quantity of water flow using quantum clusters, T. Pradeep, Annamalai Leelavathi, Mohan Udhaya Sankar, Chaudhary Amrita, Anshup, Thumu Udayabhaskararao, application no. 1521/CHE/2012, dated April 17, 2012, issued as patent no. 401784, dated July 21, 2022.
5. Structure and topology conserving transformations between two archetypal nanoparticles, T. Pradeep, K. R. Krishnadas, Ananya Baksi, Atanu Ghosh, Ganapati Natarajan application no. 201641034921, dated October 13, 2016, issued as patent no. 405913, dated September 6, 2022.

# Indian Patents (Applied)

1. Method of fabricating a conducting cloth based breath humidity sensor and applications thereof, T. Pradeep, Pillalamarri Srikrishnarka, Dasi Raaga Madhuri, Sourav Kanti Jana, Boby George, application no. 202241008331, dated February 17, 2022.
2. A selective and efficient process for the extraction of noble metals, T. Pradeep, Md Rabiul Islam, Tanmayaa Nayak, application no. 202241026274, dated May 05, 2022.
3. A method to transform crystalline minerals to nanoparticles by microdroplets, T. Pradeep, B. K. Spoorthi, Pallab Basuri, application no. 202241038282, dated July 7, 2022.
4. A method of cultivating rice without soil for its complete life cycle using nanotechnology, T. Pradeep, T.N.V.K.V Prasad application no. 202241043559, dated July 29, 2022.
5. A method for environmental arsenic detection and public awareness using human cells, T. Pradeep, Tanvi Gupte, application no. 202241049077, dated August 28, 2022.
6. Material and method for sustainable and affordable atmospheric water harvesting, T. Pradeep, Ankit Nagar; Sonali Seth, application no. 202241049229, dated August 29, 2022.
7. Vertically aligned nanoplates of atomically precise $Co_6S_8$ cluster for practical arsenic sensing, T. Pradeep, Anagha Jose, Arijit Jana, Tanvi Gupte, Keerthana Unni, Ankit Nagar, Amoghavarsha R. Kini, B.K. Spoorthi, application no. 202241076581, dated December 29, 2022.

# PCT (Applied)

1. An electrode system based on differential oxidant response for the detection of free chlorine, T. Pradeep, Kamalesh Chaudhari, Tullio Servida, Vishnu V, B. K. Spoorthi, application no. PCT/IN2022/050637, dated July 14, 2022.

# Degree Holders

## Ph.D. Graduates

- Dr. Pallab Basuri, Department of Chemistry, IIT Madras

  Generation, visualization, and understanding of microdroplets for analytical and preparative mass spectrometry

- Dr. Mohd Azhardin Ganayee, Department of Chemistry, IIT Madras

  Molecularly functionalized aminoclays: Versatile materials for new applications

- Dr. Tanvi Gupte, Department of Chemistry, IIT Madras

  Investigations into chemical and biological methods of arsenic detection

Dr. Mohd Azhardin Ganayee

Dr. Tanvi Gupte

Dr. Pallab Basuri

## MS Graduates

- Mr. Ananthu Mahendranath, Department of Metallurgical and Materials Engineering, IIT Madras

  Atomically precise cluster solids: Emerging insights into structure and properties

Mr. Ananthu Mahendranath

# Lectures Delivered

1. *Advanced materials for affordable clean water, NANOicon 2022, Inter University Centre for Nanomaterials and Devices (IUCND) Cochin University of Science and Technology, Kerala, Jan 11, 2022.
2. *Mission to save 1000 crores litres, Join the WOW Chennai, Jan 13, 2022.
3. *Water!, Jigyasa Vigyan Mahotsav Bootcamp 1 on Water conservation, February 14, 2022.
4. *Affordable clean water using advanced materials, Online workshop on "Thin Film Nanostructured Membranes on Gas Separation, Storage and Water Desalination". Indian Institute of Science Bangalore, India. Jan 20, 2022.
5. *Affordable clean water with advanced materials, IIT Alumni Industry Interaction Center, IIT Madras, Feb 5, 2022.
6. *Water – Transition to NetZero, Indo-UK symposium under SUNRISE network, February 10, 2022
7. *Nanoparticles are Molecules, CoE lecture series on Molecular materials and Functions at IIT Madras, Feb 11, 2022.
8. *Affordable clean water using advanced materials, NIT Uttarakhand, Feb 28, 2022.
9. *Affordable clean water using advanced materials, Shri Vaishnav Vidyapeeth Vishwavidyalaya, Indore, Madhya Pradesh. Feb 28, 2022.
10. *Science, technology, and innovation for sustainable clean water, IIT Roorkee. Feb 28, 2022.
11. *Science, technology, and innovation for sustainable clean water, Indian Academy of Sciences, Raman Research Institute, Bangalore. Feb 28, 2022.
12. *Water@2047: A glimpse into the challenges and opportunities, Imagining India@2047 through innovation, IIT Madras, March 7-9, 2022.
13. *Building clean water technologies from a Chemistry Laboratory Environmental Sciences and Engineering (EnSE) seminar series, Water Desalination and Reuse Research Center, KAUST. March 17, 2022
14. *Nanomolecules, SINP Materials Science Seminar Series, Saha Institute of Nuclear Physics, Kolkata March 22, 2022.
15. *Affordable clean water using advanced materials, Water Sustainability: Challenges, Technologies, and Opportunities - (IWSS 2022), Vishwa Vidyapeetham, March 24, 2022
16. *Atom dynamics in nanoparticles, Frontier Symposium-Chemistry 2022 (FSCHM 2022), IISER TVM, April 8-10, 2022.
17. *Technological advancements for achieving water sufficient gram panchayats, Azadi ka amrit mahotsav celebration of ICONIC week, Government of India Ministry of Panchayati Raj, Vigyan Bhawan, New Delhi, April 11-17, 2022.
18. *Research ethics and intellectual property rights, Stella Maris College, Chennai, May 4, 2022.
19. *Affordable clean water using advanced materials: Basic science to industry, Online ACS seminars at IIT Mandi, India. May 5, 2022.
20. Chemical reactions and dynamics in nanoparticles, LIBER Symposium 2022, Helsinki, May 12-13, 2022.

21. Beyond dimensions: Reactions between clusters, nanoparticles and bulk matter, Institute of Nanotechnology, KIT, Karlsruhe, May 16, 2021.
22. *Affordable clean water using advanced materials, The Maharaja Sayajirao University of Baroda, Vadodara, June 5, 2022.
23. From molecular acrons to Institutional Oaks, Frontier Lecture, University of Calicut. June 20, 2022.
24. Water purification technologies including arsenic removal, "International Workshop on Water Purification Technologies, Arsenic Removal from Groundwater and Integrated Water Management (IWWPT-2022), CSIR-CSMCRI, Bhavnagar, Gujarat, India June 28, 2022.
25. Water: Gaps and opportunities, 33rd Mid-Year Meeting, Indian Academy of Sciences, July 8-9, 2022.
26. Affordable clean water using advanced materials, Kannur University. July 12, 2022
27. Chemistry of atomically precise clusters, CASM 2022, NIIST Thiruvanthapuram, July 25, 2022.
28. *Water technology particularly for drinking water and Atmanirbharata, Atmanirbarata & Industry, Tamilnadu State Council for Science & Technology, July 29, 2022.
29. Complexity in the chemistry of atomically precise clusters, Indo-German workshop-2022 (IGW-CCS-2022), IIT Madras, October 5, 2022.
30. *Affordable clean water with advanced materials, RSC-IITM Desktop Seminar on Environmental Sciences, October 11, 2022.
31. Complexity in the chemistry of atomically precise clusters, AsiaNANO 2022 Asian Conference on Nanoscience & Nanotechnology, Busan, November 9-11, 2022.
32. * Affordable clean water using advanced materials, ACS Science Talks: Virtual Lecture Series No. 100, November 30, 2022.
33. Atomically precise clusters for applications, Molecular Materials and Functions Conference, IIT Madras, December 5-7, 2022.
34. Affordable clean water using advanced materials, Technische Universität Wien, December 12, 2022.
35. Affordable clean water using advanced materials, Water for life, IIT Madras, December 15-17,2022.
36. * Affordable clean water using advanced materials, International Conference on Water Resources and Arid Environments (ICWRAE 10), December 26-28, 2022.
37. Affordable clean water using advanced materials, International Conference on Nanoscience and Photonics for Medical Applications, MAHE, December 28-20, 2022.

* Online lectures

# Students' Activities

1. Dr. Tanvi Gupte has presented a poster on 'Highly sensitive $As^{3+}$ detection using electrodeposited nanostructured $MnO_x$ and phase evolution of the active material during sensing' in the 28th National Symposium in Chemistry (CRSI-NSC-28) held at IIT Guwahati, March 25-27, 2022.
2. Mr. Subrata Duary has presented a poster on '2-Mercaptonicotinic Acid-Protected Mechanoresponsive Copper Nanoclusters' in Molecular Materials and Functions conference, December 5-7, 2022.
3. Mr. Srikrishnarka Pillalamarri has delivered a talk as an invited speaker at 1st International Conference on Convergence of Interdisciplinary Science, February 19-20, 2022.
4. Mr. Sooraj B S has presented a poster on 'Study on ligand exchange induced metallicity in larger gold clusters using novel borane ligands' in International Immersion Experience (IIE) - Open House, held at IIT Madras, December 15, 2022.
5. Ms. Spoorthi Bhat has given an oral presentation on 'Ambient Microdroplet Annealing of Nanoparticles' in Students' Research Convention 2022 held at IIT Kanpur, April 05, 2022.
6. Mr. Gaurav Vishwakarma has presented a poster on 'Rapid crystallization of amorphous solid water by porosity induction' in Spectroscopy and Dynamics of Molecules and Clusters meeting held at Malpe, Karnataka, November 10-13, 2022.
7. Ms. Anagha Jose has presented a poster on 'Vertically Aligned Nanoplates of Atomically Precise $Co_6S_8$ Cluster for Practical Arsenic Sensing' in Molecular Materials and Functions conference, December 5-7, 2022.
8. Ms. Spoorthi Bhat has presented a poster on 'Ambient Microdroplet Annealing of Nanoparticles' in Chemical Research Society of India 28th National Symposium in Chemistry (CRSI-NSC-28) held at IIT Guwahati, March 25-27, 2022.
9. Ms. Jayoti Roy has presented a poster on 'Dissociative reactions of $Au_{25}(SR)_{18}$ at copper oxide nanoparticles and formation of aggregated nanostructures' in Molecular Materials and Functions conference, December 5-7, 2022.
10. Ms. Swetashree Acharya has presented a poster on 'Synthesis of molybdenum-oxo clusters via soft chemistry; it's tungsten doping and optical sensing of arsenic' in Molecular Materials and Functions conference, December 5-7, 2022.
11. Mr. Sujan Manna has won second place in the Micrograph competition in PRAKRIYA 2022, held at IIT Madras, April 25, 2022.
12. Mr. Gaurav Vishwakarma attended a workshop on "Astrochemistry and cratering in solar system." The workshop was in-person and organized at Physics Research Laboratory, Ahmedabad, from 04-10 July 2022.

13. Ms. Jayoti Roy has presented a poster on 'Gas phase ion chemistry of titanium-oxofullerene with ligated solvents' in Chemical Research Society of India 28th National Symposium in Chemistry (CRSI-NSC-28) held at IIT Guwahati, March 25-27, 2022.
14. Mr. Gaurav Vishwakarma has given an oral presentation on 'Desorption-induced evolution of cubic and hexagonal ices in an ultrahigh vacuum and cryogenic temperatures 'International conference on Chemistry and Physics at Low Temperatures, organized by the Laboratory of Molecular Spectroscopy of the Eötvös Lórand University in Budapest, July 4-6, 2022.
15. Mr. Vishal Kumar has presented a poster on 'Room temperature synthesis of nanoparticles and nanoclusters using triboelectric generator' in International Conference on Materials for Humanity held at National University of Singapore, September 19-21, 2022.
16. Ms. Paulami Bose presented a poster on 'Atom transfer between precision nanoclusters and polydispersed nanoparticles: a facile route for monodispersed alloy nanoparticles and their superstructures' in the International Conference on Materials for Humanity held at the National University of Singapore, September 19-21, 2022.
17. Mr. Ankit Nagar has presented a poster on 'Scalable drop-to-film condensation on a nanostructured hierarchical surface for enhanced humidity harvesting' in Chemical Research Society of India 28th National Symposium in Chemistry (CRSI-NSC-28) held at IIT Guwahati, March 25-27, 2022
18. Ms. Sonali Seth has presented a poster on 'Sustainable humidity harvesting for clean water' in Water for Life conference, held at IIT Madras, December 15-17, 2022.
19. Ms. Paulami Bose has presented a poster on Atom transfer between precision nanoclusters and polydispersed nanoparticles in 28th National Symposium in Chemistry (CRSI-NSC-28) held at IIT Guwahati, March 25-27, 2022.
20. Ms. Tanmayaa Nayak has presented a poster on 'Sustainable cellulose-derived materials for adsorptive removal of uranium from wastewater with faster kinetics' in Water for Life conference, held at IIT Madras, December 15-17, 2022.

# Students' Recognitions

1. Mr. Sooraj B S has received an International Immersion Experience (IIE) travel award 2022, funded by IIT Madras.
2. Mr. Gaurav Vishwakarma has received an International Immersion Experience (IIE) travel award 2022, funded by IIT Madras.
3. Ms. Jayoti Roy has received an International Immersion Experience (IIE) travel award 2022, funded by IIT Madras.
4. Dr. Pallab Basuri has received the best Thesis Award from IIT Madras.

5. Mr. Vishal Kumar has received the AWSAR award from Department of Science and Technology.
6. Dr. Tanvi Gupte has received one of the best poster awards for 'Highly sensitive $As^{3+}$ detection using electrodeposited nanostructured $MnO_x$ and phase evolution of the active material during sensing' at the NANOicon 2022 conference organized by Cochin University of Science and Technology (CUSAT), January 11-15, 2022.
7. Mr. Arijit Jana has received one of the best poster awards for 'Carborane-thiol protected tetranuclear copper nanoclusters' in NANOicon 2022 conference organized by the Cochin University of Science and Technology (CUSAT), January 11-15, 2022.
8. Mr. Gaurav Vishwakarma has received an Early Career Research Award 2022 at Indian Planetary Science Conference, March 14-16, 2022.
9. Ms. Jayoti Roy has received one of the best poster awards in Student Research Convention 2022, held at IIT Kanpur, March 4-6, 2022.
10. Mr. Srikrishnarka Pillalamarri has won 1st prize for his oral presentation in Chempius 2022, held at IIT Madras, March 13, 2022.
11. Ms. Jenifer S has received one of the best poster awards for 'Microdroplets control the orientation and chemistry of analytes' in Water for Life conference, held at IIT Madras, December 15-17, 2022.
12. Dr. Tanvi Gupte has received the best oral presentation award in Water for Life conference, held at IIT Madras, December 15-17, 2022.
13. Mr. Arijit Jana has received the best oral presentation award for 'Carborane-thiol protected tetranuclear copper nanoclusters' in Molecular Materials and Functions conference, held at IIT Madras, December 5-7, 2022.

# Alumni News

1. Dr. Indranath Chakraborty was appointed as an Assistant Professor at the School of Nano Science and Technology, IIT Kharagpur, West Bengal, India.
2. Dr. Ananya Baksi was appointed as an Assistant Professor at the Jadavpur University, West Bengal, India.
3. Dr. Depanjan Sarkar was appointed as an Assistant Professor at the Vellore Institute of Technology, Chennai, India.
4. Dr. Premkumar Selvarajan was appointed as an Assistant Professor at the Vellore Institute of Technology, Vellore, India.
5. Dr. Madhuri Jash has joined the KTH Royal Institute of Technology, Sweden as a Postdoc.

6. Dr. Angshuman Ray Chowdhuri has joined the NUS, Singapore as a Postdoc.
7. Dr. Biswajit Mondal has joined the Karlsruhe Institute of Technology, Germany as a Postdoc.
8. Dr. Mohammed Bodiuzamann has joined the King Abdullah University of Science and Technology (KAUST), Saudi Arabia as a Postdoc.
9. Dr. Sandeep Bose has joined the McGill University, Canada as a Postdoc.
10. Dr. Pallab Basuri has joined the Humboldt University of Berlin, Germany as a Postdoc.
11. Dr. Md Rabiul Islam has joined the International Centre for Clean Water (ICCW), Chennai, India as a scientist.
12. Dr. Chennu Sudhakar has joined the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bengaluru, India as a Postdoc.
13. Dr. Sritama Mukherjee has joined the KTH Royal Institute of Technology, Sweden as a Postdoc.
14. Mr. Ananthu Mahendranath has joined the University of Minnesota, USA as a Ph.D. student.
15. Ms. Subhashree Das was recruited as an Assistant Professor in Govt. College, Orissa, India.
16. Dr. Pratyusha Das has joined the University of California, Santa Barbara, USA as a Postdoc.
17. Mr. Sathvik Ajay Iyengar has received the Quad fellowship 2022.
18. Prof. Chandramouli Subramaniam has received the DST Swarnajayanti Fellowship 2022.

# Research Grants

## Ongoing projects

1. National facility of cryo-electron microscopy: Remotely operable, 24x7 for academia and industry, SERB, Rs. 28.6 crores (principal investigator) with IIT Tirupati, IISER Tirupati, IIT Palakkad, RGCB Thiruvananthapuram, Sastra Thanjavur, VIT Vellore, and MRF Chennai.
2. Carborane-protected metal nanoclusters: A new family of materials with atomic precision - DST/Czech 37 lakhs (principal investigator).
3. Understanding surface properties of atomically engineered cluster-assembled solids, SPARC project with Robin Ras and Olli Ikkala, Aalto, Finland with Tiju Thomas, IITM, Rs. 66.3 lakhs (principal investigator).
4. SUTRAM for EASY water, DST, Rs. 890 lakhs (co-principal investigator with Prof. Ligy Philip).
5. VAJRA project with Graham Cooks, Purdue University, Rs. 9.75 lakhs.
6. JC Bose Fellowship, Department of Science and Technology, 90 lakhs as (principal investigator), renewed.

7. Fingerprinting authenticity of ayurvedic preparations using ambient electrospray deposition raman spectroscopy (AERS), a home-grown method for rapid analysis, DST, Rs. 93 lakhs (principal investigator), along with Santhosh Chidangil, Manipal Academy of Higher Education (co-principal investigator).
8. Sustainable ion exchange resin-based technology for rare earth extraction, Ministry of Mines, Rs. 52 lakhs (principal investigator).
9. Atomically precise naked clusters assemblies from ligand-stabilized clusters new materials for catalysis, Department of Science and Technology, DST-DFG grant with Manfred Kappes, KIT, Rs. 72 lakhs (principal investigator).
10. pCOE on Molecular Materials and Functions, IIT Madras, Rs. 5.80 crores (principal investigator) with colleagues from IITM and other institutions (details below).

## Projects approved this year

1. Atomically Precise Materials for Sustainable Water and Energy Harvesting, SERB, Rs. 75 lakhs (principal investigator).

## Consultancy

1. Steel – Rubber adhesion improvement – Phase 2, MRF Ltd., 2019–2021, Rs. 1.2 Cr (principal investigator).

## Implementation Projects

1. Providing, fixing, and maintenance of nano material-based household water purifiers for providing in arsenic affected habitations of Punjab, Government of Punjab, Rs. 48.5 crores (principal investigator), undertaken by ICCW.
2. House-hold arsenic removal units for Government of Punjab, Rs. 4.8 crores (principal investigator), undertaken by ICCW.
3. Support of Wastewater Based Epidemiology facility at IIT Madras, In Covid Support FZE LLC, Rs.7.5 crores (principal investigator).

# Visitors

1. Dr. K. Balasubramanian, Principal Investigator and Director NFTDC, Hyderabad, Jan 6, 2022.
2. Dr. Maneesha Ramesh (Provost), Mr. B. R. Ajit (Architect), Mr. Devidasa Chaitanya (Campus Director) & Sreevalsan (PRO), Mr. Shivakumar (Head, Finance), Mr. Vishnu Vijay (DGM), Mr. A. Jayakumar, and Vijnana Bharati from Amrita University, March 10, 2022.
3. Dr. Prashanth Kumar, Plaksha University, Mohali, March 15, 2022

4. Kerala Higher Education Reforms commission team visit Prof. Sabu Thomas, (VC, MG University), Prof. Sabu Abdul Hameed, (Pro-VC, Kannur University), Prof. R. Ramakumar (Professor, TISS, Mumbai), Dr. George Varghese, (Secretary of the Higher Education Council of the govt of Kerala). Dr. Shefeeque V (research officer, Kerala state higher education council and coordinator, higher education reforms commission), April 1, 2022.
5. Mr. Naveen Unni, Managing Partner of Mckinsey, Chennai, April 27, 2022.
6. Dr. R. Bindu, Hon'ble Minister for Higher Education and Social Justice, Kerala & Smt. Sajini Mukthar (Asst. Private Secretary), Dr. V. Venu (Additional Chief Secretary), Dr. Rajasree M.S. (Vice Chancellor, Kerala Technological University), Sri. P. Shanavas, (Private Secretary), Sri. Indulal R. (Additional Private Secretary), Dr. Madhusoodhanan (Vice Chancellor, Cochin University), Prof. Gopinath Ravindran (Vice Chancellor, Kannur University), and Prof. Ajayakumar (Pro Vice-Chancellor), May 29, 2022.

Prof. Pradeep with Prof. Ariel Porat, President of Tel Aviv University, Israel and his colleagues, December 8, 2022.

7. Dr.T.N.V.K.V. Prasad, Principal Scientist (Soil Science), Principal Investigator ICAR-NASF, Acharya N.G.Ranga Agricultural University, Hyderabad, June 13, 2022.
8. Prof. Hari Srikanth, Distinguished University Professor, Department of Physics, University of South Florida, July 1, 2022.
9. Dr. Lior Asaf, Water Attache`, Embassy of Israel, New Delhi, Prof. Ariel Porat, President of Tel Aviv University, and Neeraj Gahlawat, Senior Water Resources Specialist, Embassy of Israel, New Delhi, July 21, 2022.
10. Mr. Gassan Mutwali, Senior Director, EoL Ms. Chaya Ravishankar, and Mr. Narain Madhavan from XYLEM, August 16, 2022.
11. Prof. Bhagavatula Prasad, Director of CeNS, Bangalore, August 16, 2022.
12. Prof. Sujit K. Ghosh, Department of Chemistry, IISER Pune, August 24, 2022.
13. Dr. Spike Narayan Ph.D., Member, IBM Academy of Technology, Director, Science & Technology and Director, Almaden Operations, IBM, September 9, 2022.
14. Dr. Santosh Nandan – Managing Director, Ambernath Organics Pvt Ltd, September 11, 2022.
15. The senior management team of KMML, October 7, 2022.
16. Sourabh Narang - Sales Director and Mr. Okayama- Managing Director, JEOL INDIA, October 7, 2022.

Prof. Pradeep with Dr. R. Bindu, Hon'ble Minister for Higher Education and Social Justice, Kerala, and her team May 29, 2022.

17. Prof. Ariel Porat, President of Tel Aviv University, Prof. Milette Shamir, Vice President International of Tel Aviv University, Mr. Konstantin Platonov, Asia Engagement Director, Tel Aviv University International, Dr. Gary Sussman, Director of Research and Development, December 8, 2022.
18. Prof. Paul S Weiss, Prof. Stefanie Dehnen, Prof. Manfred Kappes, Prof. Josef Breu, Prof. Shiv N. Khanna, Dr. Tomas Base, Prof. Nonappa, Prof. Amitava Patra, Prof. Biswarup Pathak, Prof. K V Adarsh, Prof. Sukhendu Mandal, Dec 4, 2022.
19. Prof. Stefanie Dehnen, Prof. Manfred Kappes, Dr. Tomas Base, Prof. Nonappa, Prof. Sukhendu Mandal, Dr. Ananya Baksi, Dr. Indranath Chakraborty, Dec 7, 2022.
20. Prof. Richard N Zare, Prof. Amit Gross, Prof. Rita Henderson, Prof. Hadas Mamane, Prof. Kartik Chandran, Dr. Samuel Chigome, Prof. C Subramaniam, Prof. Chaitanya Lekshmi Indira, Prof. Jaichander Swaminathan, Prof. E Gnanamani, Dec 17, 2022.

# Visits

1. National Institute of Technology, Tiruchirappalli (NIT-T), Guest lectures Pragyan, March 18, 2022.
2. Indian Institute of Technology, Bombay (IIT-B), Cryo-EM workshop, May 5-6, 2022.
3. Helsinki, Finland. Life Inspired Hybrid Materials (LIBER) symposium, May 11-13, 2022.
4. Tempere University, Finland, May 14, 2022.

Visit to Finland, May 11-14,2022

5. Karlsruhe Institute of Technology, Germany, May 15-17, 2022.
6. 47th Shodh Yatra Tamil Nadu joined from Paramakudi, Ramanathapuram district of Tamil Nadu to Rameshwaram with Prof. Anil K. Gupta and team, May 22-23, 2022.
7. Field trip to Kuttanad, Agriculture Division, Kerala State Planning Board to explore integrated development, May 25-27, 2022.
8. CSIR-CSMCRI, Bhavnagar, International Workshop on Water Purification Technologies, Arsenic Removal from Groundwater and Integrated Water Management (IWWPT-2022), June 28-30, 2022.
9. Farook College, Kerala, Advisory committee meeting, July 6, 2022.
10. 33rd Mid-Year Meeting of the Indian Academy of Sciences, Bengaluru, Special Session on "Basic Sciences for Sustainable Development", July 8, 2022.
11. Kannur University, Delivering the public lecture as part of lecture series organized by Research Directorate in association with IQAC of Kannur, July 12, 2022.
12. CSIR-NIIST, Thiruvananthapuram. Inaugural Plenary speaker for CASM 2022, July 25-26, 2022.

13. Israel, for a course on the management of wastewater and its sustainable reuse for irrigation, September 14-22, 2022.
14. Kerala Minerals and Metals Ltd, Kerala, to explore possibilities of collective work, September 25-27, 2022.
15. California, Atomically Precise Nanochemistry, Gordon Research Conference, Vice-chair of the conference, October 16 - 21, 2022.
16. Japan, Cryo-EM facilities of JEOL at Osaka University, to understand the current status of their Cryo-EM, November 7-9, 2022.
17. Busan, Asian Conference on Nanoscience & Nanotechnology, AsiaNANO 2022, November 9-11, 2022.
18. Visit to Vienna to receive the Prince Sultan Bin Abdulaziz International Prize for Water (PSIPW) in the 'Creativity Prize' category, Dec 9-14, 2022.
19. Visit to Hanoi, Vietnam to receive the VinFuture Prize, Dec 18-24, 2022.
20. International Conference on Nanoscience and Photonics for Medical Applications, MAHE, Manipal. Dec 28-30, 2022

# Service

- Vice President, Indian Society for Mass Spectrometry, 2014-
- Member, Executive Committee, Neutron Scattering Society of India, 2011-
- Member of the Council of Materials Research Society of India, 2011 –
- Member, Board of studies, Manipal University, 2012-
- Member, Industry Relevant R &D Expert Committee, DST, 2018-2021
- Member, Governing Council, Technology Information, Forecasting & Assessment Council (TIFAC), 2019-
- Member, Research Advisory Council, Manipal Academy of Higher Education, Manipal Member, 2018-
- Research Advisory Board, Pandit Deendayal Petroleum University, 2019-
- Member, Research Advisory Committee, IIT Ropar, 2019-
- Co-opted Member, Program Advisory Committee of SERB-SUPRA, 2019-
- Member, Technical Committee for examination and use of innovations and technologies in drinking water and sanitation sector, Department of Drinking Water and Sanitation, Ministry of Jal Shakti, 2019-2024.
- Member, Program Advisory Committee on Exponential Technologies, DST, 2020-
- Convener, Commission for the Reforms in Higher Education System, Government of Kerala, 2021-
- Chairman, Board of Governors, Institute of Nano Science and Technology, Mohali, 2021-

- Member, Editorial Board of the journals; Chemistry of Materials, ACS Nano, Analytical Chemistry, Nanoscale, Particle, Surface Innovations, International Journal of Water and Wastewater Treatment, Nanoscale Advances, and Chemical Communications.
- Associate Editor of the journal, ACS Sustainable Chemistry & Engineering, 2014–

# Upcoming Facilities

## National Facility for Cryogenic Electron Microscopy (Cryo-EM)*

A Cryo-EM facility for single particle analysis and soft materials applications, composed of two high end microscopes with rapid screening and continuous imaging capabilities to obtain structures of macromolecules and materials at angstrom resolution will be coming up at IIT Madras. We have placed the purchase orders for a Krios G4 300 kV instrument and a Talos 200i 200kV instrument, along with accessories. The facility will be housed in a new building (see below).

Status of the construction site for housing the Cryo-EM facility, December 24, 2022.

* With IIT Tirupati, IISER Tirupati, IIT Palakkad, RGCB Thiruvananthapuram, Sastra Thanjavur, VIT Vellore and MRF Chennai.

# Wastewater-Based Epidemiology (WBE)

We are establishing a new research centre that will test wastewater in a city for indicator organisms and chemicals and make the data available to the public. The facility will act as an intelligence unit to track and prevent a virus outbreak in its early stages. The data obtained from various wastewater sources and treatment facilities will be analyzed and made available to the public through dashboards. Gradually, this facility will be extended to other parts of India. We will also work on building a hydroinformatics platform for the city with appropriate modelling tools to give spatiotemporal information of the data derived from WBE studies.


ThermoFisher Scientific Q Exactive Plus Orbitrap LC-MS/MS.

The WBE facility will also be employed to detect the emerging issues of concern, such as increasing antimicrobial resistance due to excessive consumption of antibiotics. Identifying the right policies to control pharmaceuticals and personal care products will significantly improve public health. We have placed the purchase order for Q Exactive Plus Orbitrap LC-MS/MS System of ThermoFisher as of now.

We intend to help the public, policymakers, practitioners and public health officials to combat the ongoing Covid 19 pandemic through wastewater analysis. Apart from SARS-CoV-2, several other pathogens prevailing in a population can be detected through wastewater analysis. Techniques for analysis include polymerase chain reaction (PCR) and mass spectrometry (MS), combined with data analytics.

# Incubation

- **Hydromaterials** installed 100 villages water treatment units in 2022, altogether supplying arsenic and iron free water to over 900,000 people. Altogether there are 961 units of this kind operational in the country, supplying clean water to 1.2 million people. This year's highlights include: Execution of 6 new AIRP plants in Punjab; ongoing execution of 59 water treatment plants in Uttar Pradesh; ongoing installation of district-wide automation in Himachal Pradesh and ongoing installation of 2500 automatic water filters for Anganwadis in Andhra Pradesh.


- **InnoDI** expanded its reach, it has installed more than 150 units across 10 states serving clean water to over 100,000 people and saving over 100 million litres of water every year which otherwise would have gone down the drain. One of the recent installations at Kappalurl in Tamil Nadu is shown on the left. Pictured on August 15, 2021.


- **VayuJal** Technologies has installed a solar and power operated 2000 litres per day (LPD) atmospheric water harvesting unit at Engineers India Limited, Gurugram, Haryana. They now have 40, 140, 450, 1100, and 2200 LPD units in production. Highlights include: Installation completed off the grid (solar) 450 LPD unit; 34 project installations within this financial year; exported a Made in Tamilnadu product to Cyprus; awarded as one of the top 10 protech companies by HDFC Tech Innovator Challenge 2022; presented VayuJal at Dubai Expo-2020 on 28 March, 2022; awarded as Top Tech 30 startups of 2022 by Yourstory Media Tech Spark event at Taj, Bangalore; winner of AMRUT 2.0 project from Ministry of Housing & Urban Affairs; winner of Akamai-ICCW Social challenge 2022; Incubation with NASSCOM; winner of ZF Foundation-CSR Award, 2022 and awarded as emerging Entrepreneur of Tamil Nadu at Entrepreneurs Annual Meets & Awards 2022, 27 December 2022. Shown on the right is a view of the factory.

- **InnoNano Research Private Limited** is an IIT Madras-incubated company which developed AMRIT, acronym for Anion and Metal Removal by Indian Technology. AMRIT is an affordable nanotechnology-based water purifier to dispense safe and affordable drinking water at a cost <5 paise/litre. It was first introduced in the villages of Murshidabad district in West Bengal after the Arsenic Task Force of the Government of West Bengal certified and approved its use. AMRIT is installed in 2000 locations in West Bengal, Uttar Pradesh, Bihar and Karnataka providing arsenic-free drinking water to nearly 8 lakh beneficiaries. The company is not active now.

- **AquEasy Innovations Private Limited** is an Indian company incubated by IIT Madras working in the field of domestic water purification techn ologies. AquEasy currently develops contaminant specific water purifier bottle, called the 'blue bottle'. Also, the company has developed a rolling water purifier called 'roll pure' that helps in reducing the effort in water transportation and provides clean water, when the water reaches the point of use.

- **EyeNetAqua Solutions Private Limited** is a start-up company incubated at ICCW to develop and commercialize IoT-based sensing technologies for water quality monitoring. It has been recognized as the second runner-up (top 5 out of 213 companies) in the ICT Grand Challenge 2020 arranged by MeitY (CDAC, Bangalore). As a part of the challenge, a product developed as per NJJM specifications has been deployed at thirteen villages in the Ambala district of Haryana. The product has been designed and demonstrated for inline measurements of pH, TDS, residual chlorine, nitrate, pressure and volume of flow. Following this, EyeNetAqua has been selected as a Technology and Implementation Partner in AMRUT 2.0 India Watertech Startup Challenge by MOHUA. Apart from this, EyeNetAqua is actively working towards the lab-to-field translation of low-cost, colorimetric online and portable devices for multiparametric water quality testing.


- A new initiative of IIT Madras, the **International Centre for Clean Water** made tremendous progress in all its activities. We have initiated research, implementation, outreach and incubation activities. An overview of these efforts is available here. Key to these initiatives is the support of all our well-wishers, well-meaning individuals, Companies well as institutions.

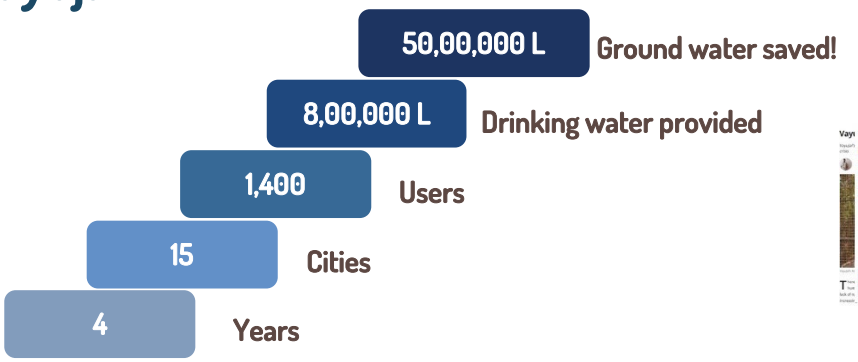
***All start-ups are co-owned by IIT Madras.***

Our initiatives and companies

# Reach of Some of our Technologies

## This pertains to last year

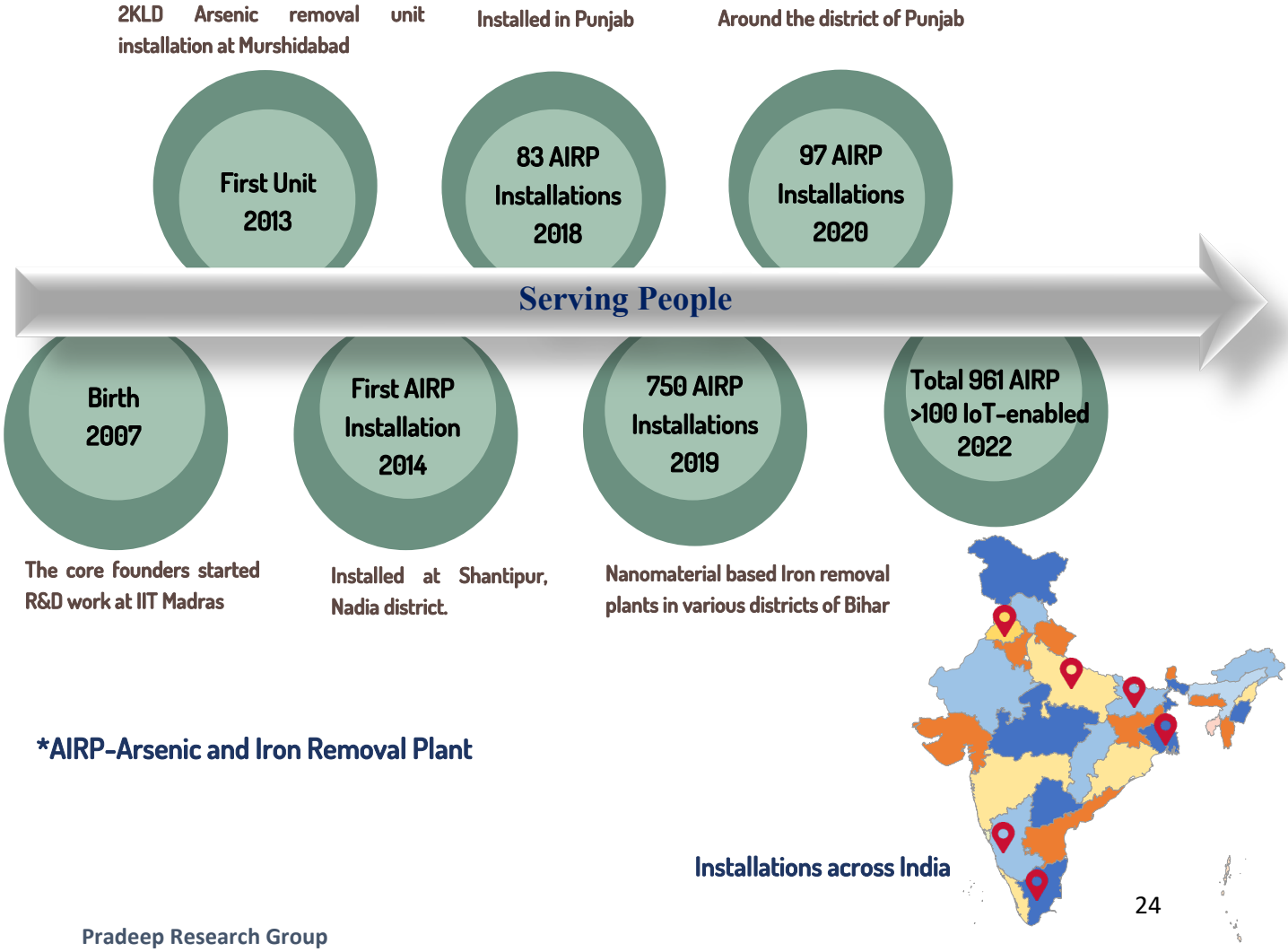
## Vayujal





Media on Vayujal

## AMRIT-Anion and Metal Removal by Indian Technology




*AIRP-Arsenic and Iron Removal Plant



Installations across India

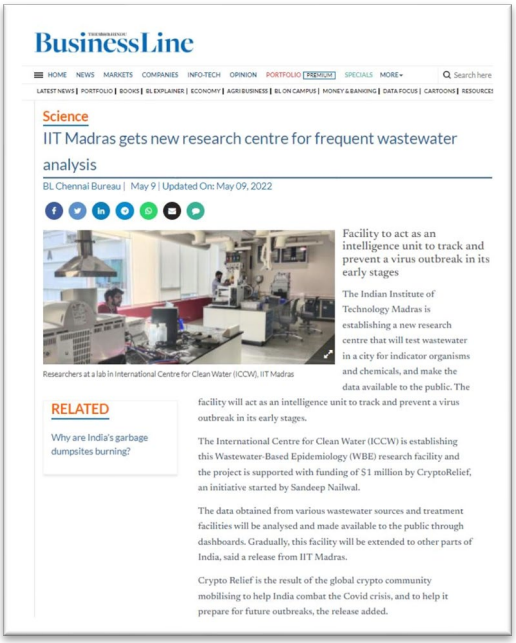
# Media Reports

India Today Web Desk
New Delhi, UPDATED: Dec 28, 2022 20:06 IST

## IIT Madras professor Padma Shri Thalappil Pradeep wins VinFuture Prize for tech to remove arsenic from groundwater

IIT Madras professor Padma Shri Thalappil Pradeep has won the VinFuture Prize, one of the largest ever annual prizes globally, for his low-cost filatration system to remove arsenic from groundwater.


*IIT Madras professor Padma Shri Thalappil Pradeep has won the VinFuture Prize, one of the largest ever annual prizes globally, for his low-cost filatration system to remove arsenic from groundwater.*



BusinessLine

Science

IIT Madras gets new research centre for frequent wastewater analysis

BL Chennai Bureau | May 9 | Updated On: May 09, 2022

Researchers at a lab in International Centre for Clean Water (ICCW), IIT Madras

Facility to act as an intelligence unit to track and prevent a virus outbreak in its early stages

The Indian Institute of Technology Madras is establishing a new research centre that will test wastewater in a city for indicator organisms and chemicals, and make the data available to the public. The facility will act as an intelligence unit to track and prevent a virus outbreak in its early stages.

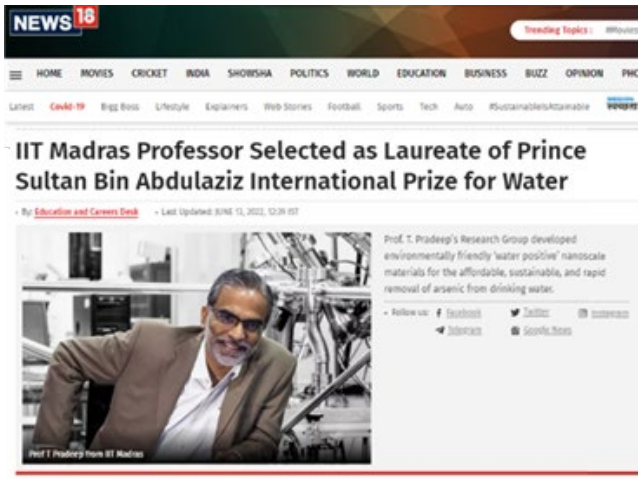
RELATED

Why are India's garbage dumpsites burning?

The International Centre for Clean Water (ICCW) is establishing this Wastewater-Based Epidemiology (WBE) research facility and the project is supported with funding of $1 million by CryptoRelief, an initiative started by Sandeep Nailwal.

The data obtained from various wastewater sources and treatment facilities will be analysed and made available to the public through dashboards. Gradually, this facility will be extended to other parts of India, said a release from IIT Madras.

Crypto Relief is the result of the global crypto community mobilising to help India combat the Covid crisis, and to help it prepare for future outbreaks, the release added.



NEWS18

## IIT Madras Professor Selected as Laureate of Prince Sultan Bin Abdulaziz International Prize for Water

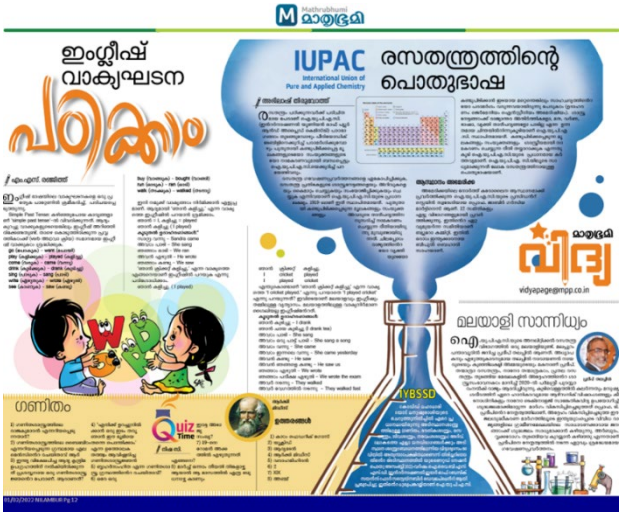
Prof. T. Pradeep's Research Group developed environmentally friendly 'water positive' nanoscale materials for the affordable, sustainable, and rapid removal of arsenic from drinking water.

The Indian Institute of Technology (IIT) Madras Prof Thalappil Pradeep has been selected as the laureate of the 10th edition of the prestigious 'Prince Sultan Bin Abdulaziz International Prize for Water' (PSIPW). He was selected for the Award under 'Creativity Prize' category given for 'breakthrough discovery' in any water-related field.

Prof. T. Pradeep's Research Group developed environmentally friendly 'water positive' nanoscale materials for the affordable, sustainable, and rapid removal of arsenic from drinking water. Prof. Pradeep has been recognized earlier with the Padma Shri, and Nikkei Asia Prize, among many others and his technologies are delivering clean water to over 1.2 crore people.

The bi-annual international scientific award was established on 21 October 2002 by Prince Sultan Bin Abdulaziz Al Saud of Saudi Arabia. The prize carries a cash component of $2,66,000 (Rs. 2 Crore Approx) besides a gold medallion, a trophy, and a certificate.

The awards ceremony will take place on September 12 at the United Nations Headquarters in New York. The award mentions Prof. T. Pradeep's team members - Avula Anil Kumar, Chennu Sudhakar, Sritama Mukherjee, Anshup, and Mohan Udhaya Sankar.




THE HINDU

## IIT Madras professor wins international prize

December 28, 2022 09:42 pm | Updated 09:42 pm IST – CHENNAI

**T. Pradeep recognised for his work on making potable groundwater accessible**

THE HINDU BUREAU

Indian Institute of Technology Madras professor T. Pradeep has been awarded the VinFuture Prize for his low-cost filtration system to remove arsenic and other heavy metals from groundwater.

VinFuture prizes are given in four categories annually and the award-winners are selected from around 1,000 nominations from 71 countries and recognise innovators from developing countries. The VinFuture Grand Prize worth $3 million includes three special prizes, each valued at $5,00,000 given to women innovators, innovators from developing countries, and innovators with outstanding achievement in emerging fields.

**This is only a selection of news reports, please see the group page for more.**
**https://pradeepresearch.org/**

# Initiatives

**Pradeep research group has started the following initiatives to disseminate the essence of science to the community at large**

## 1. Theory-Experiment Interface

**To watch the lectures please visit our youtube channel:**
**https://www.youtube.com/watch?v=HX022eoTzAQ&list=PL64fYMrIkSGw5WSREo-XKSJh8taBQ3uQc**

### Session 11 – 15/01/2022

1. **Dr. Sreeram K. Kalpathy, Department of Metallurgical and Materials Engineering delivered a talk on "Photochemical properties of Azobenzene-modified polyurea systems".**
2. **Dr. Basudev Roy, Department of Physics delivered a talk on "Study of pitch rotations in soft matter systems using optical tweezers".**
3. **Prof. Edamana Prasad, Department of Chemistry delivered a talk on "Novel 2D materials with luminescent organic molecules".**
4. **Dr. Pallab Basuri, Department of Chemistry delivered a talk on "Chemistry in microdroplets".**

### Session 12 – 19/02/2022

5. **Dr. Ashis Kumar Sen, Department of Mechanical Engineering delivered a talk on "Acoustic handling of interfaces in microfluidics".**
6. **Dr. Aravind Kumar Chandiran, Department of Chemical Engineering delivered a talk on "Halide perovskites for solar water splitting".**
7. **Dr. Kartik Chandra Mondal, Department of Chemistry delivered a talk on "Electro-chemical/Chemical Dinitrogen Reduction to Ammonia: Experimental and Theoretical calculations".**
8. **Dr. Raghavendra Sai V V, Department of Applied Mechanics delivered a talk on "Fiber optic sensors for Clinical diagnostics, Water and Food safety".**

### Session 13 – 26/03/2022

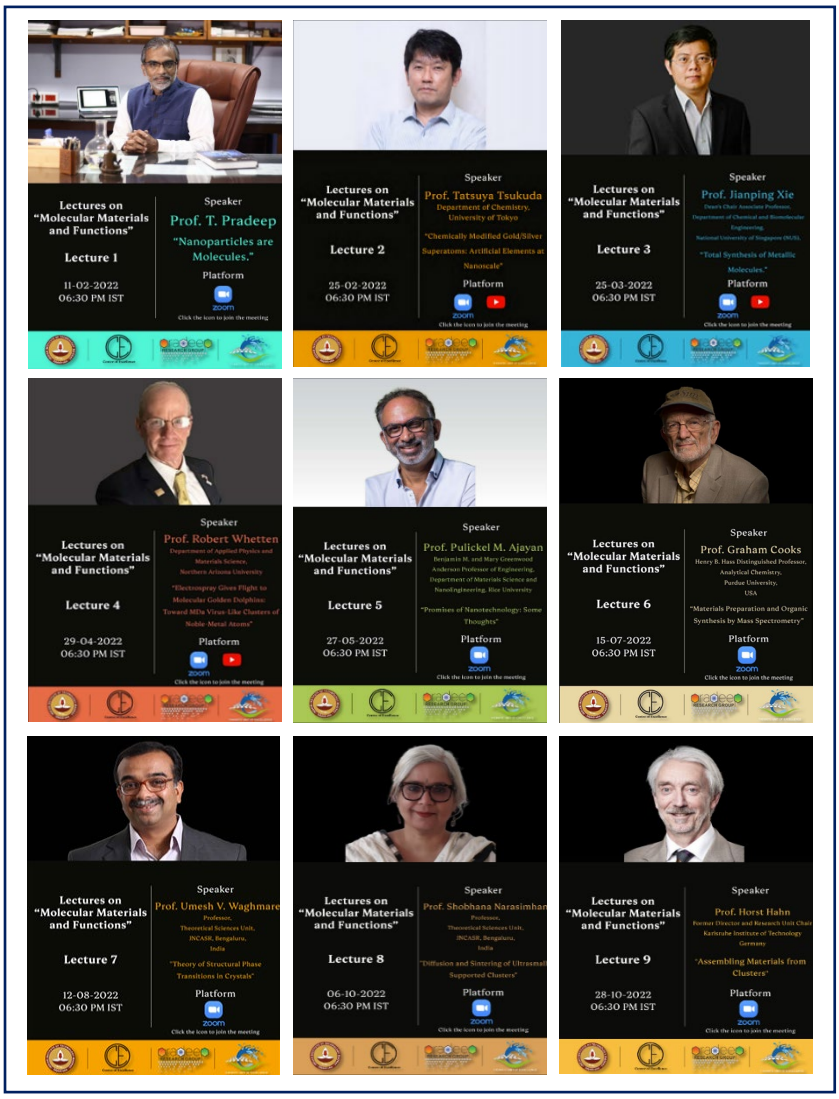
9. **Prof. Jitendra Sangwai, Department of Chemical Engineering delivered a talk on "Enhanced oil recovery using low salinity waterflooding".**
10. **Prof. Venkatesh Balasubramanian, Department of Engineering Design delivered a talk on "Journey on Road safety".**

11. **Prof. Rajakumar Balla, Department of Chemistry delivered a talk on "Laser spectroscopic methods in gas phase reactions relevant to the Earth's atmosphere".**

**Session 14 – 22/06/2022**

12. **Prof. Uday Chakkingal, Department of Metallurgical and Materials Engineering delivered a talk on "Some challenges in sheet metal forming research".**
13. **Dr. K. Sooraj, Department of Chemistry delivered a talk on "Development of High-Performance Electrode Materials for Li and Post-Li ion Batteries: Insights from Computations".**
14. **Dr. Vimal Edachery, Department of Mechanical Engineering delivered a talk on "Continously Variable Transmission: How surface topography and roughness influence lubrication, friction and scuffing".**

## 2. p-CoE on Molecular Materials and Functions lecture series




**To watch the lectures please visit our YouTube channel.**

# 3. Molecular Materials and Functions: An IIT Madras Conference

**The conference details are available at https://molmatter.org/**

# 4. Water for Life: An IIT Madras Conference

**The conference details are available at https://waterforlifeiitm.org/**

Sponsored by

AquaMAP · KENT Health Care Products · xylem Let's Solve Water · ICCW

## Water for Life

### An IIT Madras Conference - 2022

December 15-17, 2022

Campus Café Terrace Hall

NAC Rd, Indian Institute of Technology Madras,

Chennai, Tamil Nadu - 600036

**Prof. T. Pradeep**
Institute Professor
Deepak Parekh Institute Chair Professor
Department of Chemistry
IIT Madras

**Prof. Ligy Philip**
Institute Chair Professor
Department of Civil Engineering
IIT Madras

### Day 1 - December 15

| | |
|---|---|
| 08:30 AM - 09:00 AM | Registration |
| 09:00 AM - 09:15 AM | Inauguration/Prof. V. Kamakoti, Director, IITM |
| 09:15 AM - 10:45 AM | **Session 1 -** Chair: Prof. T. Pradeep<br>Prof. Richard Neil Zare<br>Prof. Rahul Raveendran Nair<br>Prof. Abhijit Patra |
| 10:45 AM - 11:00 AM | **Tea Break and Poster Arrangment** |
| 11:00 AM - 12:00 PM | **Session 2 -** Chair: Prof. Aravind Kumar Chandiran<br>Dr. J. Raghava Rao<br>Dr. S. V. Srinivasan |
| 12:00 PM - 12:45 PM | **Poster Session** |
| 12:45 PM - 01:00 PM | Group Photograph |
| 01:00 PM - 02:00 PM | **Lunch** |
| 02:00 PM - 04:00 PM | **Session 3 -** Chair: Prof. Edamana Prasad<br>Prof. V. V. Raghavendra Sai<br>Dr. S. Easwaramoorthi<br>Prof. Boby George<br>Shri Mahesh Gupta |
| 04:00 PM - 04:15 PM | **Tea Break** |
| 04:15 PM - 05:15 PM | **Session 4 -** Chair: Prof. Guhan Jayaraman<br>Prof. Kartik Chandran<br>Prof. Rita Henderson |
| 05:15 PM - 08:15 PM | Cultural Event - A trip to Music Academy<br>Dinner (up to individuals) |

### Day 2 - December 16

| | |
|---|---|
| 09:00 AM - 10:30 AM | **Session 5 -** Chair: Mr. Krishnan Narayanan<br>Prof. T. Pradeep<br>Shri Narain Madhavan/ Shri Tushar Tyagi<br>Prof. Chaitanya Lekshmi Indira |
| 10:30 AM - 10:45 AM | **Tea Break** |
| 10:45 AM - 12:15 PM | **Session 6 -** Chair: Prof. Indumathi Nambi<br>Prof. Amit Gross<br>Prof. P. C. Subumon<br>Prof. Ligy Philip |
| 12:15 PM - 01:15 PM | **Session 7 -** Chair: Mr. E. Nandakumar **(Panel Discussion)**<br>Mr. Anshup (Hydromaterials)<br>Dr. Soujit Sengupta (NGEN Water Solutions)<br>Mr. Ramesh Kumar (Vayujal Technologies)<br>Mr. Moinak Banerjee (Solinas Integrity)<br>Mr. Varun Sridharan (Greenvironment Innovation & Marketing India) |
| 01:15 PM - 02:30 PM | **Lunch** |
| 02:30 PM - 04:30 PM | **Session 8 -** Chair: Prof. Shankar Narasimhan<br>Prof. Balaji Narasimhan<br>Prof. Hadas Mamane<br>Prof. C. Subramaniam<br>Prof. L. Elango |
| 04:30 PM - 05:00 PM | **Tea Break** |
| 05:00 PM - 06:00 PM | **Session 9 -** Chair: Mr. Raghuttama Rao **(Panel Discussion)**<br>Shri T. M. Vijaya Bhaskar (IAS (retd.), Government of Karnataka)<br>Shri Narain Madhavan (Xylem)<br>Shri Ashok Natarajan (ICCW)<br>Dr. Rashmi Chansarkar (Marmon Water)<br>Dr. S. K. Sankar (Eureka Forbes) |
| 06:00 PM - 06:15 PM | Group Photograph |
| 06:15 PM Onwards | Conference Dinner |

### Day 3 - December 17

| | |
|---|---|
| 09:00 AM - 11:00 AM | **Session 10 -** Chair: Prof. Ligy Philip<br>Dr. Samuel Chigome<br>Prof. Jaichander Swaminathan<br>Prof. M. M. Shihabudheen<br>Prof. Shridharakumar Narasimhan |
| 11:00 AM - 11:15 AM | **Tea Break** |
| 11:15 AM - 12:30 PM | **Session 11 -** Chair: Prof. Rajnish Kumar **(Flash Talks)**<br>Dr. Deepanjan Sarkar<br>Dr. Gnanamani Elumalai<br>Dr. Tanvi Gupte<br>Prof. Raju K. Srinivasa/ Prof. A. Vasan<br>Mr. Pillalamarri Srikrishnarka<br>Prof. Gopala Krishna Darbha |
| 12:30 AM - 12:45 PM | Water Service in the city of Chennai and the need for linkages/Shri Jayasankar M. R. |
| 12:45 AM - 12:50 PM | Concluding Remarks/ Dr. Neelima Alam |
| 12:50 PM - 01:00 PM | Vote of Thanks/ Prof. T. Pradeep and Prof. Ligy Philip |
| 01:00 PM - 02:00 PM | **Lunch** |
| 02:00 PM onwards | Visit to IITM facilities/ Local markets/ Mahabalipuram |

Conference coordinators:
Mr. Ankit Nagar
Ph. no. +91 9840871968
Ms. Tanmayaa Nayak
Ph. no. +91 9438583353
Ms. Priya K.
Ph. no. +91 4422 57 5929
email: waterforlifeiitm@gmail.com
website: www.waterforlife.org

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# Awards and Honors

Prof. T. Pradeep has won the 10th Award (2022) of the Prince Sultan Bin Abdulaziz International Prize for Water (PSIPW).

Prof. T. Pradeep has been nominated as the National Representative for the Analytical Chemistry Division of the International Union of Pure and Applied Chemistry (IUPAC) for a period of two years, 2022-2023.

Prof. T. Pradeep receives the Prince Sultan Bin Abdulaziz International Prize for Water from H.E. Eng. Abdulrahman A. Al Fadley, the Saudi Minister of Environment, Water and Agriculture at the United Nations Office, Vienna on December 13, 2022

Prof. T. Pradeep has won the Vinfuture Special Prize for Innovators from Developing Countries.

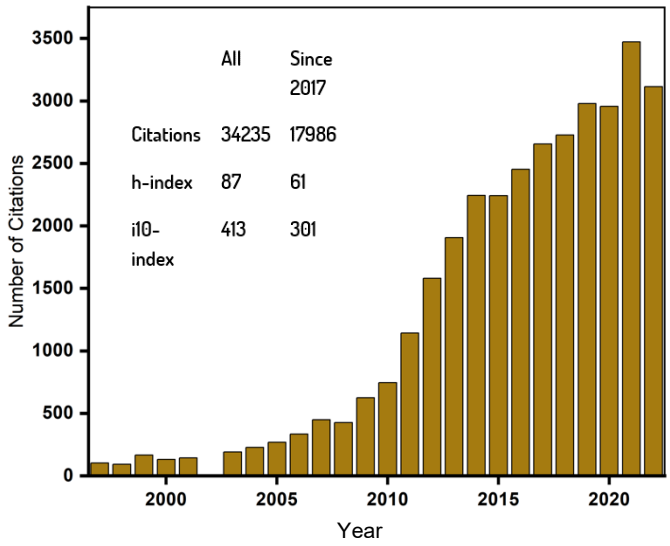

Prof. T. Pradeep receives the VinFuture Prize for Innovators from Developing Countries from Professor Thục-Quyên Nguyễn and Professor Albert P. Pisano, Co-chairs of the VinFuture Pre-screening Committee at the Hanoi Opera House, Hanoi, Vietnam on December 20, 2022.

Prof. T. Pradeep has been elected as a Fellow of the African Academy of Sciences.

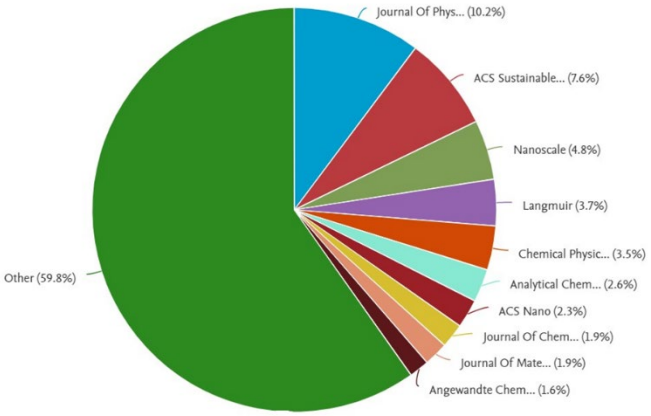
Prof. T. Pradeep has been selected for SASTRA-CNR Rao Award in Chemistry and Materials science for the year 2023.

# Publication Analysis

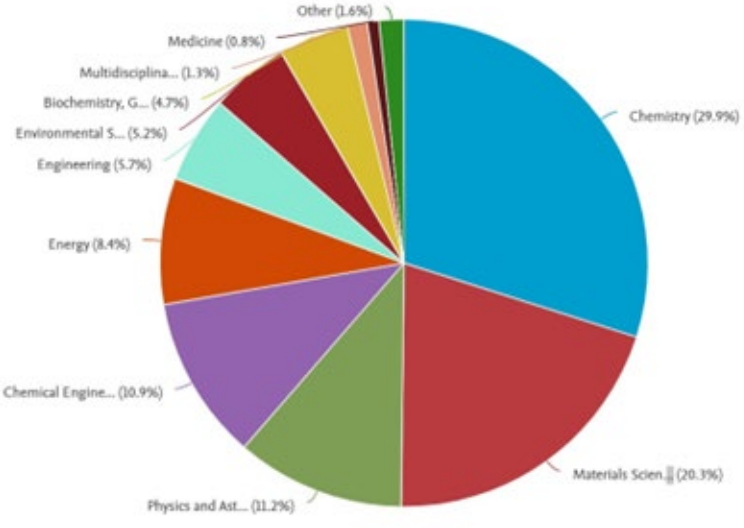
## Google Scholar

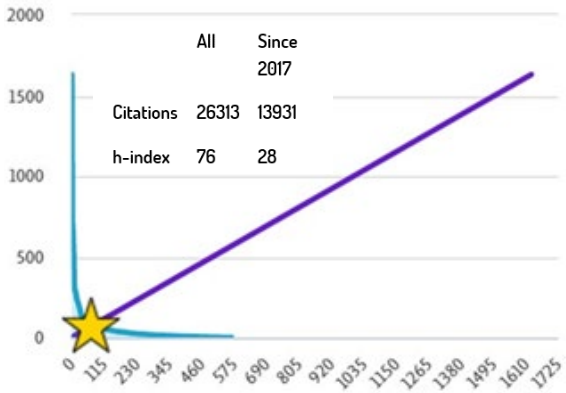



## By Source - Scopus




## Documents by subject area - Scopus




### Sources

1. Scopus, visited on December 31, 2022.
2. Google Scholar, visited on December 31, 2022.

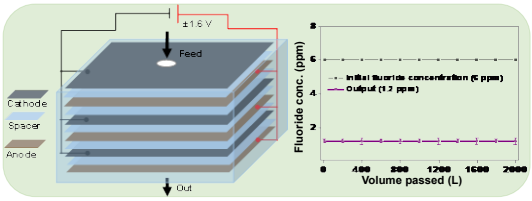
# Abstracts at a Glance

## Industrial Utilization of Capacitive Deionization Technology for the Removal of Fluoride and Toxic Metal Ions ($As^{3+/5+}$and$Pb^{2+}$)

Md Rabiul Islam, Soujit Sen Gupta, Sourav Kanti Jana, and Thalappil Pradeep

Global challenges, 2022, 6, 2100129 (DOI:10.1002/gch2.202100129)

Capacitive deionization (CDI) is an emerging desalination technology, particularly useful for removing ionic and polarizable species from water. In this context, the desalination performance of fluoride and other toxic species (lead and arsenic) present in brackish water at an industrial scale of a few kilo liters using a CDI prototype built by InnoDI Private Limited is demonstrated. The prototype is highly efficient in removing ionic contaminants from water, including toxic and heavy metal ions. It can remove fluoride ions below the World Health Organization (WHO) limit (1.5 ppm) at an initial concentration of 7 ppm in the input feed water. The fluoride removal efficiency of the electrodes (at a feed concentration of 6 ppm) deteriorates by ≈4–6% in the presence of bicarbonate and phosphate ions at concentrations of 100 ppm each. The removal efficiency depends on flow rate, initial total dissolved solids, and other co-ions present in the feed water. Interestingly, toxic species (As3+/5+ and Pb2+) are also removed efficiently (removal efficiency > 90%) by this technology. The electrodes are characterized extensively before and after adsorption to understand the mechanism of adsorption at the electrode.

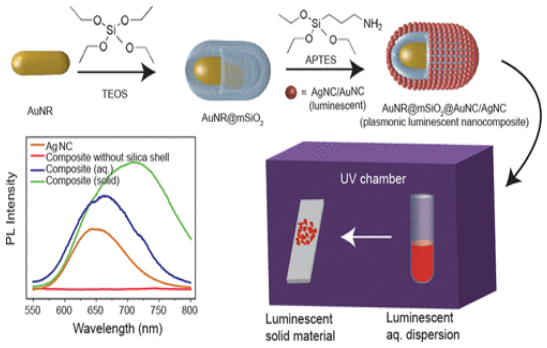



## Shell-Isolated Assembly of Atomically Precise Nanoclusters on Gold Nanorods for Integrated Plasmonic-Luminescent Nanocomposites

Amrita Chakraborty, Harsh Dave, Biswajit Mondal, Nonappa, Esma Khatun, and Thalappil Pradeep

The Journal of Physical Chemistry B, 2022, 126 (8), 1842-1851 (DOI: 10.1021/acs.jpcb.1c10207)

In this work, we integrate atomically precise noble metal nanoclusters (NCs) on gold nanorods (AuNRs) to create hybrid plasmonic-luminescent nanomaterials. Initially, we assemble luminescent Ag29(LA)12 NC (LA = lipoic acid) to silica shell encapsulated AuNRs. The resulting nanostructure shows plasmonenhanced luminescence in aqueous medium as well as in the solid state. Atomic precision of the fluorophores used in this case allows detailed characterization of individual nanocomposites by diverse techniques, including transmission electron microscopy (TEM) and 3D electron tomographic reconstruction. We extend this strategy to



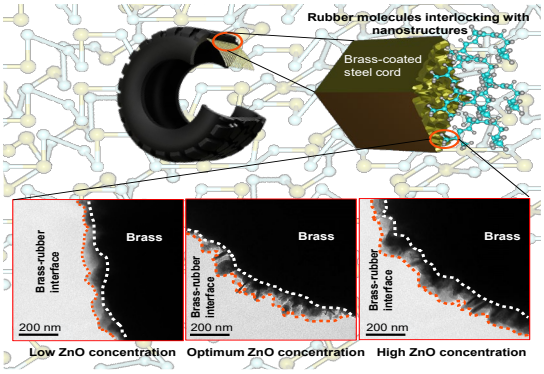

prepare similar structures with gold NC protected with bovine serum albumin (Au30BSA). These two examples demonstrate the generic nature of the present strategy in preparing plasmonic-luminescent hybrid nanostructures using atomically precise NCs.

## Role of Zinc Oxide in the Compounding Formulation on the Growth of Non-stoichiometric Copper Sulfide Nanostructures at Brass-Rubber Interface

Kannan MP, Anirban Som, Tripti Ahuja, Pillalamarri Srikrishnarka, Appukuttan Sreekumaran Nair, and Thalappil Pradeep

ACS Omega 2022, 7, 11, 9573−958 (DOI:10.1021/acsomega.1c06207)

Tire technology has evolved substantially by the introduction of brass-coated steel cords (BCSCs) in radial tires. The durability of radial tires is dependent on the integrity of the brass−rubber interface composed predominantly of nonstoichiometric copper sulfide ($Cu_{2-x}S$, where $x$ = 1 to 2) nanostructures whose morphology and characteristics are dependent upon the crucial rubber additive, ZnO. Its higher concentration impacts environmental



sustainability, while at lower levels, there is insufficient bonding between steel and the rubber thus affecting tire's safety. This brings in the need for an optimum ZnO concentration to be used in radial tires and is thus the theme of the present work. The changes in the properties of interfacial nanostructures such as morphology, thickness, crystallinity, and chemical composition were studied at various ZnO concentrations. We adopted our previously reported methodology, the "brass mesh experiment", to investigate the thickness of nanostructures at varied ZnO concentrations using transmission electron microscopy (TEM). Significant results were obtained from field-emission scanning electron microscopy (FESEM), X-ray diffraction (XRD), Raman imaging and X-ray photoelectron spectroscopy (XPS). In conjunction with a more practical experimental technique, namely the measurement of pull-out force (POF), it has been concluded that 9 parts per hundred rubber (PHR) ZnO is essential for the optimum growth of nanostructures and is considered to be the optimum for the composition studied. We believe that the scientific approach outlined in the manuscript would help the tire- and the material science communities to widen the knowledge of understanding sustainability in tire industries. It is estimated that the optimization presented here can save $400–450 million for the tire industry and 2.4 million tons of ZnO per year.

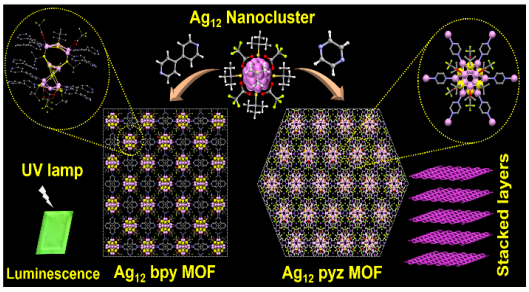
## Molecular Engineering of Atomically Precise Silver Clusters into 2D and 3D Framework Solids

Wakeel Ahmed Dar, Arijit Jana, Korath Shivan Sugi, Ganesan Paramasivam, Mohammad Bodiuzzaman, Esma Khatun, Anirban Som, Ananthu Mahendranath, Amrita Chakraborty and Thalappil Pradeep

Chem. Mater. 2022, 34, 10, 4703–4711 (DOI: 10.1021/acs.chemmater.2c00647)

Two and three-dimensional (2D and 3D) atomically precise nanocluster (NC)-based metal-organic frameworks (MOFs) with properties richer than those of NCs themselves are emerging materials. However, fabricating such materials with good stability has not been easy. In this work, a facile synthetic strategy was employed for the creation of silver NC-MOFs starting from $[Ag_{12}(TBT)_7(TFA)_4(CH_3CN)_6]^+$, facilitated by heterocyclic amines, 4, 4′-bipyridine (bpy) and pyrazine (pyz), *via* metal-metal and metal-sulphide rearrangement reactions, where TBT and TFA are tertiarybutylthiolate and trifluoroacetate, respectively. In one of the reactions, pyz ligand facilitates the

formation of a 2D framework with a trigonal crystal system, which exhibits high stability, and emits bright green luminescence at low temperature. Owing to its facile synthesis, good stability, efficient luminescence, uniform porosity, and layered structure, the resultant hexagonal 2D nanosheets can be efficiently exfoliated from parent crystals. 2D nanosheets are structurally similar to graphene. A top-down approach was employed for the exfoliation of stable 2D nanosheets with lateral dimensions in the range of 0.156 mm. In another case, the bpy ligand induces the construction of a 3D framework with an orthorhombic crystal system. Owing to its interpenetrated AB...AB structure, robustness and efficient green luminescence at room temperature, the resultant 3D MOF is capable of functioning as a high-performance luminescent sensor for selective detection of explosive analogues, 2-nitrotoluene (NT) and 2, 4-dinitrotoluene (DNT), with excellent recyclability. However, in the absence of the heterocyclic amines, a pristine AgNC was formed. Time-dependent density functional theory (TD-DFT) calculations were employed to understand the mechanism of energy transfer in AgNC-MOFs. Our strategy offers an unprecedented approach in which heterocyclic amines



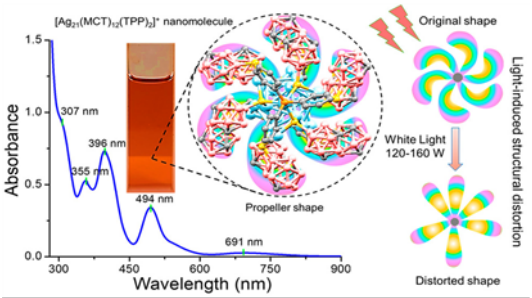

facilitate intramolecular rearrangement reactions, resulting in 2D and 3D atomically precise NC framework materials. This work not only demonstrates the creation of 2D and 3D materials but also provides new insight into the critical surface coordination chemistry controlled by heterocyclic amines for defining the morphology and properties of cluster framework.

## Carboranethiol-Protected Propeller-Shaped Photoresponsive Silver Nanomolecule

Arijit Jana, Parvathy M. Unnikrishnan, Ajay K. Poonia, Jayoti Roy, Madhuri Jash, Ganesan Paramasivam, Jan Machacek, Kumaran Nair Valsala Devi Adarsh, Tomas Base, and Thalappil Pradeep

Inorg. Chem. 2022, 61, 23, 8593–8603 (DOI:10.1021/acs.inorgchem.2c00186)

We report the synthesis, structural characterization, and photophysical properties of a propeller-shaped Ag21 nanomolecule with six rotary arms, protected with m-carborane-9-thiol (MCT) and triphenylphosphine (TPP) ligands. Structural analysis reveals that the nanomolecule has an Ag13 central icosahedral core with six directly connected silver atoms and two more silver atoms connected through three Ag–S–Ag bridging motifs. While 12 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 a silver sulfide staple motif is opposite to the orientation of carborane ligands, resembling the existence of a bidirectional rotational orientation in the nanomolecule. Careful analysis reveals that the orientation of carborane ligands on the cluster's surface resembles an assembly of double rotors. The zero circular dichroism signal indicates its achiral nature in solution. There are multiple absorption peaks in its UV–vis absorption spectrum, 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 with increasing collision energy. Its multiple optical



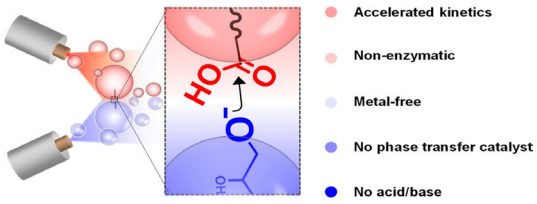

absorption features are in good agreement with the theoretically calculated spectrum. The cluster shows a narrow near-IR emission at 814 nm. The Ag21 nanomolecule is thermally stable at ambient conditions up to 100 °C. However, white-light illumination (lamp power = 120–160 W) shows photosensitivity, and this induces structural distortion, as confirmed by changes in the 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 carriers, spread over a broad wavelength region of 520–650 nm. The formation of core-centered long-lived carriers in the excited state is responsible for the observed light-activated structural distortion.

# Accelerated Non-Enzymatic Fatty Acid Esterification during Microdroplet Collision: A Method for Enhanced Sustainability

Pallab Basuri, Jenifer Shantha Kumar, Subhashree Das, and Thalappil Pradeep

ACS Sustainable Chem. Eng. 2022, 10, 26, 8577–8587 (DOI:10.1021/acssuschemeng.2c02070)

Accelerated non-enzymatic and metal-free "reaction and extraction" of sugar esters at the interface of two immiscible liquid microdroplets is demonstrated. The bimolecular reaction occurs by collision of microdroplets originating from two home-built electrospray sonic ion sources, carrying sugar molecules in water and long-chain fatty acids in toluene, respectively. Our method shows that the rate of reaction is enhanced ~107 times in comparison to the bulk, initiated by ultrasonic activation. Such a high rate of reaction in the microdroplets can be attributed to factors such as surface activity, concentration enhancement, partial solvation, and temperature-assisted dehydration of the species occurring in microdroplets. We provide evidence for an interfacial nucleophilic addition–elimination reaction mechanism. This method of synthesis is extended to 18 similar reactions. Microdroplet synthesis offers a sustainable method for biphasic reactions, eliminating the need for phase transfer reagents and activating agents such as acids/bases, metals, or enzymes.

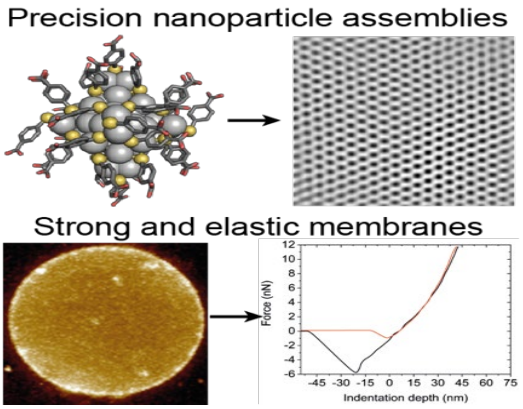


## Strong and elastic membranes via hydrogen bonding directed self-assembly of atomically precise nanoparticles

Anirban Som, Alessandra Griffo, Indranath Chakraborty, Hendrik Hähl, Biswajit Mondal, Amrita Chakraborty, Karin Jacobs, Päivi Laaksonen, Olli Ikkala, Thalappil Pradeep, Nonappa

Small, 2022, 2201707 (DOI:10.1002/smll.202201707

Two-dimensional (2D) nanomaterials have provided an extraordinary palette of mechanical, electrical, optical, and catalytic properties. Ultranthin 2D nanomaterials have classically been produced via exfoliation, deposition, or advanced synthesis using a handful of starting materials. Thus, there is a need to explore more generic avenues to expand the feasibility to the next generation 2D materials beyond atomic and molecular-level covalent networks. In this context, self-assembly of atomically precise noble nanoparticles could, in principle, suggest modular approaches for new generation 2D materials, provided ligand engineering allows symmetry breaking and directional internanoparticle interaction. Here we demonstrate the self-assembly of silver nanoclusters (NCs) capped with p-mercaptobenzoic acid ligands ($Na_4Ag_{44}$-$pMBA_{30}$) into large area free-standing membranes by trapping the NCs in a transient solvent layer at air-solvent interfaces. The patchy distribution of ligand bundles



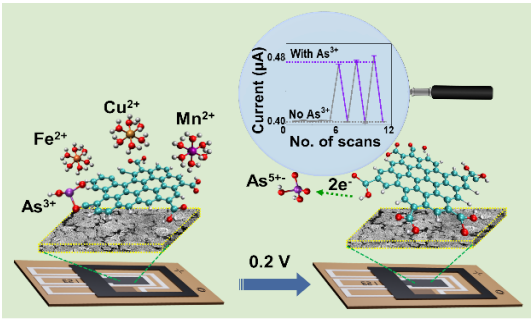

facilitates symmetry breaking and preferential intralayer hydrogen bondings resulting in strong and elastic membranes. The membranes with Young´s modulus of 14.5 ± 0.2 GPa can readily be transferred to different substrates. The assemblies allow detection of Raman active antibiotic molecules with high reproducibility without any need for substrate pretreatement.

## Selective and Practical Graphene-Based Arsenite Sensor at 10 ppb

Sourav Kanti Jana, Kamalesh Chaudhari, Md Rabiul Islam, Ganapati Natarajan, Tripti Ahuja, Anirban Som, Ganesan Paramasivam, Addanki Raghavendra, Chennu Sudhakar, and Thalappil Pradeep

ACS Appl. Nano Mater. 2022, 5, 11876−11888 (DOI:10.1021/acsanm.2c02860)

Arsenic detection in field water samples at concentrations of relevance with affordable and simple equipment is of global interest. We report a bio-mimetic electrode using electrochemically reduced graphene oxide (ERGO) for highly selective and sensitive reagent-free arsenite ($As^{3+}$) detection in field water samples, down to ten parts per billion levels, enabling measurement of drinking water quality affordably for millions of arsenic affected people. This electronically and structurally optimized ERGO electrode shows selective detection of $As^{3+}$ in both phosphate buffered saline (PBS, pH~7) and field water samples, even though over 100 times larger conductivity and total dissolved solids (TDS), respectively are present in them. Raman and FTIR spectroscopies were used to understand the mechanism of selectivity and sensitivity. The sensing mechanism involved two processes, namely, selective binding of $As^{3+}$ with the -COOH groups of ERGO followed by its electro-oxidation by an applied potential. Density functional theory (DFT) and force-field calculations were used to obtain crucial insights into the site selectivity and mechanism of oxidation of $As^{3+}$. A two-



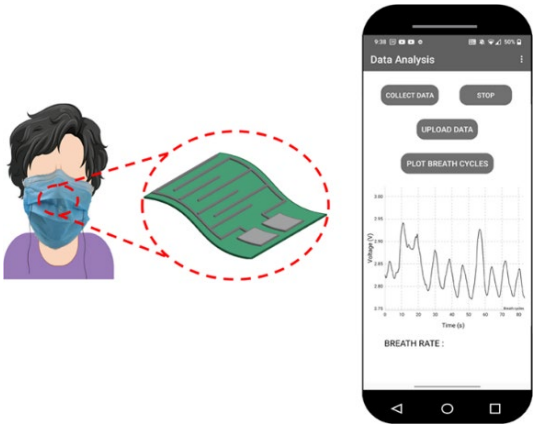

electron transfer process from $As^{3+}$ to ERGO followed by associative O ligand addition to $As^{3+}$ by a ketone oxygen atom, and concomitant regeneration of -COOH group is presented. The ion selectivity depends both on structural and electronic factors. Firstly, the compact pyramidal-shaped $As^{3+}$ species may closely approach the edge -COOH functional group to a greater extent than the other ions enabling covalent binding of the As center with the ketone O atom. Furthermore, closer proximity of the lowest unoccupied molecular orbital (LUMO) acceptor level of the positively-charged ERGO and the highest occupied molecular orbital (HOMO) donor level of the $As^{3+}$ species suggests that a uniquely-selective resonant charge-transfer effect occurs between the $As^{3+}$ species and ERGO.

## Toward continuous breath monitoring on a mobile phone using a frugal conducting cloth-based smart mask

Pillalamarri Srikrishnarka, Raaga Madhuri Dasi, Sourav Jana, Tripti Ahuja, Jenifer Shantha Kumar, Ankit Nagar, Amoghavarsha Kini, Boby George, and Thalappil Pradeep

ACS Omega 2022, 7, 47, 42926–42938 (DOI: 10.1021/acsomega.2c05017)

A frugal humidity sensor that can detect changes in the humidity of exhaled breath of individuals has been fabricated. The sensor comprises a humidity-sensitive conducting polymer that is in situ formed on a cloth that acts as a substrate. Interdigitated silver electrodes were screen-printed on the modified cloth, and conducting threads connected the electrodes to the measurement circuit. The sensor's response to changing humidity was measured as a voltage drop across the sensor using a microcontroller. The sensor was capable of discerning between fast, normal, and slow breathing based on the response time. A response time of ~1.3 s was observed for fast breathing. An Android-based mobile



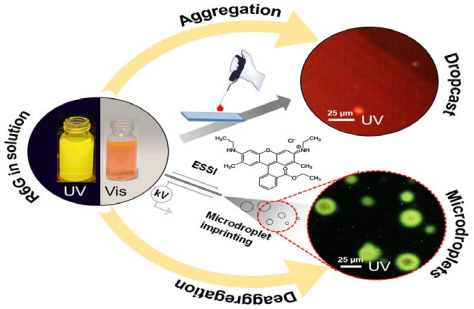

application was designed to collect sensor data *via* Bluetooth for analysis. A time series classification algorithm was implemented to analyze patterns in breathing. The sensor was later stitched onto a face mask, transforming it into a smart mask that can monitor changes in the breathing pattern at work, play, and sleep.

## Aggregation of molecules is controlled in microdroplets

Pallab Basuri, Jenifer Shantha Kumar, Keerthana Unni, Sujan Manna, and Thalappil Pradeep

Chem. Comm.,2022, 58, 12657-12660. (DOI: 10.1039/D2CC04587G)

Molecular de-aggregation was observed at the air/water interface of aqueous microdroplets. We probed this phenomenon using dyes such as Rhodamine 6G (R6G), Rhodamine B, acridine orange, and fluorescein, which show aggregation-induced shift in fluorescence. The fluorescence micrographs of microdroplets derived from the aqueous solutions of these dyes show that they are monomeric at the air/water interface, but highly aggregated at the core. We propose that rapid evaporation of the solvent influences the de-aggregation of molecules at the air–water interface of the microdroplets

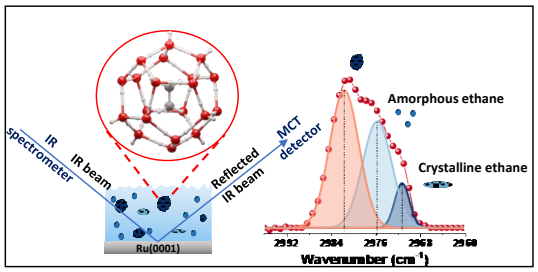



## Formation of Ethane Clathrate Hydrate in Ultrahigh Vacuum by Thermal Annealing

Bijesh K. Malla, Gaurav Vishwakarma, Soham Chowdhury, Premkumar Selvarajan, and Thalappil Pradeep

J. Phys. Chem. C 2022, 126, 42, 17983–17989 (DOI: 10.1021/acs.jpcc.2c06264)

The existence of many molecules in the form of clathrate hydrates (CHs) in ultrahigh vacuum (UHV) and cryogenic conditions has not been explored adequately. In the present study, a detailed investigation by reflection absorption infrared spectroscopy confirmed that the three phases of ethane, i.e., amorphous, crystalline, and CH, coexist in a




vapor-deposited ethane–water mixture at 60 K in UHV. Experiments were conducted with vapor-deposited ice films at 10 K, which were

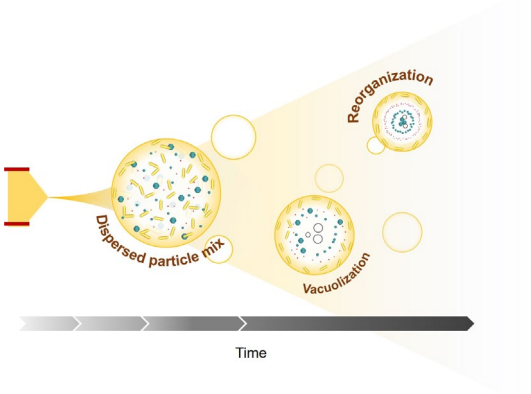
annealed to 60 K for tens of hours, and the IR spectral evolution was monitored systematically. Upon maintaining the system at 60 K, three phases of ethane were seen to coexist, but a gradual increase in the hydrate phase was noticed. The evolution of ethane CH from the amorphous ethane–water ice mixture was observed for the very first time in UHV under cryogenic conditions. The formation of the CH was further confirmed by temperature-programmed desorption (TPD) mass spectrometry. Quantum chemical calculation suggested the formation of $5^{12}6^2$ cage of structure I CH in the ice matrix. The formation of ethane CH in a thin ice film at such a low temperature under UHV suggests its existence in the cometary environment.

## Spatial reorganization of analytes in charged aqueous microdroplets

Pallab Basuri, Amrita Chakraborty, Tripti Ahuja, Biswajit Mondal, Jenifer Shantha Kumar, and Thalappil Pradeep

Chem. Sci., 2022, 13 ,13321-13329 (DOI: 10.1039/D2SC04589C)

Imprinted charged aqueous droplets of micrometer dimensions containing spherical gold and silver nanoparticles, gold nanorods, proteins and simple molecules were visualized using dark-field and transmission electron microscopies. With such studies, we hoped to understand the unusual chemistry exhibited by microdroplets. These droplets with sizes in the range of 1–100 μm were formed using a home-built electrospray source with nitrogen as the nebulization gas. Several remarkable features such as mass/size-selective segregation and spatial localization of solutes in nanometer-thin regions of microdroplets were visualized, along with the formation of micro–nano vacuoles. Electrospray parameters such as distance between the spray tip and surface, voltage and nebulization gas pressure influenced particle distribution within the droplets. We relate these features to unusual phenomena such as the enhancement of rates of chemical reactions in microdroplets.

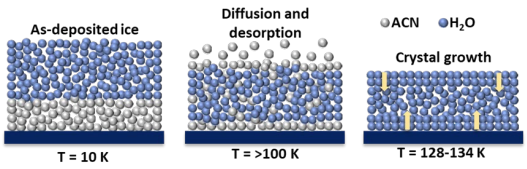


## Rapid crystallization of amorphous solid water by porosity induction

Gaurav Vishwakarma, Bijesh K. Malla, Rabin Rajan Methikalam, and Thalappil Pradeep

Phys. Chem. Chem. Phys., 2022, 24, 26200-26210 (DOI: 10.1039/D2CP02640F)

Rapid crystallization of amorphous solid water (ASW) is often associated with crystallization that initiates at random nucleation sites in the bulk and expands in all directions. In this work, by preparing sandwich films of acetonitrile (ACN) and ASW in the form of ACN@ASW and ASW@ACN in an ultrahigh vacuum (UHV), we demonstrate a new method for rapid crystallization of ASW via ACN diffusion-desorption induced porosity in the ASW matrix even in the window of 128-134 K, well below the normal crystallization temperature of 155 K. By placing an HDO (5% $D_2O$ in $H_2O$) probe layer in ASW, we found that when ACN diffuses and desorbs through ASW, it induces ASW crystallization where the crystal grows both from the top and from the bottom simultaneously into the bulk. Crystallization kinetics and activation energy ($E_a$) for the formation of crystalline ice (CI) were evaluated using the Avrami equation and were compared with the previous reports. The evaluated $E_a$ was ~53 kJ $mol^{-1}$, close to the $E_a$ of crystal growth (47-56 kJ·$mol^{-1}$) and it suggested the absence of a nucleation process and supported rapid crystallization. Such occurrence of CI due to diffusion of ACN suggests a possible mechanism for the former's existence in many astrophysical environments.




## Ion-Exchanging Graphenic Nanochannels for Macroscopic Osmotic Energy Harvesting

Ankit Nagar, Md Rabiul Islam, Kartheek Joshua, Tanvi Gupte, Saurav Kanti Jana, Sujan Manna, Tiju Thomas and Thalappil Pradeep

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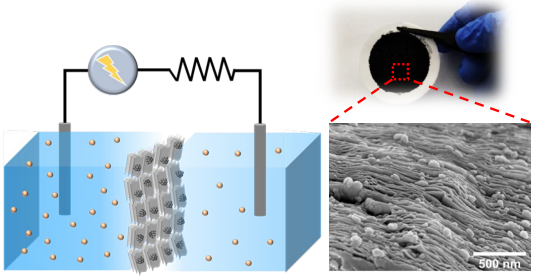
The Gibbs free energy difference between seawater and river water can be tapped by selective ion transport across charged nanochannels, referred to as reverse electrodialysis (RED). However, existing single pore and micro-/ nano- fluidic RED systems

have shown poor prospects for scalability and practical implementation. Herein, we present a macroscopic RED system, utilizing a cation- or an anion-selective membrane. The membranes comprise reduced graphene oxide (rGO) nanosheets decorated uniformly with $TiO_2$ nanoparticles. The nanosheets are covalently functionalized with polystyrene (PS), and subsequently linked to sulfonate or quaternary amine functional groups to obtain cation- and anion- selectivity, respectively. The membranes show excellent ion transport properties along with high power densities demonstrated under artificial salinity gradients. The cation-exchange membrane (CEM) delivered a power density of 448.7 mW $m^{-2}$ under a 500-fold concentration gradient, while anion-exchange membrane (AEM) produced a substantial power output of 177.8 mW $m^{-2}$ under a similar gradient. The




efficiencies ranged from 10.6% to 42.3% for CEM, and 9.7% to 46.1% in the case of AEM. Testing under varying pH conditions revealed higher power output under acidic conditions and substantial power output across the entire pH range, rendering them practically viable for sustainable energy harvesting in acidic and alkaline wastewaters.

## Human Skin-Cell-Based Sensor for Environmental Arsenic Detection and for Creating Social Awareness

Tanvi Gupte, Suryalakshmi Pandurangan, Md Rabiul Islam, Pillalamarri Srikrishnarka, Ankit Nagar, Niraikulam Ayyadurai, Tiju Thomas, Thalappil Pradeep

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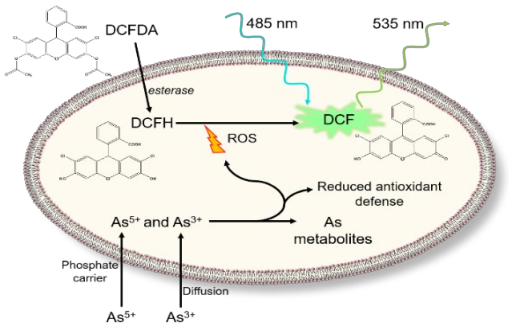
Arsenic (As) toxicity is a significant threat to global public health. Moreover, lack of social awareness and understanding of the impact of As in the affected communities are also of concern. Therefore, sub-ppm level detection of As in environmental waters and associated public awareness are crucial for remediation programs. We developed a sustainable As sensing methodology by merging the fundamental concepts of As cytotoxicity with



an alternative approach for selectivity. A cellular platform was prepared on an electrospun scaffold using As-sensitive keratinocyte cells. Arsenic-induced reactive oxygen species (ROS) were quantified using a fluorimetric probe, 2′,7′-dichlorofluorescin diacetate, commonly used to detect oxidative stress within cells. Experiments were conducted with a mixture of arsenite and arsenate, the predominant forms of As present in natural conditions, in 1:1 ratio. We also quantified unknown As concentrations in real water samples. The selectivity to As was achieved by exposing the contaminated water composed of several ions to an As adsorbing material, namely, confined metastable 2-line ferrihydrite (CM2LF). An adsorption-desorption protocol enabled As extraction in field conditions. The ROS resulting from cells' responses to the As extract was used as the signature of As concentration. The sensor could precisely quantify even 5 ppb of As in tap water and the theoretical limit of detection (LOD) was 2.7 ppb. A sustainable device using the cellular platform is proposed for As detection in field conditions that can also be used for social awareness, demonstrating the impact of As on human biology in affected regions.

## Phosphine protected atomically precise silver-gold alloy nanoclusters and their luminescent superstructures

Madhuri Jash, Arijit Jana, Ajay K. Poonia, Esma Khatun, Papri Chakraborty, Ankit Nagar, Tripti Ahuja, K.V. Adarsh, and Thalappil Pradeep

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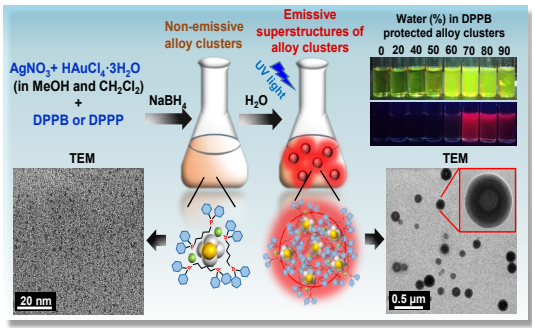
Superstructures made by assemblies of metal nanoclusters (NCs) have gained interest due to their atomic precision and exciting photophysical properties. Although there are some reports of cluster assembled materials of NCs protected with thiols, the preparation of stable thiol-free analogs is largely unexplored due to the poor stability of such structures. Herein we report the synthesis of




phosphine protected alloy NCs of silver with varying gold doping and superstructures of such systems. We show that alloying of

phosphine protected silver clusters with gold results in comparatively more stable clusters than weakly ligated hydride and phosphine co-protected silver clusters. Two new Ag-Au alloy cluster series, $[Ag_{11-x}Au_x(DPPB)_5Cl_5O_2]^{2+}$, x = 1-10 ($Ag_{11-x}Au_x$ in short) and $[Ag_{15-x}Au_x(DPPP)_6Cl_5]^{2+}$, x = 1-6 ($Ag_{15-x}Au_x$ in short) have been synthesized using two different phosphines, DPPB (1,4-bis(diphenylphosphino)butane) and DPPP (1,3-bis(diphenylphosphino)propane), respectively. These alloy clusters possess aggregation-induced emission (AIE) property, which was unexplored till now for phosphine protected silver clusters. Visibly non-luminescent methanol solution of these clusters showed strong red luminescence in presence of water, due to formation of cluster-assembled spherical hollow superstructures without any template. Solvophobic effect along with π···π and C-H···π interactions in the ligand shell make the alloy NCs assemble compactly within the hollow spheres. The assembly makes them highly emitting due to the restriction of intramolecular motion. The emissive states of the alloy clusters show many-fold increase in lifetime in presence of water. Femtosecond transient absorption studies revealed the lifetime of the excited state charge carriers in their monomeric and aggregated states. Apart from enriching the limited family of phosphine protected silver alloy NCs, the work also provides a new strategy to build controlled assembly of NCs with tailored luminescence. These materials could be new phosphors for applications in composites, sensors, thin films, and photonic materials.

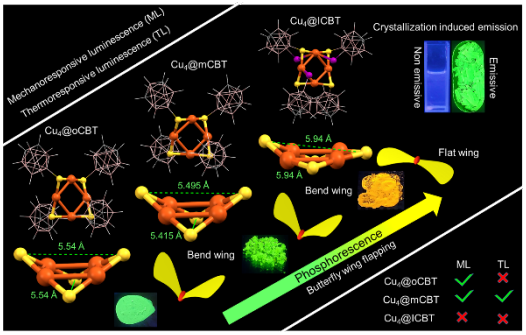
## Carborane-thiol protected copper nanoclusters: Stimuli-responsive materials with tunable phosphorescence

Arijit Jana, Madhuri Jash, Wakeel Ahmed Dar, Jayoti Roy, Papri Chakraborty, Ganesan Paramasivam, Sergei Lebedkin, Kaplan Kirakci, Sujan Manna, Sudhadevi Antharjanam, Jan Machacek, Monika Kucerakova, Sundargopal Ghosh, Kamil Lang, Manfred M. Kappes, Tomas Base and Thalappil Pradeep

Chem. Sci., (DOI:10.1039/D2SC06578A)

Atomically precise nanomaterials with tunable solid-state luminescence attract global interest. In this work, we present a new class of thermally stable isostructural tetranuclear copper nanoclusters (NCs), shortly $Cu_4$@oCBT, $Cu_4$@mCBT and $Cu_4$@ICBT, protected by nearly isomeric carborane thiols: *ortho*-carborane-9-thiol, *meta*-carborane-9-thiol and *ortho*-carborane 12-iodo 9-thiol, respectively. They have a square planar $Cu_4$ core and a butterfly-shaped $Cu_4S_4$ staple, which is appended with four

respective carboranes. For $Cu_4$@ICBT, strain generated by the bulky iodine substituents on the carboranes makes the $Cu_4S_4$ staple flatter in comparison to other clusters. High-resolution electrospray ionization mass spectrometry (HR ESI-MS) and collision energy-dependent fragmentation, along with other spectroscopic and microscopic studies confirm their molecular structure. Although none of these clusters show any visible luminescence in solution, bright μs-long phosphorescence is observed in crystalline form. The $Cu_4$@oCBT and $Cu_4$@mCBT NCs are green emitting with quantum yields (Φ) of 81 and 59 %, respectively, whereas $Cu_4$@ICBT is orange emitting with a Φ of 18 %. Density functional theory (DFT) calculations reveal the nature of their respective electronic transitions. The green luminescence of $Cu_4$@oCBT and $Cu_4$@mCBT clusters get shifted to yellow after mechanical grinding, but it is regenerated after exposure to solvent




vapor, whereas the orange emission of $Cu_4$@ICBT is not affected by mechanical grinding. Structurally flatten $Cu_4$@ICBT didn't show mechonoresponsive luminescence in contrast to other clusters, having bent $Cu_4S_4$ structures. $Cu_4$@oCBT and $Cu_4$@mCBT are thermally stable up to 400 °C. The $Cu_4$@oCBT retained green emission even upon heating to 200 °C under ambient conditions, while $Cu_4$@mCBT changed from green to yellow in the same window. This is the first report on structurally flexible carborane thiol appended $Cu_4$ NCs having stimuli-responsive tunable solid-state phosphorescence behavior.

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