# ANNUAL REPORT 2024











# 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

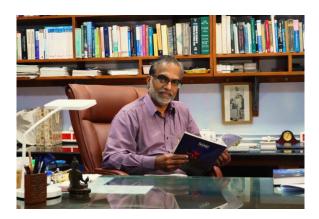
Fax: +91-44-22570545/0509

Email: <a href="mailto:pradeep@iitm.ac.in">pradeep@iitm.ac.in</a>

Laboratories: DST Unit of Nanoscience

and Thematic Unit of Excellence

Web: <a href="https://pradeepresearch.org/">https://pradeepresearch.org/</a>



Our struggle is to be creative every day.

#### Ph.D. students

- A. Suganya\*
- Amoghavarsha R. Kini
- Anagha Jose
- Anubhav Mahapatra
- Atrayee Datta
- Bijesh K. Malla
- B. S. Sooraj
- Deepak Kumar Patel\*

- Harshita Nagar
- Keerthana Unni
- Khusboo Saluja
- Riya Dutta
- Samapti Mondal
- Sinchan Mukhopadhyay
- Soham Chowdhury
- Sonali Seth

- Subrata Bag
- Subrata Duary
- Sujan Manna
- Swetashree Acharya
- Tanmayaa Nayak
- Vivek Yadav
- \* Jointly advised students

#### MS students

• S. Sudhir

#### Postdoctoral fellows/ Project associates

- Dr. Anirban Som
- Dr. A. Parthasarathy
- Dr. Anish R Nath
- Dr. Lopamudra Acharya
- Dr. Rival Jose
- Dr. Sourav Kanti Jana
- Karthika Kalyansundar
- S. Jayaram

#### International visiting fellows

- Dr. Egor Moses
- Dr. Nebil Omri

#### Administrative officer

• K. Priya

#### M.Sc./Visiting students

- Saloni Gupta
- Usha
- P. Jamshiya Sulthana
- Devansh Paliwal
- Abhijit Gupta
- Ankita Sasmal<sup>\$</sup>
- V. Sneha<sup>\$</sup>

- S. Srijina<sup>\$</sup>
- Aastha Thapa<sup>\$</sup>
- K. M. Hanoona
- P. K. Jabin Shabanu<sup>\$</sup>
- K. S. Aswathi \$
- Sparsh Saraswat<sup>\$</sup>
- Teena J Mathew<sup>\$</sup>

- Sofia Sara Baji<sup>\$</sup>
- Gayathri Goud<sup>\$</sup>
- Swathi V. Iyer<sup>\$</sup>
- S. Radhika Bharathi\$
- Lalchhanchhuaha\$
- Hminga Fanai<sup>\$</sup>
- \$ Students from other institutions

#### **Project technicians**

- S. Balamurugan
- S. Bhanupriya
- C. Meyyarasan
- Gokul Raja
- T. Venkatesan
- M. Dhananjayan

#### International joint students/Postdocs

- Suzan Kagan\*
- Sapir Assayag
- Alexandra Skliarevskaja
- Itay Eldar
- Dr. Maya Khatun

\* Jointly advised PhD student from Tel Aviv University

#### Lab attendants

- Chitra Ganavel
- Merlin Martin
- Sasikala Sudhakar

#### Centre of Excellence (CoE) on Molecular Materials and Functions

#### CoE fellows

- Dr. Depanjan Sarkar
- Dr. Mathew Joseph
- Dr. Ramya Dwivedi
- Dr. Rahul Kumar

micriational joint students, rostages

# What's Inside

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# Glimpses of 2024



The Book, "Technological Solutions for Water Sustainability: Challenges and Prospects: Towards a Water-Secure India" edited by Ligy Philip, Thalappil Pradeep, and S. Murty Bhallamudi, was released by Shri M.K. Narayanan, 19<sup>th</sup> Governor of West Bengal and former NSA, on March 22, 2024.



Inauguration of ANRF National facility of Cryo-EM at IIT Madras, by Prof. Abhay Karandikar, Secretary, DST, along with Prof. V. Kamakoti, Director, IIT Madras, and Prof. T. Pradeep, on August 28, 2024.



Participants of the 11<sup>th</sup> edition of AsiaNano Conference on Nanoscience and Nanotechnology, IIT Madras held during September 23–25, 2024.



Participants of the 1<sup>st</sup> International Symposium on Cryo-Electron Microscopy, IIT Madras, on August 10, 2024.



Participants of the 2<sup>nd</sup> edition of the Centre of Excellence International Winter School on Molecular Materials and Functions 2024, IIT Madras held during December 4–8, 2024.



Participants of the 2<sup>nd</sup> edition of Centre of Excellence International Conference on Molecular Materials and Functions 2024, IIT Madras held during December 9–11, 2024.



Participants of the 2<sup>nd</sup> edition of the International Conference on Water for Life 2024, IIT Madras held during December 12–14, 2024.



Prof. T. Pradeep becomes the 23<sup>rd</sup> foreign member from India to be elected to the United States National Academy of Engineering (NAE), on September 25, 2024. This is one of the highest professional distinctions. The picture was taken at the dinner of the class of 2024.



IIT Madras organized a hands-on workshop on Microcrystal Electron Diffraction (MicroED) after the 1<sup>st</sup> International Symposium on Cryo-Electron Microscopy 2024, held during August 11–13, 2024.



International Advisory Board (IAB) of the Centre of Excellence on "Molecular Materials and Functions", IIT Madras, held on December 8, 2024. Our coinvestigators and several world leaders in the area participated.



India-Germany discussion meeting on International Research Training Groups, fostering new opportunities for bilateral scientific advancements, IIT Madras, December 11, 2024, supported by our DST-DFG project.

# **Awards and Honours**



Prof. T. Pradeep was honoured with the prestigious 'CRS Gold Medal' by the Chirantan Rasayan Sanstha for his academic achievements at the symposium on "Science Beyond Boundaries: Invention, Discovery, Innovation, and Society - Rasayan 18", Christ University, Bangalore, January 29, 2024.



Prof. T. Pradeep receiving the prestigious Eminent Engineer Award 2023 in the Research & Consultancy category of the Engineering Council of India (ECI), New Delhi, April 29, 2024.



Prof. T. Pradeep receiving the 'Prof. M.V. Pylee Award 2023' for the distinguished academician in India, May 30, 2024. It was instituted by the Cochin University of Science and Technology (CUSAT), presented by honourable ministers of Kerala State Dr. R. Bindu and P. Rajeeve and Anil Sahasrabudhe, Chairman, National Educational Technology Forum (NETF), in presence of the VC of CUSAT.



Prof. T. Pradeep has been elected as a fellow of Academia Europaea in 2024.

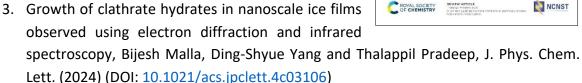


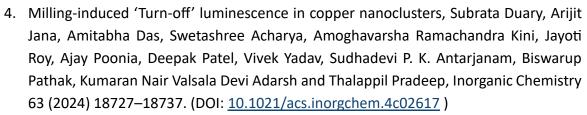
Prof. T. Pradeep being induced as a fellow of the US National Academy of Engineering by its President John L. Anderson and Chair Errol B. Davis, NAS Building, Washington DC, September 26, 2024.

Prof. T. Pradeep was honoured with "Acharya Prafulla Chandra Ray Memorial Award 2023" by the Indian Chemical Society at the JECRC University, Jaipur, Rajasthan, December 21, 2024 (to be received in person in 2025).

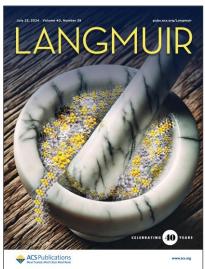
#### **Publications**

- Stable dimer intermediates during intercluster reactions of atomically precise nanoclusters, Swetashree Acharya, Jayoti Roy, Diptendu Roy, Biswarup Pathak and Thalappil Pradeep, J. Phys. Chem. C. (2024) (Just accepted)
- Simulated interstellar photolysis of N<sub>2</sub>O ice: selectivity in photoproducts, Bijesh Malla, Soham Chowdhury, Devansh Paliwal, Hanoona K. M., Gaurav Vishwakarma, Rabin Methikkalam and Thalappil Pradeep, J. Phys. Chem. C. (2024) (DOI: 10.1021/acs.jpcc.4c06624)



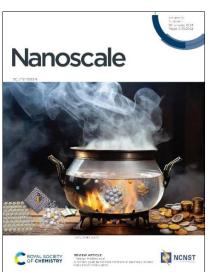


- Nanocluster reaction-driven in-situ transformation of colloidal nanoparticles to mesostructures, Paulami Bose, Pillalamarri Srikrishnarka, Matias Paatelainen, Nonappa, Amoghavarsha Ramachandra Kini, Anirban Som, and Thalappil Pradeep, Nanoscale (2024). (DOI: 10.1039/D4NR02820A)
- 6. Enhanced electrical output in an electrostatic generator using charged water, Vishal Kumar, Pillalamarri Srikrishnarka, Ramamurthy Nagarajan, and Thalappil Pradeep, ACS

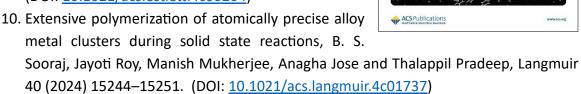


Sustain. Chem. Eng. 12 (2024) 13106–13115. (DOI: 10.1021/acssuschemeng.4c01860)

- 7. Multicolor photoluminescence of Cu<sub>14</sub> clusters modulated using surface ligands, Arijit Jana, Subrata Duary, Amitabha Das, Amoghavarsha Ramachandra Kini, Swetashree Acharya, Jan Machacek, Biswarup Pathak, Tomas Base and Thalappil Pradeep, Chem. Sci. 15 (2024) 13741–13752. (DOI: 10.1039/D4SC01566E)
- 8. From solution to microstructures in minutes: microdroplet-derived stand-alone TiO2 surfaces for simultaneous water harvesting and treatment, Keerthana Unni, Jenifer Shantha Kumar, Anirban Som,



- Depanjan Sarkar, Thalappil Pradeep, ACS Sustainable Chem. Eng. 12 (2024) 11957–11967. (DOI: 10.1021/acssuschemeng.4c02806)
- Cysteine-protected antibacterial spheroids of atomically precise copper clusters for direct and affordable arsenic detection from drinking water, Jenifer Shantha Kumar, Arijit Jana, Jayathraa Raman, Hema Madhuri Veera, Amoghavarsha Ramachandra Kini, Jayoti Roy, Sourav Kanti Jana, Tiju Thomas and Thalappil Pradeep, ES&T Letters 11 (2024) 831–837. (DOI: 10.1021/acs.estlett.4c00264)



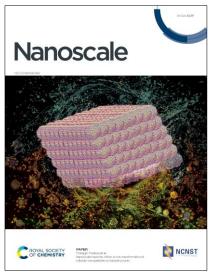
- 11. Partitioning photochemically formed CO₂ into clathrate hydrate under interstellar conditions, Gaurav Vishwakarma, Bijesh Malla, Rajnish Kumar and Thalappil Pradeep, PCCP 26 (2024) 1600 −16016. (DOI: 10.1039/D4CP01414F)
- 12. Interparticle anti-galvanic reactions of atomically precise silver nanoclusters with plasmonic gold nanoparticles: interfacial control of atomic exchange, Paulami Bose, Jayoti Roy, Vikash Khokhar, Biswajit Mondal, Ganapati Natarajan, Sujan Manna, Vivek Yadav, Anupriya Nyayban, Sharma S. R. K. C. Yamijala, Nonappa and Thalappil Pradeep, Chem. Mater. 36 (2024) 7581–7594. (DOI: 10.1021/acs.chemmater.4c00620)
- 13. Observing atomically precise nanocluster aggregates in solution by mass photometry, Jayoti Roy, Ila Marathe, Vicki Wysocki and Thalappil Pradeep, Chem. Commum. 60 (2024) 6655–6658. (DOI: 10.1039/D4CC00363B)
- 14. Interfacial growth of large area single-crystalline silver sheets through ambient microdroplets, Depanjan Sarkar, Anirban Som, Keerthana Unni, Sujan Manna, and



15. Spontaneous weathering of natural minerals in charged water microdroplets forms nanomaterials, B. K. Spoorthi, Koyendrila Debnath, Pallab Basuri, Ankit Nagar, Umesh V. Waghmare and Thalappil Pradeep, Science, 384 (2024) 1012–1017. (DOI: 10.1126/science.adl3364)

CM CHEMISTRY OF MATERIALS

16. Spontaneous  $\alpha$ -C-H carboxylation of ketones by gaseous  $CO_2$  at the air-water interface of aqueous microdroplets, Pallab Basuri, Sinchan Mukhopadhyay, K. S. S. V. Prasad Reddy, Keerthana Unni, B. K. Spoorthi, Jenifer Shantha Kumar, Sharma S. R. K. C. Yamijala and



Thalappil Pradeep, Angew. Chem. 63 (2024) e202403229. (DOI: 10.1002/anie.202403229)

17. Formation and dissociation of dimethyl ether clathrate hydrate in interstellar ice mimics, Bijesh Malla, Gaurav Vishwakarma, Soham Chowdhury, Samir Nayak, Sharma S. R. K. C. Yamijala and Thalappil Pradeep, J. Phys. Chem. C, 128 (2024) 2463–2470. (DOI: 10.1021/acs.jpcc.3c07792)

# Editorials (2024)

- Reintroducing the INTRODUCTION: how to write a compelling introduction for the ACS sustainable family of journals, Audrey Moores, Jingwen Chen, Bala Subramaniam, Michael KC Tam, Elizabeth J. Biddinger, Dean Brady, Danielle Julie Carrier, Ivet Ferrer, Nicholas Gathergood, Hongxian Han, Ive Hermans, King Kuok Mimi Hii, Bing Joe Hwang, Milad Kamkar, Kevin Leonard, Watson Loh, Say Chye Joachim Loo, Andrew C. Marr, Michael A.R. Meier, Ryuhei Nakamura, Graham N. Newton, Thalappil Pradeep, Kotaro Satoh, Wil V. Srubar III, Ning Yan, Asha James, Mihir Jha, Atal Shivhare, Julio F. Serrano, and Peter Licence, ACS Sustainable Chem. Eng. 12 (2024) 8581–8583. (DOI: 10.1021/acssuschemeng.4c04252)
- Managing water, the mother of resources: thoughts on world water day 2024, Thalappil Pradeep, Michael K. C. Tam and Julio F. Serrano, ACS Sustainable Resour. Manage. 1 (2024) 368–369. (DOI: 10.1021/acssusresmgt.4c00096)
- 3. Fireside chat with Man Mohan Sharma: Catalysis for sustainability, Milad Kamkar, Thalappil Pradeep and Julio F. Serrano, ACS Sustainable Resour. Manage. (2024) (DOI: <a href="https://doi.org/10.1021/acssusresmgt.4c00502">10.1021/acssusresmgt.4c00502</a>)

# **Patents Granted**

# **Indian patents**

- 1. Synthesis of protein protected luminescent metal clusters and retaining the bioactivity of the protein, Pradeep, Debasmita Ghosh, Mohammad Bodiuzzaman, Anirban Som, Ananya Baksi, Atanu Ghosh, and Jyotirmoy Ghosh, application no. 201841049925, dated December 31, 2018, issued as patent no. 495343, issued on January 5, 2024.
- 2. A method of detection of low concentration of analytes by superhydrophobic pre concentration paper spray ionization mass spectrometry (SHPPSI MS), T. Pradeep, Pallab Basuri, Avijit Baidya and Tripti Ahuja, application no. 201741047403, dated December 30, 2017, issued as patent no. 504588, issued on January 31, 2024.
- 3. A smartphone based fluoride-specific sensor for rapid and affordable colorimetric detection and precise quantification at sub-ppm levels for field applications, Thalappil Pradeep, Sritama Mukerjee, Manav Shaw and Kamalesh Choudhuri, application no.

- 202041026054, dated June 20, 2020, issued as patent no. 536268, issued on April 30, 2024.
- 4. A method to transform crystalline minerals to nanoparticles by microdroplets, T. Pradeep, B. K. Spoorthi and Pallab Basuri, application no. 202241038282, dated July 7, 2022, issued as patent no. 539562, issued on May 28, 2024.

# **Patents Applied**

- 1. Method of preparing assembled spheroids of copper nanoclusters for ultra-trace arsenic detection, Thalappil Pradeep, Tiju Thomas, Jenifer Shantha Kumar and Arijit Jana, application no. 202441041750, dated May 29, 2024.
- 2. Method of making nanoparticles from natural minerals in high-pressure water jets, T. Pradeep and B. K. Spoorthi, application no. 202441041814, dated May 29, 2024.
- 3. Electrospray deposited anisotropic alloy catalysis for efficient nitrate reduction in wastewater, Thalappil Pradeep, Aswathi K. S., Depanjan Sarkar, Keerthana Unni, Sourav Kanti Jana, Anirban Som, Soham Chowdhury, Sinchan Mukhopadhyay, application no. 202441104803, dated December 31, 2024.
- A method of efficient transformation of crystalline minerals to nanoparticles by saltcontaining microdroplets, Thalappil Pradeep, Jamshiya Sulthana P, Anubhav Mahapatra, B. K. Spoorthi, Depanjan Sarkar, application no. 202441104922, dated December 31, 2024.

# **PCT Applied**

- 1. Material and method for sustainable and affordable atmospheric water harvesting, Thalappil Pradeep; Ankit Nagar; Sonali Seth, application no. WO2024047666 A1, dated March 7, 2024.
- Vertically aligned nanoplates of atomically precise Co<sub>6</sub>S<sub>8</sub> 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. WO2024142079 A1, dated April 7, 2024.

# **Degree Holders**

# Ph.D. Graduates

- 1. Dr. Paulami Bose, Department of Chemistry, IIT Madras, 2024, "Interdimensional Chemistry of Atomically Precise Nanoclusters: A path to Functional Materials".
- 2. Dr. Vishal Kumar, Department of Chemistry and Department of Chemical Engineering, IIT Madras, 2024, "Studies on Physical and Chemical Changes by Triboelectricity".
- 3. Dr. Jayoti Roy, Department of Chemistry, IIT Madras, 2024, "Probing Chemical Interactions of Atomically Precise Nanoclusters with Mass Spectrometry".

- 4. Dr. B. K. Spoorthi, Department of Chemistry, IIT Madras, 2024, "Transformation of Molecules and Materials in Microdroplets".
- 5. Dr. S. Jenifer, Department of Chemistry and Department of Metallurgical and Materials Engineering, IIT Madras, 2024, "Studies on Aggregation in Microdroplets and Nanoclusters and Protein Binding for Arsenic Detection in Water".
- 6. Dr. Anil Kumar Avula, Department of Chemistry, IIT Madras, 2024, "Materials for Arsenic and Fluoride: A Study of Affordable and Sustainable Nanocomposites for Clean Water".







Dr. Vishal

Dr. Paulami Bose

Dr. B. K. Spoorthi







Dr. Anil Kumar Avula

Dr. S. Jenifer

Dr. Jayoti Roy

# **MS** Graduates

1. Ramesh Kumar Soni, Department of Chemistry, IIT Madras, 2024, "Fabrication of Pilot Plant and Scale Manufacture of Cellulose-Based Nanomaterial for Arsenic Removal".



Ramesh Kumar Soni

# **Lectures Delivered**

- 1. Affordable clean water using advanced materials, IITACB Saturday Webinar, January 13, 2024 (webinar).
- 2. Atomically precise clusters, Rasayan 18, Christ University, Bengaluru, January 29–30, 2024.
- 3. Atomically precise clusters: new advancements, Department of Chemistry, Purdue University, West Lafayette, February 1, 2024.
- 4. Affordable clean water using advanced materials, Engineering & Institute of Sustainable Future, Purdue University, West Lafayette, February 2, 2024.
- 5. Materials for water, Discussion with VT India Centre for Research & Innovation, February 2, 2024 (online).
- 6. Clathrate hydrates in interstellar environment, Department of Chemistry, University of Houston, Houston, February 9, 2024.
- 7. Atomically precise clusters: Towards megadalton molecules, 3<sup>rd</sup> DAE-BRNS Symposium on Current Trends in Analytical Chemistry (CTAC-2023), BARC, Mumbai, March 8, 2024.
- 8. Research excellence to impact, my story, Malaviya Mission Teacher Training Programme, IIT Madras, March 11–15, 2024.
- 9. Empowering India: Ideas for action by scientists and engineers, IIT Jammu, March 17, 2024 (with Krishnan Narayanan).
- 10. Roadmap to impactful innovation: my story, ITC Lifesciences & Technology Centre, Bangalore, May 10, 2024.
- 11. Affordable clean water using advanced materials, Eni Award Lectures, FEEM premises, Milan, May 21, 2024.
- 12. Empowering people using advanced materials, Prof. M. V. Pylee Award 2023, CUSAT, Cochin, May 30, 2024.
- 13. Carboranethiols: versatile ligands for atomically precise clusters, Penn State University, University Park, June 12, 2024.



Prof. T. Pradeep delivering a guest lecture on "Roadmap to Impactful Innovation" at ITC Life Science & Technology Centre, Bangalore, on May 10, 2024.

- 14. Can microdroplets make soil?,

  Department of Chemistry, Purdue University, West Lafayette, June 17, 2024.
- 15. Treatment methods for arsenic, JJM Assam Lecture, IITM, June 20, 2024.
- Can microdroplets make soil?, 11th National Conference on Recent Trends in Materials
   Science and Technology 2024, IIST, Thiruvananthapuram, June 26, 2024.
- 17. Can microdroplets make soil?, University of Calicut, Calicut, June 27, 2024.
- 18. Can microdroplets make soil?, International Conference on Materials and Membranes for Water and Energy, CSMCRI, Bhavnagar, July 10–12, 2024.
- 19. Can microdroplets make soil?, INST Mohali, July 16, 2024.

- 20. Can microdroplets make soil?, MIT World Peace University, Pune, July 19, 2024.
- 21. Can microdroplets make soil?, IISER Bhopal, July 29, 2024.
- 22. Can microdroplets make soil?, Bangaluru India Nano, Bengaluru, August 3, 2024.
- 23. Treatment methods for arsenic, India-Israel workshop, ICCW, IIT Madras, August 6, 2024.
- 24. Can microdroplets make soil?, IIT Madras Colloquium, IIT Madras, August 7, 2024.
- 25. Molecular acorns to institutional oaks, Stella Maris College at 60, Chennai, August 29, 2024.



Prof. T. Pradeep, after delivering a talk on "Can water microdroplets make soil?" at the Department of Chemistry, IISER Bhopal, July 29, 2024.

- 26. Affordable clean water using advanced materials, FINERAC Presentation, August 29, 2024.
- 27. Affordable clean water using advanced materials, Teachers' Day Lecture, IIT Kharagpur, September 5, 2024.
- 28. Can microdroplets make soil?, Chemistry Department, IIT Kharagpur, September 6, 2024.
- 29. Affordable clean water using advanced materials, University of Oklahoma, Norman, September 25, 2024.
- 30. Can microdroplets make soil?, University of Oklahoma, Norman, September 27, 2024.
- 31. Can microdroplets make soil? A path to sustainable nanotechnology, University at Buffalo, Buffalo, October 1, 2024.
- 32. Affordable clean water using advanced materials, RENEW, University at Buffalo, Buffalo, October 2, 2024.
- 33. Affordable clean water using advanced materials, As2024, KIT Bhubaneswar, October 2, 2024.
- 34. Can microdroplets make soil?, KIT

  South Campus, Karlsruhe, October 17, 2024.
- 35. Affordable clean water using advanced materials, KIT North Campus, Karlsruhe, October 18, 2024.
- 36. Can microdroplets make soil? A path to sustainable nanotechnology, W for W Foundation, Webinar, October 25, 2024.



Prof. T. Pradeep delivering 'Catalyzing Conservations' talk on the topic of "Affordable clean water using advanced materials" at the University at Buffalo's RENEW Institute, October 2, 2024.

- 37. Glimpses of my work, lecture for students at the Department of Medical Sciences & Technology, IIT Madras, November 7, 2024.
- 38. Affordable clean water using advanced materials, (Chemistry) Meet 2024, Connecting at Konark, November 13, 2024.
- 39. Unlocking entrepreneurial potential in the water sector, ICCW Online, November 16, 2024.
- 40. Wastewater-based epidemiology, MoHUA India-Israel Presentation, IIT Madras, November 18, 2024.
- 41. Carboranethiol-based clusters, EFCS, Farook College, Calicut, December 2–3, 2024.



Lecture for students at the Department of Medical Sciences & Technology, IIT Madras, November 7, 2024.

- 42. Atomically precise metals clusters, CoE Winter School, IIT Madras, December 4, 2024.
- 43. Can microdroplets make soil?, CoE Winter School, IIT Madras, December 5, 2024.
- 44. Carboranethiol-based clusters, 2<sup>nd</sup> CoE Conference, IIT Madras, December 9–11, 2024.
- 45. Can microdroplets make soil?, 2<sup>nd</sup> Water for Life Conference, IIT Madras, December 12–14, 2024.
- 46. Can microdroplets make soil?, Conference on Advances in Catalysis for Energy and Environment (CACEE-2024), TIFR, Mumbai, December 16–20, 2024.
- 47. Matter in confinement Clusters, microdroplets and clean water, Gitam University, Visakhapatnam, December 19, 2024.
- 48. Can microdroplets make soil?, ICL Presentation, December 24, 2024 online.
- 49. Can microdroplets make soil?, Chem 24, IACS, Kolkata, December 27, 2024.

# Students' Activities

- 1. Bijesh Kumar Malla has given an oral presentation on "Photochemistry of Molecular
- Ices Under Ultrahigh Vacuum and Cryogenic Conditions," at the Physical Research Laboratory, Ahmedabad, India, January 5–7, 2024.
- B. S. Sooraj visited the laboratory of Dr. Rodolphe Antoine, Institut Lumiere Materie, University of Claude Bernard Lyon 1, Lyon, France, January 23–February 8, 2024.
- Soham Chowdhury presented a poster titled "Clathrate hydrates in simulated interstellar medium" at the 42<sup>nd</sup> meeting of the



Mr. B. S. Sooraj with Dr. Rodolphe Antoine, Institut Lumiere Materie, University of Claude Bernard Lyon 1, France January, 2024.

Astronomical Society of India (ASI) 2024, IISc., Bangalore, January 31–February 4, 2024.

- 4. Bijesh Kumar Malla visited Houston to work with Dr. Ding-Shyue Yang at the Department of Physical Chemistry, University of Houston, January—April, 2024.
- 5. Deepak Kumar Patel presented a poster titled "Macropolyhedral syn-B<sub>18</sub>H<sub>22</sub>, the 'Forgotten' Isomer" at the Gordon Research Conference (GRC) on Atomically Precise Nanochemistry, Galveston, Texas, USA, February 2–9, 2024.
- 6. Anagha Jose presented a poster titled "Vertically Aligned Nanoplates of Atomically Precise Co<sub>6</sub>S<sub>8</sub> Cluster for Practical Arsenic Sensing" at the Gordon Research Seminar (GRS) on Atomically Precise Nanochemistry, Galveston, Texas, USA, February 3–4, 2024.



Mr. Bijesh Kumar Malla with Dr. Ding-Shyue Yang, University of Houston, Houston, January-April, 2024.

- 7. Swetashree Acharya has given an oral presentation on "Soft Synthesis of Molybdenum-oxo Clusters and Their Applications for Clean Water" at the Gordon Research Seminar (GRS) on Atomically Precise Nanochemistry, Galveston, Texas, USA, February 3–4, 2024.
- 8. Subrata Duary has given an oral presentation on "A Few Atomic Copper Nanoclusters with 'Turn off' Luminescence by Ambient Mechanical Grinding" at the Gordon Research Seminar (GRS) on Atomically Precise Nanochemistry, Galveston, Texas, USA, February 3–4, 2024.
- 9. Swetashree Acharya presented a poster titled "Formation of Metastable Dimers in the Reactions of Atomically Precise MAg<sub>24</sub>(DMBT)<sub>18</sub> (M= Ag, Au, Pd, Pt) and Ag<sub>29</sub>(BDT)<sub>12</sub> Clusters" at the Gordon Research Conference (GRC) on Atomically Precise Nanochemistry, Texas, USA, February 4–9, 2024.
- 10. Amoghavarsha R. Kini presented a poster titled "Nanomechanical Properties of Crystals of Cu<sub>4</sub> with Enhanced Hardness in Low-Density Isomorphs" at the Gordon



Ms. Anagha Jose with Prof. Jennifer S. Brodbelt, UT Austin, Texas, February 12 - April 29, 2024.

- Research Conference (GRC) on Atomically Precise Nanochemistry, Galveston, Texas, USA, February 4–9, 2024.
- 11. Anagha Jose presented a poster titled "Vertically Aligned Nanoplates of Atomically Precise Co<sub>6</sub>S<sub>8</sub> Cluster for Practical Arsenic Sensing" at the Gordon Research Conference (GRC) on Atomically Precise Nanochemistry, Galveston, Texas, USA, February 4–9, 2024.
- 12. Subrata Duary presented a poster titled "A Few Atomic Copper Nanoclusters with 'Turn off' Luminescence by Ambient Mechanical Grinding" at

- the Gordon Research Conference (GRC) on Atomically Precise Nanochemistry, Galveston, Texas, USA, February 4–9, 2024.
- 13. Anagha Jose visited UT Austin, Texas, to work with Prof. Jennifer S. Brodbelt, February 12–April 29 2024.
- 14. Deepak Kumar Patel visited Institute of Physics and Institute of Inorganic Chemistry of Czech Academy of Science to work with Dr. Monika Kučeráková and Dr. Tomas Base March–December, 2024.
- 15. Riya Dutta has given an oral presentation at a webinar on Earth Day, organised by ICCW, IIT Madras, April 22, 2024.
- 16. Sujan Manna visited MIT, USA, to work with Prof. Loza Tadesse, Department of Mechanical Engineering, April–July, 2024.
- 17. Vivek Yadav has given an oral presentation on "Atomically Precise Carboranethiol-Protected Ag<sub>17</sub>, AuAg<sub>16</sub>, Ag<sub>13</sub>Cu<sub>4</sub> and AuAg<sub>12</sub>Cu<sub>4</sub> Nanocl usters" at the 7<sup>th</sup> International Symposium on Monolayer-Protected Clusters (ISMPC), Penn State University, USA, June 12–14, 2024.



Mr. Sujan Manna with Prof. Loza Tadesse, MIT, USA. April–July, 2024.

- 18. Vivek Yadav has presented a poster titled "Atomically Precise Carboranethiol-Protected Ag<sub>17</sub>, AuAg<sub>16</sub>, Ag<sub>13</sub>Cu<sub>4</sub> and AuAg<sub>12</sub>Cu<sub>4</sub> Nanoclusters" at the 7<sup>th</sup> International Symposium on Monolayer-Protected Clusters (ISMPC), Penn State University, USA, June 12–14, 2024.
- 19. Deepak Kumar Patel visited the laboratory of Prof. Holger Braunschweig at Julius-Maximilians-University of Würzburg, Würzburg, Germany, June 2024.
- 20. Deepak Kumar Patel visited Karlsruhe Institute of Technology, Germany to work with Prof Manfred M. Kappes, June 2024.
- 21. Deepak Kumar Patel visited the Elettra Synchrotron Trieste facility, Italy and worked



Mr. Deepak Kumar Patel with Dr. Monika Kučeráková and Dr. Tomas Base at Elettra Synchrotron Trieste facility in Italy, June 2024.

- with Dr. Monika Kučeráková and Dr. Tomas Base, June 2024.
- 22. Vivek Yadav has presented a poster titled "Atomically Precise Carboranethiol-Protected Ag<sub>17</sub>, AuAg<sub>16</sub>, Ag<sub>13</sub>Cu<sub>4</sub> and AuAg<sub>12</sub>Cu<sub>4</sub> Nanoclusters" at the Gordon Research Conference (GRC) 2024 on Noble Metal Nanoparticles, Mount Holyoke College in Massachusetts, US, June 16–21, 2024.
- 23. S. Sudhir hosted a four-day program on entrepreneurship conducted by Thinkstartup at IITM Research Park, IIT Madras, July 3, 2024.

- 24. Keerthana Unni presented a poster titled "From Solutions to Microstructures in Minutes: Microdroplet Derived Stand-Alone TiO<sub>2</sub> Surfaces for Simultaneous Water Harvesting and Treatment" at the 33<sup>rd</sup> CRSI National Symposium in Chemistry (CRSI-NSC), Hyderabad, July 4–6, 2024.
- 25. Soham Chowdhury has given an oral presentation on "Composition-Dependent Clathrate Hydrate Formation of Trimethylene Oxide and Consequences of Dissociation" in the International Conference on Chemistry and Physics at Low Temperatures 2024, Niseko, Hokkaido, Japan, July 6–11, 2024.
- 26. Bijesh Kumar Malla has given an oral presentation on "Insights into Interstellar Ice Photochemistry: Cryogenic Laboratory Studies" in the International Conference on Chemistry and Physics at Low Temperatures 2024, Niseko, Hokkaido, Japan, July 6–11, 2024.
- 27. Sujan Manna presented a poster titled "Surface Enhanced Raman Spectroscopy of Atomically Precise Nanoclusters" at the Gordon Research Conference on Plasmonics and Nanophotonics, Newry, Maine, USA, July 7–12, 2024.
- 28. Sujan Manna gave a talk on "Raman spectroscopy" at the summer school, Tadesse lab, MIT, USA, July 17–18, 2024.
- 29. Keerthana Unni is visiting Purdue University to work with Prof. R. Graham Cooks, Purdue, August 2024–August 2025.
- 30. S. Sudhir conducted a workshop for YouthIdeathon 2024, a Startup Workshop at The Lords International School and Sana Model School, Chennai, August 13, 2024.
- 31. Subrata Duary visited the Stanford Linear Accelerator Center (SLAC), Stanford University, USA, to get trained in cryo-EM (Single Particle Analysis/SPA) technique under the supervision of Prof. Wah Chiu, August—November, 2024.
- 32. Sujan Manna has delivered an invited talk on "Ambient Morphology-Preserved Doping of Cu(0) to Anisotropic Gold Nanoparticles Through Reactions with Atomically Precise Nanoclusters" at the 11<sup>th</sup> Asian Conference on Nanoscience and Nanotechnology (AsiaNANO) 2024, IIT Madras, September 25, 2024.
- 33. Vivek Yadav has given an oral presentation on "Clustering of Clusters" at the 11<sup>th</sup> Asian Conference on Nanoscience and Nanotechnology (AsiaNANO) 2024, IIT Madras, September 25, 2024.
- 34. Tanmayaa Nayak presented a poster titled "Cellulose-Derived Nanomaterials for Affordable and Rapid Remediation of Uranium in Water" at the 9<sup>th</sup> International Congress and Exhibition on Arsenic in the Environment (As 2024), KIIT-DU, Odisha, October 20–24, 2024.
- 35. Sonali Seth presented a poster titled "Biopolymer-Based Adsorbent for Uranium Removal from Water" at the 9<sup>th</sup> International Congress and Exhibition on Arsenic in the Environment (As 2024), KIIT-DU, Odisha, October 20–24, 2024.
- 36. Bijesh Kumar Malla presented a poster on "Formation of Clathrate Hydrates under Simulated Interstellar Conditions" at the SoPhyc-Physical Chemistry Symposium 2024, IIT Bombay, October 22–25, 2024.

- 37. Amoghavarsha R. Kini has given an oral presentation on "Atomically Precise Nanoclusters: From Structure to Functions" at the Chemistry in-House Symposium (CiHS) 2024, IIT Madras, October 29, 2024.
- 38. Vivek Yadav presented a poster titled "Atomically Precise Carboranethiol-Protected Ag<sub>17</sub>, AuAg<sub>16</sub>, Ag<sub>13</sub>Cu<sub>4</sub> and AuAg<sub>12</sub>Cu<sub>4</sub> Nanoclusters" at the Chemistry in-House Symposium (CiHS) 2024, IIT Madras, October 29, 2024.
- 39. B. S. Sooraj Presented a poster titled "Ligand Dependent Metallicity in Au<sub>144</sub> Nanoclusters Unveiled by Excited State Electron Dynamics" at the 5<sup>th</sup> International Conference on Emerging Advanced Nanomaterials (ICEAN 2024), Newcastle, Australia, November 4–8, 2024.
- 40. Sujan Manna presented a poster titled "Surface Enhanced Raman Spectroscopy of Atomically Precise Nanoclusters" at the FCS-OWLS conference, IIT Bombay, November 16–21, 2024.
- 41. Atrayee Datta, Anubhav Mahapatra and Riya Dutta visited the Satish Dhawan Space Centre (SDSC) SHAR, Sriharikota, the Spaceport of India, November 21, 2024.
- 42. Sonali Seth presented a poster titled "Biopolymer-Based Adsorbent for Uranium Removal from Water" at the International Winter School 2024 on Frontiers in Materials Science, JNCASR, Bangalore, December 2–6, 2024.
- 43. Samapti Mondal participated in the International Winter School 2024 on Frontiers in Materials Science, JNCASR, Bangalore, December 2–6, 2024.
- 44. Swetashree Acharya has given an oral presentation on "Reactions of Nanoclusters" at the 2<sup>nd</sup> edition of CoE International Conference on Molecular Materials and Functions 2024, IIT Madras, December 9–11, 2024.
- 45. Amoghavarsha R. Kini has given an oral presentation on "Nanomechanical Investigations of Crystals of Cu<sub>4</sub> Nanocluster Isomorphs: Enhanced Hardness of the Low-Density Analogue" at the 2<sup>nd</sup> edition of CoE International Conference on Molecular Materials and Functions 2024, IIT Madras, December 9–11, 2024.
- 46. Vivek Yadav presented a poster titled "Site-Specific Substitution in Atomically Precise Carboranethiol-Protected Nanoclusters and Concomitant Changes in Electronic Properties" at the 2<sup>nd</sup> edition of CoE International Conference on Molecular Materials and Functions 2024, IIT Madras, December 9–11, 2024.
- 47. Harshita Nagar presented a poster titled "Rapid Determination of the Atomic Structure of Small Copper Nanoclusters with MicroED" at the 2<sup>nd</sup> edition of CoE International Conference on Molecular Materials and Functions 2024, IIT Madras, December 9–11, 2024.
- 48. B. S. Sooraj has given an oral presentation on "Ligand Dependent Metallicity in Au<sub>144</sub> Nanoclusters Unveiled by Excited State Electron Dynamics" at the 2<sup>nd</sup> edition of CoE International Conference on Molecular Materials and Functions 2024, held at IIT Madras, India, December 9–11, 2024.

- 49. Anagha Jose has given an oral presentation on "Vertically Aligned Nanoplates of Atomically Precise  $Co_6S_8$  Cluster for Practical Arsenic Sensing" at the  $2^{nd}$  edition of International Conference on Water for Life 2024, IIT Madras, December 12–14, 2024.
- 50. Sinchan Mukhopadhyay presented a poster titled "Spontaneous  $\alpha$ -C–H Carboxylation of Ketones by Gaseous CO<sub>2</sub> at the Air-water Interface of Aqueous Microdroplets" at the 2<sup>nd</sup> edition of the International Conference on Water for Life 2024, IIT Madras, December 12–14, 2024.
- 51. Tanmayaa Nayak has given an oral presentation on "Cellulose-Derived Nanomaterials for Affordable and Rapid Remediation of Uranium in Water" at the 2<sup>nd</sup> edition of the International Conference on Water for Life 2024, IIT Madras, Chennai, December 12–14, 2024.
- 52. Sonali Seth presented a poster titled "Biopolymer-Based Adsorbent for Uranium Removal from Water" at the 2<sup>nd</sup> edition of the International Conference on Water for Life 2024, IIT Madras, December 12–14, 2024.
- 53. Vivek Yadav presented a poster titled "Site-Specific Substitution in Atomically Precise Carboranethiol-Protected Nanoclusters and Concomitant Changes in Electronic Properties" at the Conference on Advances in Chemistry for Energy and Environment (CACEE), TIFR Mumbai, December 16–20, 2024.

# Students' Recognitions

- 1. Dr. B. K. Spoorthi has received the Best Thesis Award of Chemistry Department, IIT Madras at the 2024 convocation, July 19, 2024.
- 2. Keerthana Unni has received the best poster Award for "From Solutions to Microstructures in Minutes:
  - Microstructures in Minutes:
    Microdroplet Derived Stand-Alone TiO<sub>2</sub>
    Surfaces for Simultaneous Water
    Harvesting and Treatment" at the 33<sup>rd</sup>
    CRSI National Symposium in Chemistry
    (CRSI-NSC), Hyderabad, July 4–6, 2024.
- Amoghavarsha R. Kini has received the International Immersion Experience (IIE) travel award 2024, funded by IIT Madras.



Dr. B. K. Spoorthi has received the Best Thesis Award of Chemistry Department, IIT Madras, July 29, 2024.

- 4. Swetashree Acharya has received the <sup>29, 2024.</sup>
  International Immersion Experience (IIE) travel award 2024, funded by IIT Madras.
- 5. Riya Dutta and Sujan Manna won the Asian Paint Alchemy competition held in Mumbai, March 15, 2024.
- 6. Bijesh Kumar Malla has received the best poster award for "Formation of Clathrate Hydrate under Simulated Interstellar Conditions" at the Physical Chemistry Chemical Physics (PCCP) at the SoPhyc-Physical Chemistry Symposium 2024, IIT Bombay, India, October 22–25, 2024.

- 7. Amoghavarsha R. Kini won the best oral presentation award for "Atomically Precise Nanoclusters: From Structure to Functions" at the Chemistry in-House Symposium (CiHS)-2024, IIT Madras, October 29, 2024.
- 8. Sujan Manna has received the International Immersion Experience (IIE) travel award 2024, funded by IIT Madras.
- 9. Sujan Manna became one of the top 20 finalists in the 'Science in Focus' competition organized by India Science Fest, IISER Pune, November 2024.
- 10. Vivek Yadav has received the best poster award for "Atomically Precise Carboranethiol-Protected Ag<sub>17</sub>, AuAg<sub>16</sub>, Ag<sub>13</sub>Cu<sub>4</sub> and AuAg<sub>12</sub>Cu<sub>4</sub> Nanoclusters" at the 2<sup>nd</sup> edition of CoE International Conference on Molecular Materials and Functions 2024, IIT Madras, December 9–11, 2024.
- 11. S. Sudhir became one of the finalists in the 'Build to Innovate: Rural-Agri Challenge' by IITM Incubation Cell, June 15, 2024.
- 12. S. Sudhir became the runner up in the 'Next Gen Digital Action', a global youth initiative part of Digital Tech Summit 2024 to enable diverse youth-led ideas, perspectives and action on digital technologies transforming societies, hosted by DTU, Denmark, October 31, 2024.
- 13. Harshita Nagar has received the best poster award for "Rapid Determination of the Atomic Structure of Small Copper Nanoclusters with MicroED" at the 2<sup>nd</sup> edition of CoE International Conference on Molecular Materials and Functions 2024, IIT Madras, 9–11, December 2024.
- 14. Deepak Kumar Patel has received the best poster award for "Molecular Rotor with Conformation-Dependent Dipole Moment" at the 2<sup>nd</sup> edition of CoE International Conference on Molecular Materials and Functions 2024, IIT Madras, December 9–11, 2024.
- 15. Vivek Yadav won a recognition for asking most interesting questions at the Conference on Advances in Chemistry for Energy and Environment (CACEE), TIFR, Mumbai, December 16–20, 2024.

# **Alumni News**

- 1. Dr. Bindhu Alappat has joined as the Vice President of Academic Affairs at Holy Family University, USA.
- 2. Dr. Tanvi Gupte has joined as a postdoc at Columbia University, USA.
- 3. Dr. Tripti Ahuja has joined as a postdoc in CSIR-CDRI, Lucknow.
- 4. Dr. Gaurav Vishwakarma has joined as a postdoc at National University of Singapore.
- 5. Dr. Vishal Kumar has joined as a postdoc at National Taiwan University, Taiwan.
- 6. Dr. Jayoti Roy has joined as a postdoc at Karlsruhe Institute of Technology, Germany.
- 7. Dr. B. K. Spoorthi has joined as a postdoc at Purdue University, USA.
- 8. Mr. Devansh Paliwal has joined as a doctoral student at ETH Zurich, Switzerland.
- 9. Ms. K. S. Aswathi has joined as a doctoral student at Texas A&M University, USA.
- 10. Ms. Karthika Kalyansundar has joined as a doctoral student at Ohio University, USA.

- 11. Dr. Anish R. Nath has joined as a senior executive at MRF Limited, Chennai.
- 12. Mr. S. Jayaram has joined as a technical officer MA3 grade at MRF Limited, Chennai.

#### **Research Grants**

#### **Ongoing Projects**

- 1. JC Bose Fellowship, DST 2015–2020; renewed 2021, DST, Rs. 90 lakhs.
- 2. Fingerprinting authenticity of ayurvedic preparations by ambient electrospray deposition Raman spectroscopy, SHRI proposal, DST, Rs. 53.8884 and 41.3656 lakhs for IITM and Manipal Academy of Higher Education respectively. (principal investigator with Santhosh Chidangil, Manipal, Co-PI)
- 3. Atomically precise naked cluster assemblies from ligand-stabilized clusters: New materials for catalysis, DST/DFG, Rs. 72.028 lakhs. (principal investigator, with Manfred Kappes)
- 4. 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 Tanavur, VIT Vellore and MRF Chennai.
- 5. Carborane-protected metal nanoclusters: A new family of materials with atomic precision DST/Czech, Rs. 37 lakhs. (principal investigator, with Tomas Base)
- 6. Centre of Excellence on Molecular Materials and Functions, Ministry of Education, Rs. 16.8 crores. (principal investigator)
- 7. Atomically precise materials for sustainable water and energy harvesting, SERB, Rs. 75.32 lakhs. (principal investigator)

Others, such as R&D Awards, technology development, CSR grants, and instrument maintenance activities, are also managed as projects.

#### Consultancy

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

#### **Implementation Projects**

There are several other implementation projects taken through the International Centre for Clean Water.

# **Visitors**

- 1. Mr. Girish Agarwal, Dr. Pooja Agarwal, Dr. Gaurav Singh and Mr. Faraz Farooqui, Crypto Relief, January 6, 2024.
- 2. Dr. Mamata Bangera, Birkbeck, University of London, January 16, 2024.

- Joseph Cheriyan, Deputy General Manager Secretarial-CSR-ESG, Dr. A. Sreekumaran Nair, Corporate Manager (R&D), MRF, January 19, 2024.
- 4. Shri Kailash Karthik N, IAS, Mission Director, Jal Jeevan Mission, Assam, Varadharajan Ranganathan, TDK Ventures Innovation Hub, and Dr. Shubhra Shukla, Jivass Technologies, January 25, 2024.
- Prof. Roop Mahajan, Professor, Department of Materials Science and Engineering, Former Director of Institute for Critical Technology and Applied



Prof. T. Pradeep and Gaurav Sing (seated), CEO, Blockchain for Impact, with the team during the launch of 'Q Exactive Plus' as a part of the Waste Water Based Epidemiology (WBE) Project, IIT Madras, January 6, 2024.



Prof. Roop Mahajan, Former Director of Institute for Critical Technology and Applied Sciences; and Dr. M.K. Padmanabhan, Director of the Virginia Tech, February 10, 2024.

Sciences, Prof Emeritus Virginia Tech, and Dr. M.K. Padmanabhan, Director of Virginia Tech, India, February 10, 2024.

- 6. Prof. Suresh Bhargava, Distinguished Professor, AM Member of Order of Australia (Queens Civilian Honour 2022), Director for CAMIC, STEM College, RMIT University, February 22, 2024.
- 7. ENI team Sara Scagliotti, Andrea Lainati, Andrea Bartolini, Ilaria Reitano, February 22–23, 2024
- 8. Dr. Venugopal Vijaykrishnan, Dr. Gayathri Subramanyam, Dr. Devi Sirisha Janni, ITC Life Science & Technology Centre, Bangalore, March 15, 2024.
- 9. Ms. Noa Amsalem, Water Attaché- International

Development Cooperation (MASHAV) and David Emanuel Kasman, Project Manager from Consulate General of Isreal, March 19, 2024.



Prof. T. Pradeep, with Kailash Karthik N, Mission Director at Jal Jeevan Mission, Varadharajan Ranganathan, TDK Ventures Innovation Hub and Nandakumar E, ICCW, January 25, 2024.



Prof. T. Pradeep, with Prof. Suresh Bhargava, Distinguished Professor, AM - Member of Order of Australia, Director for CAMIC, STEM College, RMIT University, February 22, 2024.

- 10. Dr. Aysha Swapna, Principal of Farook College, Dr. T. Shalina Begum, Dr. Reji Thomas, Mr. Mohammed Nishad Maniparambath, Mrs. S. Bodhy Krishna, Mrs. T. P. Shabna and Dr. M. Yoosuf Ameen, Farook College, Kerala, March 20, 2024.
- 11. Shri. M.K. Narayanan, 19th Governor of West Bengal and former NSA, March 22, 2024.
- 12. Dr. Sudip Chakraborty, Reader F, Harish-Chandra Research Institute (HRI), an Aided Institute of Department of Atomic Energy (DAE), Allahabad, May 5, 2024.



Prof. T. Pradeep, with ENI team members (Ilaria Reitano (left) and Sara Scagliotti, Andrea Lainati, Andrea Bartolini (right), with M. Udhaya Shankar and Prof. T. Pradeep, February 23, 2024.



Prof. T. Pradeep with Dr. Venugopal Vijaykrishnan, Dr. Gayathri Subramanyam and Dr. Devi Sirisha Janni, ITC Life Science & Technology Centre, Bangalore, March 15, 2024.

- 13. Mr. Ramasamy Narayanan, Head, Sustainability; Mr. Nareshkumar Katakam, Senior Manager, Sustainability; Monisha Suyenlai, Assistant Manager, Sustainability, A Sreekumaran Nair, Corporate Manager, R&D; MRF, May 24, 2024.
- 14. Mr. Bhajan Singh, NSF India, June 5, 2024.
- 15. Prof. Gaurav Chopra, Associate Professor, Department of Chemistry, Purdue Institutes for Drug Discovery, Cancer Research, Neuroscience, Immunology, Purdue University, June 21, 2024.
- 16. Dr. Soumyabrata Roy, Research Scientist,

Ajayan Research Group, Materials Science & Nanoengineering, Rice University, USA, June 22, 2024.

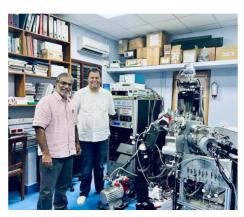


Prof. T. Pradeep, with Shri. M. K. Narayanan, 19<sup>th</sup> Governor of West Bengal, March 22, 2024.



Prof. T. Pradeep, with Mr. Ramasamy Narayanan -Head, Mr. Nareshkumar Katakam -Senior Manager, Monisha Suyenlai, Assistant Manager, Sustainability and A Sreekumaran Nair - Corporate Manager, R&D, May 24, 2024.

- 17. Mr. K.K. Mishra, President of Product & Business Development, Mr. Hemang Patel, G.M (R&D), 20 Microns Nano Minerals Limited, Gujrat, July 23, 2024.
- 18. Dr. Ajay Chandak, Certified Energy Auditor & Renewable Energy Expert, Chandak Innovations LLP, Shamgiri, August 5, 2024.
- 19. Suzan Kagan, visiting PhD student from Tel Aviv University, coordinated the course ID5011, People's Water Data, and also participated in several measurements in the field, August–November, 2024.



Prof. T. Pradeep with Prof. Gaurav Chopra, Associate Professor at Purdue University, June 21, 2024.

- 20. Prof. Kuruvilla Joseph, outstanding Professor & Dean, Indian Institute of Space Science and Technology (IIST), September 6, 2024.
  - 21. Prof. Sabu Thomas, former VC of MG University, September 11, 2024.
  - 22. Dr. Tofayel Ahmed, Associate Professor 'E', Saha Institute of Nuclear Physics, October 7, 2024.
  - 23. Prof. S. Chandrasekaran, Department of Organic Chemistry, IISc Bangalore, November 5, 2024.
  - 24. Prof. Dr. Mukundan Thelakkat, Professor of Applied Functional Polymers, University of Bayreuth, Germany, November 10, 2024.



Suzan Kagan, visiting PhD student from Tel Aviv University, collecting water quality data as a part of the course, 'People's Water Data', August–November, 2024.

25. Prof. T. Venkatesan, Senior Advisor, office of Vice President for Research and Partnerships, Founding Director of Center for Quantum Research and Technology, Prof. of Physics and ECE, University of Oklahoma, November 14, 2024.



Prof. T. Pradeep with Prof. Sabu Thomas, former VC of MG University, September 11, 2024.



Prof. S. Chandrasekaran, Professor of Organic Chemistry, IISc Bangalore, had an interaction with students of the group, November 5, 2024.



Prof. Mukundan Thelakkat, Professor of Applied Functional Polymers, University of Bayreuth, Germany, delivered talk at IIT Madras, November 10, 2024.



Prof. T. Pradeep and his students with Prof. T. Venkatesan, Director of the Center for Quantum Research and Technology, University of Oklahoma, November 14, 2024.

- 26. Dr. Ruchi Gupta, Associate Professor in Biosensors, Global Engagement Lead for School of Chemistry, University of Birmingham, November 25, 2024.
- 27. Prof. Arieh Ben-Naim, Department of Physical Chemistry, The Hebrew University of Jerusalem, December 4, 2024.



Prof. T. Pradeep with Padma Vibhushan Dr. R. A. Mashelkar, FRS; Prof. V. Kamakoti, Director of IITM, and Prof. Rajnish Kumar, Director's Office, IIT Madras, December 8, 2024.



Prof. Arieh Ben-Naim, Professor at the Hebrew University of Jerusalem, with Prof. K. Mangala Sunder and Prof. T. Pradeep at the Department of Chemistry, IIT Madras, December 26, 2024. He gave two talks in Chemistry on December 23 and 26, 2024.

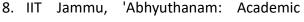
28. Padma Vibhushan Dr. R. A. Mashelkar, FRS, December 8-9, 2024.

Several other visitors came for the four conferences we conducted during the year.

# **Visits**

- 1. Venus Safety & Health Pvt. Ltd., Mumbai, January 2, 2024.
- 2. Stella Maris College (Autonomous), Chennai, as the chief guest for the Graduation Day, January 10, 2024.
- 3. Christ University, Bangalore, to receive the CRS Gold Medal Award in the Symposium: "Science Beyond Boundaries: Invention, Discovery, Innovation and Society Rasayan 18", January 29, 2024.
- 4. Department of Chemistry, Purdue University, February 1, 2024 and Environmental and Ecological Engineering, Purdue University, February 2, 2024.

- Galveston, Texas, USA, chair of the Gordon Research Conference (GRC) on Atomically Precise Nanochemistry, February 4–9, 2024.
- 6. IIT Bombay, Mumbai, Chair of the Symposium of Cryo-EM Facility, March 8, 2024.
- 7. Bhabha Atomic Research Centre (BARC), Mumbai, the 3<sup>rd</sup> DAE-BRNS Symposium on Current Trends in Analytical Chemistry (CTAC-2023), March 8, 2024.

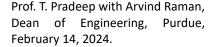




Prof. T. Pradeep with all the participants at the Gordon Research Conference, Texas, USA, February 4–9, 2024. Prof. Pradeep was the Chair of the conference.

Leadership Program on behalf of the Ministry of Education of India, March 15–19, 2024.

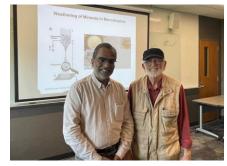
- 9. Stella Maris College (Autonomous), Chennai, SMC Research Council Advisory meeting, March 22, 2024.
- 10. IISER Pune, progress review meeting of SUPRA, April 9, 2024.
- 11. INST, Mohali, 18th BoG meeting, April 12, 2024.
- 12. Delhi, the nominations of INSA Fellowship (IYA, IAF, IDL-1, and IDL-2 for the year 2024), April 24, 2024.
- 13. Delhi, to receive the Eminent Engineers' Award 2023 Research & Consultancy category by Engineering Council of India, April 29, 2024.
- 14. ITC Life Science & Technology Centre, Bangalore, for a guest lecture, May 10, 2024.



- 15. University of Bayreuth, Germany, May 15-19, 2024.
- 16. Milan, Italy, Scientific Commission annual meeting of the Prize Commission of Eni Award 2024 edition at FEEM premises, May 20, 2024.
- 17. SANJOG 2024-Workshop for Children of Army JCs/Jawans and Family, IIT Madras, June 9, 2024.



Prof. T. Pradeep with the researchers at ITC, Bangalore, May 10, 2024.



Visit to Purdue. Prof. T. Pradeep with Prof. Graham Cooks, after a talk, June 17, 2024.

- 18. Cochin University of Science and Technology, Kerala, to receive the 'Prof. M. V. Pylee
  - Award' for the distinguished academician in India for the year 2023, May 30, 2024.
- 19. Penn State University, Pennsylvania, USA, the 7<sup>th</sup> International Symposium on Monolayer Protected Clusters (ISMPC24), June 12–14, 2024.
- 20. Visit to Purdue University, June 15–18, 2024.
- 21. IIST, Thiruvananthapuram, the 11th National Conference on Recent Trends in



Meeting on WTC project at Nallampatti, Tamil Nadu, August 4, 2024.



Prof. T. Pradeep with Prof. Horst Hahn at the Advanced Radar Research Centre, University of Oklahoma, September 26, 2024.

Materials Science and Technology, June 26, 2024.

- 22. Calicut University, Kerala, National Conference on Advanced Materials (NCAM) 2024, June 27, 2024.
- 23. CSIR-CSMCRI Bhavnagar, Gujarat, International Conference on Materials and Membranes for Water and Energy (ICMMWE)-2024, July 10–12, 2024.
- 24. MIT World Peace University (MIT-WPU), Pune, first National Scientists Round Table Conference (NSRTC 2024) for Viksit Bharat 2047, July 19, 2024.
- 25. IISER Bhopal, attended the technical review meeting and delivered a talk at the Department of Chemistry, July 29, 2024.
- 26. Bangalore, as a plenary speaker in the 13th Edition of Bengaluru India Nano, August 3, 2024.
- 27. Nallampatti, Tamil Nadu, for meeting on WTC project, Au gust 4, 2024.
- 28. Pondicherry, along with Mr. Ashok Natarajan, meeting with Dr. Dhinadayalan, Secretary PWD, August 21, 2024.



US National Academy of Engineering (NAE) Annual Meeting 2024, with the class of 2024, September 29, 2024.



Prof. T. Pradeep with Krishna Rajan, SUNY Distinguished Professor, Thomas Thundat, SUNY Empire Innovation Professor and Haiqing Lin, Professor, University at Buffalo, October 2, 2024.

- 29. Stella Maris College, Chennai, Diamond Jubilee of the Department of Chemistry, August 29, 2024.
- 30. 19<sup>th</sup> BoG meeting (online) of INST, Mohali, August 30, 2024.
- 31. IIT Hyderabad, National Programme on Nano Science & Technology (NPNST), a brainstorming session for the preparation of a vision document on advanced materials, September 2–3, 2024.
- 32. IIT Kharagpur, institute lecture at the School of Nano Science and Technology, September 5, 2024.



Prof. T. Pradeep with Thomas Thundat, and Amit Goyal, SUNY Empire Innovation Professors, University at Buffalo, October 3, 2024.



At Eni Award 2024 prize giving ceremony in front of Palazzo del Quirinale in Rome, Italy, October 15, 2024.

- 33. University of Oklahoma, to deliver lectures and explore collaborations, September 24–27, 2024.
- 34. Washington, D.C., USA, invited to the National Academy of Engineering (NAE) Annual Meeting-2024, September 28–30, 2024.
- 35. University at Buffalo, New York, as a distinguished speaker for the RENEW 'Catalyzing Conversations' talk, October 1–3, 2024.
- 36. Bangalore, an innovation tour for the course ID5031: Innovation and

Entrepreneurship – a multidisciplinary approach, October 8, 2024.

- 37. Palazzo del Quirinale in Rome, Italy, for the Eni Award 2024 prize giving ceremony, October 14, 2024.
- 38. Visit to KIT, Germany, as part of the International Excellence Award, October 15–19, 2024.
- 39. Meeting with Rahul Mammen Mappillai, Managing Director, MRF Ltd, October 30, 2024.



Prof. T. Pradeep with Prof. Thomas Hirth, Vice President at KIT, and Prof. Manfred M. Kappes, KIT, Germany, October 2024.



Prof. T. Pradeep with Rahul Mammen Mappillai (left), Managing Director, MRF Ltd, October 30, 2024.



At the National Conference on Emerging Frontiers in Chemical Science (EFCS)-2024, Farook College, Kerala, December 2–3, 2024.

- 40. Konark, Odisha, for the Chemistry Meet 2024 at Lotus Eco Beach Resort, November 13, 2024.
- 41. Participated in the one-day symposium, in connection with the anniversary celebrations on the completion of the 60<sup>th</sup> year of the journal Chemical Communications, Royal Society of Chemistry at IIT Madras, November 18, 2024.
- 42. Sacred Heart College, Thevara, Kerala, as an invited keynote speaker in the 23<sup>rd</sup> Prof. K.
   V. Thomas Endowment National Seminar on Frontiers in Materials Science, November 27, 2024.



Prof. T. Pradeep with Prof. Krishna, Dean and Prof. GVR Sharma, Director, Faculty Development at GITAM University, Visakhapatnam, December 4, 2024.

- 43. Farook College, Kerala, chairman of the National Conference on Emerging Frontiers in Chemical Sciences (EFCS), December 2–3, 2024.
- 44. Conducted International Advisory Board (IAB) of the Centre of Excellence on



Prof. T. Pradeep with Dr. Anil Kakodkar as part of the CACEE-2024 event, TIFR, Mumbai, December 16, 2024.

- "Molecular Materials and Functions at IIT Madras, December 8. 2024.
- 45. Tata Institute of Fundamental Research (TIFR) Mumbai, conference on Advances in Catalysis for Energy and Environment (CACEE-2024), December 16, 2024.
- 46. GITAM Deemed to be University, Hyderabad, delivered a distinguished lecture followed by interaction with the faculty members to discuss the possibilities of advanced research at GITAM facilities, December 19, 2024.
- 47. JECRC University, Jaipur, Rajasthan, for the 'Acharya Prafulla Chandra Ray Memorial Award 2023' at the 61<sup>st</sup> ACC 2024 Annual Convention of Chemists and International Conference, December 19–21, 2024 (to be received in 2025).
- 48. IACS Kolkata, Chem24, December 27, 2024.

#### **Services**

- 1. Chairman, Board of Governors, Institute of Nano Science and Technology, Mohali, 2021–2024.
- 2. Member, Research Advisory Council, Manipal Academy of Higher Education, Manipal Member, 2018–
- 3. Research Advisory Board, Pandit Deendayal Petroleum University, 2019-
- 4. 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.
- Associate Editor of the journal, ACS Sustainable Resource Management, 2024
   Chemistry of Materials, 2018–; ACS Nano, 2018–; Nanoscale Advances, 2019–; Clean Water, 2020–; Chemical Communications, 2020–2024; Environmental Science: Water Research & Technology, 2023–; ACS Environmental Science and Technology 2024–; The Journal of Physical Chemistry Letters, 2024–

#### Incubation

Hydromaterials has installed village water treatment units, altogether supplying arsenic and iron-free water to over 1000,000 people. In many places, we have addressed uranium contamination as well. Altogether, there are around 1700 units of this kind operational in our country, supplying clean water to 1.4 million people. This year's highlights include: ongoing execution of 59 village water



treatment plants in Uttar Pradesh, ongoing installation of district-wide automation in Himachal Pradesh, successful installation of 2,500 water filters for Anganwadis and ongoing installation of 5,850 automatic water filters for Anganwadis and schools in Andhra Pradesh. For more details, please visit <a href="https://hydromaterials.in/">https://hydromaterials.in/</a>

VayuJal Technologies has installed a solar and grid power operated 2000 litres per day (LPD) atmospheric water harvesting unit at Engineers India Limited, Gurugram, Haryana, and at Gram Vikas - Brahmapur, Odisha. They have five variants of atmospheric water generators now with daily drinking water production from 43 to 2800 liters per day. VayuJal now has 130 machines in 29 states in India and Europe & Sri Lanka, catering to more than 4800



VayuJal was awarded the Climate Smart Innovation Exhibition & Award (CSI) 2024, organised by Solar Decathalon India at Infosys, Mysore.

people with drinking Water from Air. VayuJal is catering to industry segment leaders such as ITC Chola, ITC Life Science, Toyota Industries, Tata Communications, NASSCOM, IIT Madras, IIT Jammu, DRL-DRDO, IOCL, HPCL, Shell, JCBL, Tata Reality, L&T, Sify, etc. Highlights include: winner of the Climate Smart Innovation Exhibition & Award (CSI) 2024 - Organised by Solar Decathalon India at Infosys-Mysore.; winner of the NASSCOM Foundation Climate Tech Challenge – 2024. For more details, please visit <a href="https://vayujal.com/">https://vayujal.com/</a>

- AquEasy Innovations Private Limited is an Indian company incubated by IIT Madras working in the field of domestic water purification technologies. AquEasy currently develops contaminant specific water purifier bottles, 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. For more details, please visit <a href="https://www.ynos.in/startup/aqueasy">https://www.ynos.in/startup/aqueasy</a>
- EyeNetAqua Solutions Private Limited is a start-up company incubated at ICCW to develop and commercialize IoT-based sensing technologies for water quality monitoring. In the past EyeNetAqua has demonstrated inline measurements of pH, TDS, residual chlorine, nitrate, pressure and volume of flow for source water quality monitoring. For more details, please visit <a href="https://www.eyenetaqua.com/">https://www.eyenetaqua.com/</a>

### Centres

#### International Centre for Clean Water (ICCW)

across the country. In

The International Centre for Clean Water (ICCW), an initiative of IIT Madras has completed five years of its existence. Located at the IIT Madras Research Park, the Centre has developed and implemented technologies for real-time water quality and flow monitoring to support the Indian government's ambitious plans to implement Drink from Tap facilities

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Installation of CDI technologybased drinking water system in Gandhipura.

partnership with the Embassy of Israel, New Delhi, ICCW has initiated capacity-building programs for senior officials of the Ministry of Urban and Housing Affairs.

For the industrial sector, ICCW has developed solutions for recovery of materials and clean water from effluents, evaluated water initiatives and conducted water audits and certification programmes to help them in their quest for "Net Zero Water". ICCW has completed a household water security study for Ramanthapuram district and implemented over 130 safe drinking water solutions for communities, using emerging technologies that save carbon and water footprints,

with awareness programmes and behavioural change initiatives. Impact assessment for these projects and projects of other organisations has been added to the portfolio.

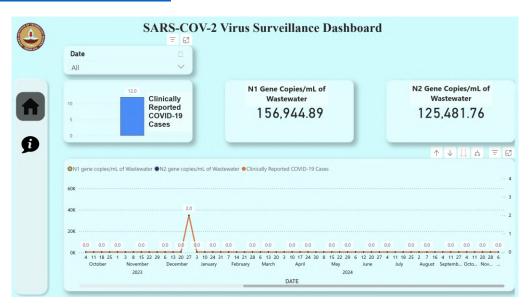
ICCW strengthened its support for startups by creating a Waterpreneur Studio – an ecosystem dedicated to startups in the water sector. Over 20 startups are being mentored at various stages of their evolution with a panel of experts. ICCW's international forays include being the India Challenge Owner for the 4<sup>th</sup> edition of the Atal Innovation Mission -Innovation Centre Denmark Challenge, and an MOU with Feng China University, Taiwan to bring sustainable water solutions to India. For more details, please visit <a href="https://iccw.world/">https://iccw.world/</a>

#### Wastewater-Based Epidemiology (WBE)

We have established a new research centre to test municipal wastewater for pathogens and chemicals and make the data available to the public and other potential stakeholders. This facility acts as an intelligence unit to track and prevent disease outbreaks in its early stages.

The WBE study is performed by analyzing biological and chemical human urinary biomarkers in wastewater. The WBE tool tracks pollutants, pesticides, licit and illicit drugs, and personal care products to which the population is exposed.

We recently created an online dashboard to track SARS-CoV-2 viruses circulating in IIT Madras community. The samples are analysed once a week and the data for the whole year are on the dashboard. An image of the dashboard is shown below. For more details, please visit <a href="https://usedwateranalytics.org/">https://usedwateranalytics.org/</a>



ANRF National Facility for Cryo-Electron Microscopy

DST-ANRF has set up a world-class cryo-electron microscopy facility at IIT Madras to provide a platform for researchers in and around IIT Madras.

We have initiated the setup of a cryo-electron microscopy imaging suite equipped with state-of-the-art infrastructure. We provide high-resolution analysis of a variety of samples, including

those from life sciences, materials science, and environmental sciences, to obtain new insights. For more details, please visit <a href="https://cryoem.iitm.ac.in/">https://cryoem.iitm.ac.in/</a>



SERB-ANRF national facility of cryo-EM: Krios G4 (left) and Talos F200i (right) at IIT Madras.

This year, we organized the 1<sup>st</sup> International Symposium on Cryo-Electron Microscopy, followed by a hands-on workshop on Microcrystal Electron Diffraction (MicroED) by Prof. Brent L. Nannenga, Associate Professor of Chemical Engineering, Arizona State University.



The details of the cryo-EM symposium are available at <a href="https://cryoem.iitm.ac.in/conference/">https://cryoem.iitm.ac.in/conference/</a>

#### Centre of Excellence (CoE) on Molecular Materials and Functions

We have built a sustainable centre with global visibility on molecular matter, focusing on atomically precise clusters and gas hydrates, to seed, nurture, and expand cutting-edge science and technology in respective areas, collectively with the best people across the world, with the involvement of the next generation.

As a part of this centre, we organized international winter schools, international conferences, lecture series, technical talks and lab visits. Some of these activities of 2024 are shown in the following pages. For more details, please visit <u>coe-on-molecular-materials-and-functions</u>

# Activities of Centre of Excellence (CoE) on molecular materials and functions

#### 1. Technical Talks

Talk-1: "MDa mass spectrometry for materials science" by Ms. Anagha Jose, IIT Madras, January 18, 2024.



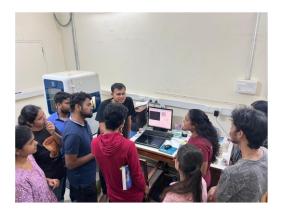
#### 2. Lab Visits

I. Visit to the lab of Prof. T. Pradeep, DST Unit of Nanoscience and Technology, Thematic Unit of Excellence, and SERB National Facility of Cryo-Electron Microscopy, Department of Chemistry, IIT Madras, January 25, 2024.





II. Visit to the lab of Prof. Pijush Ghosh, Department of Mechanical Engineering, IIT Madras, on March 14, 2024.



III. Visit to the lab of Prof. Rajnish Kumar, Department of Chemical Engineering, IIT Madras, April 18, 2024.





IV. Visit to the lab of Prof. Thangavelu Palaniselvam, Department of Chemistry, IIT Madras, June 6, 2024.



3. CoE Winter School on Molecular Materials and Functions 2024

The details of winter school are available at <a href="https://molmatter.org/coe-winter-school-2024/">https://molmatter.org/coe-winter-school-2024/</a>



4. CoE International Conference on Molecular Materials and Functions 2024

The conference details are available at <a href="https://molmatter.org/conference-2024/">https://molmatter.org/conference-2024/</a>



5. International Conference on Water for Life 2024

The conference details are available at <a href="https://waterforlifeiitm.org/">https://waterforlifeiitm.org/</a>

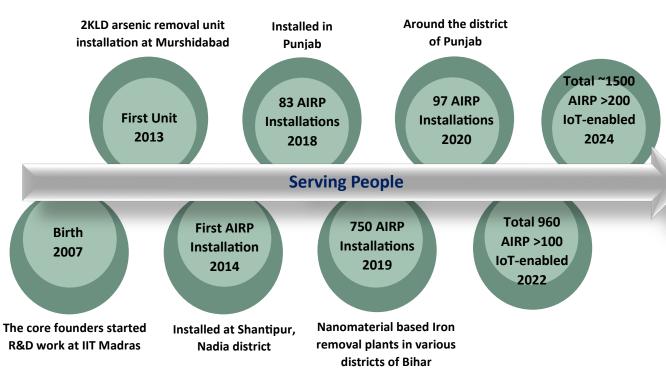


### Reach of Some of Our Technologies

VayuJal



### AMRIT- Anion and Metal Removal by Indian Technology



AIRP- Arsenic and Iron Removal Plant

Installations across India



### Media Reports (only a few)

### IIT-M unveils hybrid course to increase water literacy

Padmaja.J≇timesgroup.com

Chennai: In order to create water-literate citizens, IIT Madras has unveiled a hybrid four-month certificate course — Water Quality — An Approach to People's Water Data.

Apart from teaching students, this course will help create a database of ground, surface and piped water quality. said TPradeep, chemistry professor with IIT-M and one of the five instructors of the course. The institute has partnered with Tel Aviv University in Israel for the course.

As a pilot project, IIT Madras trained students of Stella Maris College, Madras Christian College and some students from Erode. It tested the water quality in 300 houses in Chennai and Erode and uploaded the data online. "Major findings from the previous exercise were that people were unaware about water quality and they believed that water from reverse osmossi is pure," said Prof Pradeep.

Now, IIT-M has launched water quality in 300 houses in Chemai and Erode and uploaded the data online. "Majorfindings from the previous exercise were that people were unaity and they believed that water from reverse osmosis is pure," said Pradeep.

Now, IIT-M has launched nees, coliform, nitrate, chlorideetc.

"This course is a deep-dive on water quality. Also, the course will generate water data. If we have 150 students, we will generate water data. If we have 150 owater sample data," said Pradeep.

Now, IIT-M has launched



this course to expand the initithis course to expand the initiative. Theory classes will be conducted online and offline about water quality and its impact on human health. The offline practicals involve each student picking 10 houses and testing water quality, including measuring the pH, hardness, coliform, nitrate, chloride etc.

affected by water quality
Students can have a certificate from ITF-Mon water quality, which will add to their resumes, and they can apply to water or food testing centres, shared Pradeep.
The course will entail a fee of 1.500, which will be refunded after course completion. The fee will also include field test kits. For practicals, the students will be assigned the closest colleges or labs, said Prof Pradeep.
The course can pick cities like Chemnal, Trichy and Combatore for offline practicals, said Swaminathan.
Minimum eligibility for the course is final year of bachelors of science or engineering. The registration forms are on the NPTEL website and he last date to register is January 18. Classes will begin from January 26, on Mondays, Tuesdays and Wednesdays, between 5pm and 5.50pm.

### IIT Chennai launches groundbreaking wastewater-based epidemiology project

Led by a team of distinguished researchers at IIT Chennai, this pioneering initiative seeks to revolutionize community health through a data-driven preventive healthcare approach using wastewater surveillance.

Updated: January 17, 2024 02:49 IST











### 'Outstanding work': IIT-M team makes mineral nanoparticles with water



♥ CHENNAI A 26°C

#### THE TIMES OF INDIA

#### IIT-Madras offering multi-disciplinary course in innovation and entrepreneurship

A Ragu Raman / TNN / Jul 23, 2024, 20:28 IST







CHENNAI: Indian Institute of Technology- Madras (IIT - Madras) is offering a four-month certificate course in 'Innovation and Entrepreneurship - A Multi-disciplinary Approach' aimed at final-year science and engineering students.

### THEMAHINDU

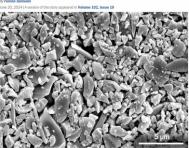
### Prof. M.V. Pylee Award for T. Pradeep

Published - March 12, 2024 08:12 pm IST - KOCH

THE HINDU BUREAU



#### Charged microdroplets turn minerals into nanoparticles





### Clean-water-for-all crusader Professor Thalappil Pradeep of IIT-Madras elected international member of US National Academy of Engineering

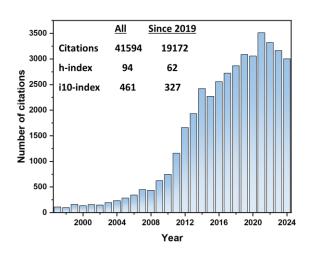
Professor Pradeep was bestowed the honour for his contributions to cluster chemistry and the discovery and implementation of affordable drinking water

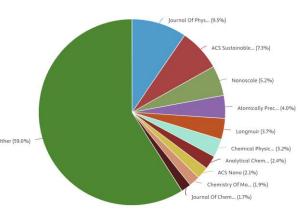


### **Publication Analysis**

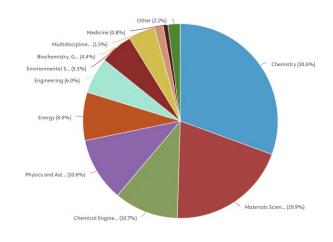
### Google Scholar

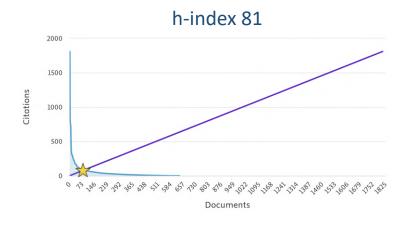






### Scopus - Document by subject





#### Sources

- 1. Google Scholar visited on December 30, 2024.
- 2. Scopus visited on December 30, 2024.

### Abstracts at a Glance

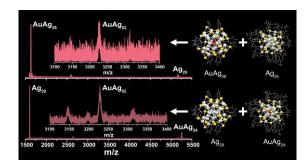
## Stable Dimer Intermediates During Intercluster Reactions of Atomically Precise Nanoclusters

Swetashree Acharya, Jayoti Roy, Diptendu Roy, Biswarup Pathak\* and Thalappil Pradeep\*

J. Phys. Chem. C, 2024. (Just accepted)

Intercluster reactions involving atomically precise noble metal nanoclusters (NCs) in solution, closely resembling reactions between molecules, are important for exploring chemistry at the nanoscale. In the present study, we conducted reactions between  $[Ag_{29}(1,3-BDT)_{12}]^{3-}(1,3-BDT=1,3$ benzenedithiol) and center-doped  $[MAg_{24}(2,4-DMBT)_{18}]^{q}$  (q = 1 for M = Ag, Au; and q = 2 for M = Pd, Pt; 2,4-DMBT = 2,4-dimethylbenzenethiol) NCs in solution. For the first time, we report the formation of stable dimers, formed between two NCs with mixed metal-ligand interfaces. The dimeric species formed were [MAg53xBDT12DMBT18-y]3- ( $x \ge 0$  and  $y \ge 0$ ), with 16 electrons in their valence shells. Here, the dimers were formed irrespective of the nature of the central atom in the NC, although the compositions were different depending on the central atom. These dimers were stable in solution for ~2 days.

The dithiol protected [Ag<sub>29</sub>BDT<sub>12</sub>]<sup>3-</sup> part was more stable in the dimers, during monothiol fragmentation than the protected [MAg<sub>2 4</sub>DMBT<sub>18</sub>]<sup>q-</sup> part. UV/vis spectroscopic and mass spectrometric analyses, along with density functional theory (DFT) calculations were used to understand the dimers. Our work has highlighted the importance of the cluster interface in the stability of the dimer formed. Probing such stable dimers formed during intercluster reactions can help us understand the reaction mechanism in greater detail.



#### Simulated Interstellar Photolysis of N<sub>2</sub>O Ice: Selectivity in Photoproducts

Bijesh K. Malla, Soham Chowdhury, Devansh Paliwal, Hanoona KM, Gaurav Vishwakarma, Rabin Rajan J. Methikkalam, and Thalappil Pradeep\*

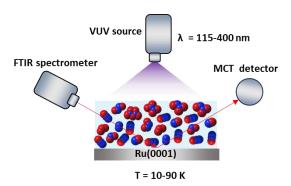
J. Phys. Chem. C, 2024. (Just accepted) (DOI: <u>10.1021/acs.jpcc.4c06624</u>)

Thermal diffusion and recombination control the kinetics of photochemical reactions of reactive radicals formed by ultraviolet photon irradiation in interstellar ices. Here, we show that upon vacuum ultraviolet photolysis, N<sub>2</sub>O ice produces

 $O_3$  and several oxides of nitrogen, such as NO, NO<sub>2</sub>, N<sub>2</sub>O<sub>2</sub>, N<sub>2</sub>O<sub>3</sub>, N<sub>2</sub>O<sub>4</sub>, and N<sub>2</sub>O<sub>5</sub> in interstellar ice mimics. Photoproducts within the bulk and on the surface were analyzed using reflection absorption infrared spectroscopy and Cs<sup>+</sup> ion-based

secondary ion mass spectrometry, while desorbed species were studied using temperature-programmed desorption spectrometry. Notably, thermal annealing of the photo-irradiated ice to 90 K resulted in a significant increase in NO and N<sub>2</sub>O<sub>3</sub>. Photoirradiation at 10 K revealed the dominance of three atom photoproducts, such as NO2 and O3. In contrast, irradiation at 50 K significantly enhanced the production of four or higher atom photoproducts (N2O2, N2O3, N2O4, and N2O5). This behavior is attributed to the restricted diffusion of reactive radicals and unstable oxygen species (O and O<sub>3</sub>) at which confines radical-radical 10 reactions to three or fewer atom

photoproducts, whereas higher temperatures facilitate oxygen and other radical diffusion and recombination, yielding heavier photoproducts. These results throw light on the thermal diffusion effects on the kinetics of photoproducts in interstellar ice mimics.

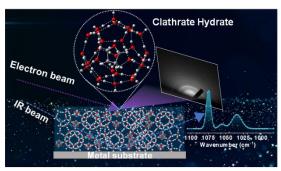


# Growth of Clathrate Hydrates in Nanoscale Ice Films Observed Using Electron Diffraction and Infrared Spectroscopy

Bijesh K. Malla, Ding-Shyue Yang\*, and Thalappil Pradeep\*

J. Phys. Chem. Lett., 2024 (Just accepted) (DOI: 10.1021/acs.jpclett.4c03106)

Clathrate hydrates (CHs) are believed to exist in cold regions of space, such as comets and icy moons. While spectroscopic studies have explored their formation in similar laboratory conditions, direct structural characterization using diffraction techniques has remained elusive. We present the first electron diffraction study of tetrahydrofuran (THF) and 1,3-dioxolane (DIOX) CHs in the form of nanometer-thin ice films under ultrahigh vacuum at cryogenic temperatures. By using reflection high-energy electron diffraction, we show that THF CH grows readily on various substrates during thermal annealing of an amorphous ice mixture of THF and water, and the formation is independent of the nature of the substrate. The growth of DIOX CHs on



an Au (111) substrate is similar. Comparison of electron diffraction patterns with calculated XRD patterns indicates that THF and DIOX form structure II CH (5<sup>12</sup>6<sup>4</sup>) with a lattice constant of ~17.2 Å (cubic, Fd m). Both CHs were also grown on Ru(0001) and were examined by reflection absorption infrared spectroscopy. A direct comparison of diffraction data with infrared spectra as a function of temperature further demonstrates the

strength of multiple probes in examining complex systems possessing diverse molecular interactions.

### Milling-Induced 'Turn-off' Luminescence in Copper Nanoclusters

Subrata Duary, Arijit Jana, Amitabha Das, Swetashree Acharya, Amoghavarsha Ramachandra Kini, Jayoti Roy, Ajay Kumar Poonia, Deepak Kumar Patel, Vivek Yadav, P. K. Sudhadevi Antharjanam, Biswarup Pathak\*, Adarsh Kumaran Nair Valsala Devi\*, and Thalappil Pradeep\*

Inorg. Chem., 63, 2024, 18727–18737. (DOI: 10.1021/acs.inorgchem.4c02617)

Atomically precise copper nanoclusters (NCs) attract research interest due to their intense photoluminescence, which enables their applications in photonics, optoelectronics, and sensing. Exploring properties requires carefully designed clusters with atomic precision and a detailed understanding of their atom-specific luminescence properties. Here, we report two copper NCs,  $[Cu_4(MNA)_2(DPPE)_2]$  and  $[Cu_6(MNA-H)_6]$ , shortly Cu<sub>4</sub> and Cu<sub>6</sub>, protected by 2mercaptonicotinic acid (MNA-H<sub>2</sub>) and 1,2bis(diphenylphosphino)ethane (DPPE), showing "turn-off" mechanoresponsive luminescence. Single-crystal diffraction reveals that in the Cu<sub>4</sub> cluster, two Cu<sub>2</sub> units are appended with two thiols, forming a flattened boat-shaped Cu<sub>4</sub>S<sub>2</sub> kernel, while in the Cu<sub>6</sub> cluster, two Cu<sub>3</sub> units form an adamantane-like Cu<sub>6</sub>S<sub>6</sub> kernel. High-resolution electrospray ionization mass spectrometry studies



reveal the molecular nature of these clusters. Lifetime decay profiles of the two clusters show the average lifetimes of 0.84 and 1.64 µs, respectively. These thermally stable Cu NCs become nonluminescent upon mechanical milling but regain their emission upon exposure to solvent vapors. Spectroscopic data of the clusters match well with their computed electronic work expands structures. This collection of thermally stable and mechanoresponsive luminescent coinage metal NCs, enriching the diversity and applications of such materials.

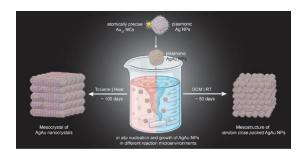
## Nanocluster Reaction-Driven in Situ Transformation of Colloidal Nanoparticles to Mesostructures

Paulami Bose, Pillalamarri Srikrishnarka, Matias Paatelainen, Nonappa, Amoghavarsha Ramachandra Kini, Anirban Som, and Thalappil Pradeep\*

Nanoscale, 2024. (DOI: 10.1039/d4nr02820a)

Atomically precise noble metal nanoclusters (NCs) are molecular materials known for their precise composition, electronic structure, and unique optical properties, exhibiting chemical reactivity. Herein, we demonstrated a simple one-pot method for fabricating self-assembled Ag-Au bimetallic mesostructures using a reaction between 2-phenylethanethiol (PET)-protected atomically precise gold NCs and colloidal silver nanoparticles (Ag NPs) tunable in а reaction microenvironment. The reaction carried out in toluene at 45 °C with constant stirring at 250 revolutions per minute (RPM) vielded a thermally micronsized cuboidal mesocrystals of self-AgAu@PET assembled nanocrystals. However, the reaction in dichloromethane at room temperature with constant stirring at 250 RPM resulted in a self-assembled

mesostructure of randomly close-packed NPs. AgAu@PET Using a host of experimental techniques, including optical electron microscopy, optical absorption spectroscopy, and light scattering, we studied the nucleation and growth processes. Our findings highlight a strategy to utilize precision and plasmonic NP chemistry in tailored microenvironments, leading customizable bimetallic hybrid three dimensional nanomaterials with potential applications.



### **Enhanced Electrical Output in an Electrostatic Generator Using Charged Water**

Vishal Kumar, Pillalamarri Srikrishnarka, Ramamurthy Nagarajan\*, and Thalappil Pradeep\*

ACS Sustainable Chem. Eng., 12, 2024, 13106–13115(DOI: 10.1021/acssuschemeng.4c01860)

Electrostatic charging of water, particularly at the water-hydrophobic interface, continues to perplex researchers despite centuries of work. Recent advancements in energy harvesting, materials synthesis, and sensing employing electrohydrodynamic generated processes have renewed interest in the electrostatic charging of water. This work aims to understand the charging of water from an energyharvesting perspective. We used a singleelectrode electrostatic generator initially to demonstrate enhancement of the electric output with the addition of water. Through several control measurements. established that the enhancement was a result of the electrostatic charging of water.



The role of electrode wettability and pH on the electric output was studied. The effect of pH on the charging of water was correlated with the output voltage. The system was extended to a double-electrode electrostatic generator (DE-EG) to expand the applicability of the technique and increase the output. Using

the DE-EG, we demonstrated the influence of an electric field on the charging of water. The electricity thus produced was used to power multiple light-emitting diodes. Furthermore, the technique was employed to treat wastewater containing a dye using

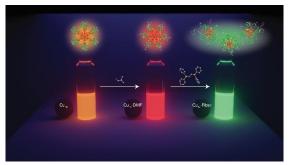
a 3D-printed linear actuator. The insights presented are useful in enhancing the performance of water-based EGs and could help to better understand various electrohydrodynamic processes.

# Multicolor Photoluminescence of Cu<sub>14</sub> Clusters Modulated Using Surface ligands

Arijit Jana, Subrata Duary, Amitabha Das, Amoghavarsha Ramachandra Kini, Swetashree Acharya, Jan Machacek, Biswarup Pathak\*, Tomas Base\* and Thalappil Pradeep\*

Chem. Sci., 15, 2024, 13741–13752. (DOI: <u>10.1039/D4SC01566E</u>)

Copper exhibit unique nanoclusters structural features and their molecular assembly results in diverse photoluminescence properties. In this study, we present ligand-dependent multicolor luminescence observed in a Cu<sub>14</sub> cluster, primarily protected by orthocarborane-9,12-dithiol (o-CBDT), featuring an octahedral Cu<sub>6</sub> inner kernel enveloped by eight isolated copper atoms. The outer layer of the metal kernel consists of six bidentate o-CBDT ligands, in which carborane backbones are connected through μ<sub>3</sub>-sulphide linkages. The initially prepared Cu<sub>14</sub> cluster, solely protected by six o-CBDT ligands, did not crystallize in its native form. However, in the presence of N,N-dimethylformamide (DMF), the cluster crystallized along with six DMF molecules. Single-crystal X-ray diffraction (SCXRD) revealed that the DMF molecules were directly coordinated to six of the eight capping Cu atoms, while oxygen atoms were bound to the two remaining Cu apices in antipodal positions. Efficient tailoring of the cluster surface with DMF shifted its luminescence from yellow to bright red.



Luminescence decay profiles showed fluorescence emission for these clusters, originating from the singlet states. Additionally, we synthesized microcrystalline fibers with a onedimensional assembly of DMF-appended Cu<sub>14</sub> clusters and bidentate DPPE linkers. These fibers exhibited bright greenishphosphorescence emission, vellow originating from the triplet state, indicating the drastic surface tailoring effect of secondary ligands. Theoretical calculations provided insights into the electronic energy levels and associated electronic transitions for these clusters. This work demonstrated dynamic tuning of the emissive excited states of copper nanoclusters through the efficient engineering of ligands

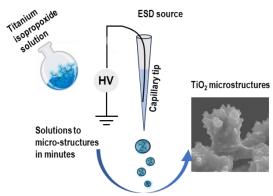
### From Solution to Microstructures in Minutes: Microdroplet-Derived Stand-Alone TiO<sub>2</sub> Surfaces for Simultaneous Water Harvesting and Treatment

Keerthana Unni, Jenifer Shantha Kumar, Anirban Som, Depanjan Sarkar\* and Thalappil
Pradeep\*

ACS Sustainable Chem. Eng., 12, 2024, 11957–11967.

(DOI:10.1021/acssuschemeng.4c02806)

We present a straightforward and ecofriendly method to transform a titanium tetraisopropoxide (TTIP) solution into superhydrophobic TiO<sub>2</sub> microstructures by ambient microdroplet deposition. At lower temperatures the micropillars amorphous TiO<sub>2</sub> act as nucleation sites for condensing humidity to form droplets. However, the microstructures facilitate efficient water runoff despite TiO<sub>2</sub>'s hydrophilic character by a combination of hydrophobicity surface and gravity. Additionally, the photocatalytic surface resists biofilm formation and degrades the contaminants, offering longterm collection of safe water and its purification, which has been demonstrated



with examples. We demonstrate that the microdroplet-based methodology developed for the conversion of solution into microdroplets can also be applied to other metal oxides, including CuO and ZnO, highlighting the universality of the process.

# **Cysteine-Protected Antibacterial Spheroids of Atomically Precise Copper Clusters for Direct and Affordable Arsenic Detection from Drinking Water**

Jenifer Shantha Kumar, Arijit Jana, Jayathraa Raman, Hema Madhuri Veera, Amoghavarsha Ramachandra Kini, Jayoti Roy, Saurav Kanti Jana, Tiju Thomas and Thalappil Pradeep\*

Environ. Sci. Technol. Lett., 11, 2024, 831–837. (DOI: 10.1021/acs.estlett.4c00264)

Rapid and naked-eye detection of water-borne contaminants using molecularly precise nanomaterials has emerged as a promising strategy to reduce the impact of chemical pollution. This study presents a luminescence-based arsenic (As) sensor, eliminating the need for sample preparation. Incorporating red-emitting spheroidal cluster-assembled superstructures (CASs), comprised of

by I-cysteine (I-Cys) and 1,2-

Cu<sub>17</sub> nanoclusters (Cu<sub>17</sub>NCs), coprotected

bis(diphenylphosphino) ethane (DPPE) ligands, the sensor exhibits notable sensitivity toward arsenite ( $As^{3+}$ ) and ( $As^{5+}$ ) ions. A detection limit of 1 ppb in tap water was achieved through luminescence-based quenching. Remarkably, it demonstrates selective detection of As amidst common interfering metal ions such as  $Cd^{2+}$ ,  $Hg^{2+}$ ,  $Fe^{3+}$ ,  $Pb^{2+}$ ,  $Cu^{2+}$ , and  $Cr^{3+}$ . A sensor disc made of CASs coated on nonwoven polypropylene (PP) mats has been devised for practical field applications. Electron

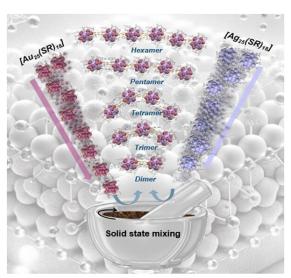
microscopy reveals disrupted morphology of the spheroids due to As interaction. Moreover, the CASs exhibit significant antibacterial efficacy against Gramnegative Escherichia *coli* and Grampositive Staphylococcus aureus and antibiofilm properties against Bacillus *subtilis*. This research highlights the effectiveness of atomically precise clusters for a practical application with direct societal relevance.

## Extensive Polymerization of Atomically Precise Alloy Metal Clusters During Solid State Reactions

B. S. Sooraj, Jayoti Roy, Manish Mukherjee, Anagha Jose and Thalappil Pradeep\*

Langmuir, 40, 2024, 15244–15251. (DOI: 10.1021/acs.langmuir.4c01737)

Exploring the reactions between atomically precise metal clusters consequences of such reactions has been an exciting field of research during the past decade. Initial studies in the area were on reactions between clusters in the solution phase, which proceed through the formation of dimers of reacting clusters. In the present work, we examine the interaction between two atomically precise clusters, [Au25(PET)18] and [Ag25(DMBT)18] -, in the solid state, and where PET DMBT 2-2,4phenylethanethiol and dimethylbenzenethiol, respectively. The experiments were performed different ratios of these two clusters, and it was inferred that the kinetics of the reactions were faster compared with reactions in the solution. The metal exchange between these two clusters, due to their interactions in the solid state, leads to the formation of dimers, trimers,



tetramers, and polymers of atomically precise alloy metal clusters. We observed polymer entities up to hexamers, which were observed for the first time. Control experiments revealed that metal exchange is a key factor leading to polymerization. Our work points to a new approach for synthesizing polymers of atomically precise alloy metal clusters.

## Partitioning Photochemically Formed CO<sub>2</sub> into Clathrate Hydrate under Interstellar Conditions

Gaurav Vishwakarma, Bijesh K. Malla, Rajnish Kumar\* and Thalappil Pradeep\*

Phys. Chem. Chem. Phys., 26, 2024, 16008–16016. (DOI: 10.1039/D4CP01414F)

Clathrate hydrates (CHs), host-guest compounds of water forming hydrogenbonded cages around guest molecules, are now known to exist under interstellar conditions. Experimental evidence demonstrated that prolonged thermal treatment of a solid mixture of water and CO<sub>2</sub>/CH<sub>4</sub> produces CHs at 10-30 K under simulated interstellar conditions. However, in the current study, we show that CO<sub>2</sub> produced photochemically by vacuum ultraviolet irradiation of H<sub>2</sub>O-CO mixtures at 10 K and  $\sim 10^{-10}$  mbar, gets partitioned into its CH phase and a matrix phase embedded in amorphous ice. The process occurring under simulated interstellar conditions was studied at different temperatures and H<sub>2</sub>O-CO compositions. The formation of CO<sub>2</sub> CH and other photoproducts was confirmed using infrared reflection absorption **UV-induced** spectroscopy. The photodesorption event of CO<sub>2</sub> may provide



the mobility required for the formation of CHs, while photoproducts like methanol can stabilize suc h CH structures. Our study suggests that new species originating during such energetic processing in ice matrices may form CH, potentially altering the chemical composition of astrophysical environments.

# Interparticle Antigalvanic Reactions of Atomically Precise Silver Nanoclusters with Plasmonic Gold Nanoparticles: Interfacial Control of Atomic Exchange

Paulami Bose, Jayoti Roy, Vikash Khokhar, Biswajit Mondal, Ganapati Natarajan, Sujan Manna, Vivek Yadav, Anupriya Nyayban, Sharma S. R. K. C. Yamijala\*, Nonappa\*, and Thalappil Pradeep\*

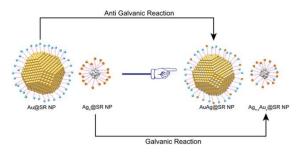
Chem. Mater., 36, 2024, 7581–7594. (DOI: 10.1021/acs.chemmater.4c00620)

This work demonstrates that antigalvanic reactions (AGRs) between thiol-protected plasmonic gold nanoparticles (NPs) and atomically precise silver nanoclusters (NCs) are an interfacial chemistry-driven

phenomenon. We reacted 2,4-dimethylbenzenethiol (DMBT)-protected Au NPs (average diameter of 4.46  $\pm$  0.64 nm) with atomically precise [Ag<sub>25</sub>(DMBT)<sub>18</sub>]<sup>-</sup> NC and obtained

bimetallic AgAu@DMBT alloy NPs. Systematic investigations with optical absorption spectroscopy, high-resolution transmission/scanning transmission electron microscopy, elemental and mapping revealed the reaction-induced morphological and compositional transformation in NPs. Furthermore, we show that such AGRs get restricted when geometrically rigid interfaces are used. For this, we used 1,3-benzenedithiol (BDT)protected Au@BDT NPs and  $[Ag_{29}(BDT)_{12}(TPP)_4]^{3-}$ NCs (TPP triphenylphosphine). Electrospray ionization mass spectrometric (ESI MS) studies revealed that the interparticle reaction proceeds via metal-ligand and/or metal exchange, depending on the

interface. Density functional theory (DFT) calculations and molecular docking simulations were used to understand the interactions and reaction energetics leading to favorable events. Interfacial chemistry of this kind might offer a one-pot synthetic strategy to create ultrafine bimetallic NP-based hybrid materials with potential optoelectronic and catalytic applications.

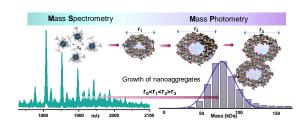


# Observing Atomically Precise Nanocluster Aggregates in Solution by Mass Photometry

Jayoti Roy, Ila Marathe, Vicki Wysocki and Thalappil Pradeep\*

Chem. Commun., 60, 2024, 6655-6658. (DOI: 10.1039/D4CC00363B)

We report the first mass photometric characterization of nanoaggregates of atomically precise nanoclusters (NCs) in solution. The differently-sized nanoaggregates of silver-gold alloy NCs,  $[Ag_{11-x}Au_x(DPPB)_5Cl_5O_2]^{2+}[x =$ **DPPB** 1,4bis(diphenylphosphino)butane], formed in examined solution, were by mass photometry (MP) with protein calibration. In addition, we conducted MP studies of varying solvent composition to understand the structural evolution of nanoaggregates. The masses of nanoaggregates were correlated to structures of 15 to 50 nm diameter observed in cryo-electron microscopy.

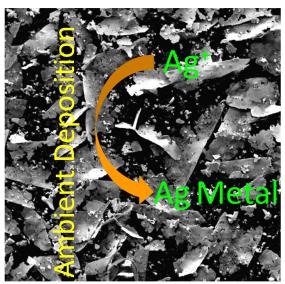


# Interfacial Growth of Large Area Single-Crystalline Silver Sheets Through Ambient Microdroplets

Depanjan Sarkar\*, Anirban Som, Keerthana Unni, Sujan Manna, and Thalappil Pradeep\*

Small, 2024, 2400159. (DOI: 10.1002/smll.202400159)

We report the creation of micrometersized sheets of silver at the air-water interface by direct deposition electrospray-generated silver ions (Ag+) on an aqueous dispersion of reduced graphene oxide (RGO), in ambient conditions. In the process of electrospray deposition (ESD), an electrohydrodynamic flow is created in the aqueous dispersion, and the graphene sheets assemble, forming a thin film at the air-water interface. The deposited Ag+ coalesce to make single-crystalline Ag sheets on top of this assembled graphene layer. Fast neutralization of Ag+ forming atomic Ag, combined with their enhanced mobility on graphene surfaces, presumably facilitates the growth of larger Ag clusters. Moreover, restrictions imposed by the interface drive the crystal growth in two dimensions. By controlling the precursor salt concentration, RGO concentration, deposition time, and ion current, the dimensionality of the Ag sheets could be tuned. These Ag sheets are effective substrates for surface-enhanced Raman spectroscopy (SERS), as demonstrated by the successful detection of methylene blue at nanomolar concentrations.



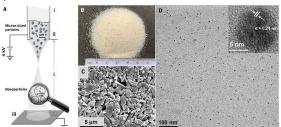
# Spontaneous Weathering of Natural Minerals in Charged Water Microdroplets forms Nanomaterials

B. K. Spoorthi, Koyendrila Debnath, Pallab Basuri, Ankit Nagar, Umesh V. Waghmare, and Thalappil Pradeep\*

Science, 384, 2024, 1012–1017. (DOI: 10.1126/science.adl3364)

In this work, we show that particles of common minerals break down spontaneously to form nanoparticles in charged water microdroplets milliseconds. We transformed micron-sized natural minerals like quartz and ruby into 5- to 10-nanometer particles when integrated into aqueous microdroplets generated via electrospray. We deposited the droplets on a substrate, which allowed characterization. nanoparticle determined through simulations that quartz undergoes proton-induced slip,

especially when reduced in size and exposed to an electric field. This leads to particle scission and the formation of



silicate fragments, which we confirmed with mass spectrometry. This rapid weathering process may be important for soil formation, given the prevalence of charged aerosols in the atmosphere.

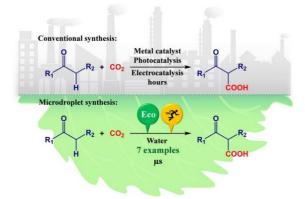
### Spontaneous α-C−H Carboxylation of Ketones by Gaseous CO₂ at the Air-Water Interface of Aqueous Microdroplets

Pallab Basuri\*, Sinchan Mukhopadhyay\*, K.S.S.V. Prasad Reddy, Keerthana Unni, B. K. Spoorthi, Jenifer Shantha Kumar, Sharma S.R.K.C. Yamijala, and Thalappil Pradeep\*

Angew. Chem. Int. Ed., 63, 2024, e202403229. (DOI: 10.1002/anie.202403229)

We present a catalyst-free route for the reduction of carbon dioxide integrated with the formation of a carbon-carbon bond at the air/water interface of negatively charged aqueous microdroplets, at ambient temperature. The reactions proceed through carbanion generation at the  $\alpha$ -carbon of a ketone followed by nucleophilic addition to CO<sub>2</sub>. Online mass spectrometry reveals that the product is an β-ketoacid. Several factors, such as the concentration of the reagents, pressure of CO<sub>2</sub> gas, and distance traveled by the droplets, control the kinetics of the reaction. Theoretical calculations suggest that water in the microdroplets facilitates

this unusual chemistry. Furthermore, such a microdroplet strategy has been extended to seven different ketones. This work demonstrates a green pathway for the reduction of CO<sub>2</sub> to useful carboxylated organic products.

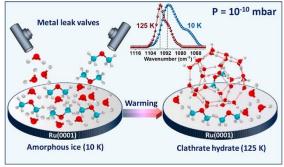


## Formation and Dissociation of Dimethyl Ether Clathrate Hydrate in Interstellar Ice Mimics

Bijesh K. Malla, Gaurav Vishwakarma, Soham Chowdhury, Samir Kumar Nayak, Sharma S. R. K. C. Yamijala, and Thalappil Pradeep\*

J. Phys. Chem. C, 128, 2024, 2463–2470. (DOI: 10.1021/acs.jpcc.3c07792)

Clathrate hydrates (CHs) are believed to exist within interstellar environments, potentially contributing to the preservation of diverse volatile compounds within icy bodies across the cosmos. In this study, using reflection absorption infrared spectroscopy, we show the formation of dimethyl ether (DME) CH from a vapordeposited DME—water amorphous ice mixture. Experiments were conducted in



an environment mimicking interstellar conditions: ultrahigh vacuum ( $P \sim 5 \times 10^{-}$ 

 $^{10}$  mbar) and cryogenic conditions ( $T\sim 10-150~$  K). Thermal annealing of the amorphous ice mixture to a higher temperature ( $T\sim 125~$  K) resulted in the formation of CH. Quantum chemical calculations suggested the formation of  $5^{12}6^4$  cages of structure II CH. Subsequent investigations into the dissociation of DME CH unveiled its transformation into hexagonal ice, requiring a substantial

activation energy of 68.04 kJ mol<sup>-1</sup>. Additionally, confirmation of the formation and dissociation of CH was supported by temperature-programmed desorption mass spectrometry. These results significantly advance our understanding of the existence of CHs under extreme conditions relevant to an interstellar medium.

### Acknowledgements

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