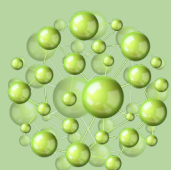




# ANNUAL REPORT 2023



THEMATIC UNIT OF EXCELLENCE



Center of Excellence on  
**Molecular Materials  
and Functions**

Please visit the links for the annual reports of  
[2014](#), [2015](#), [2016](#), [2017](#), [2018](#), [2019](#), [2020](#), [2021](#), [2022](#)

## Our team

### Thalappil Pradeep

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



Our struggle is to be creative every day.

### Ph.D. and MS Students

- |                        |                        |                      |
|------------------------|------------------------|----------------------|
| • A. Anil Kumar        | • Harshita Nagar       | • Subrata Duary      |
| • A. Suganya           | • Jayoti Roy           | • Sujan Manna        |
| • Amoghavarsha R. Kini | • Keerthana Unni       | • Swetashree Acharya |
| • Anagha Jose          | • Paulami Bose         | • Tanmayaa Nayak     |
| • Anubhav Mahapatra    | • Riya Dutta           | • Vishal Kumar*      |
| • Atrayee Datta        | • S. Jenifer           | • Vivek Yadav        |
| • Bijesh K. Malla      | • Sinchan Mukhopadhyay | • Ramesh Kumar*      |
| • B. K. Spoorthi       | • Samapti Mondal       | • S. Sudhir*         |
| • B. S. Sooraj         | • Sonali Seth          |                      |
| • Deepak Kumar Patel*  | • Soham Chowdhury      |                      |

\*Jointly advised students

### Postdoctoral Fellows/ Project Associates

- |                          |                         |
|--------------------------|-------------------------|
| • Dr. Anish R Nath       | • Karthika Kalyansundar |
| • Dr. Anupriya Nyayban   | • Anshupriya            |
| • Dr. Sourav Kanti Jana  | • Vikash Khokhar        |
| • Dr. Anirban Som        | • Rima Chandra          |
| • Dr. A. Parthasarathy   | • Asmitha Shri          |
| • Dr. Gaurav Vishwakarma | • Ashmit Verma          |

### Administrative Officer

- K. Priya

### International Visiting Faculty

- Dr. Nebil Omri

### M.Sc./ Visiting Students

- |                                   |                                    |  |
|-----------------------------------|------------------------------------|--|
| • Devansh Paliwal                 | • P Vijithra <sup>\$</sup>         | • Suzan Kagan <sup>\$\$</sup>                  |
| • Abhijit Gupta                   | • Jayathraa Raman <sup>\$</sup>    | • Shakked Ben Giat <sup>\$\$</sup>             |
| • Sakshi Khandare <sup>\$</sup>   | • G Goutham Krishna <sup>\$</sup>  | • Timor Lichtman <sup>\$\$</sup>               |
| • Mohd. Shafeeullah <sup>\$</sup> | • C Anagha <sup>\$</sup>           | • Tohar Izikson <sup>\$\$</sup>                |
| • Shree Lakshmi <sup>\$</sup>     | • K S Adhya Lakshmi <sup>\$</sup>  | • Kazutaka Oiwa <sup>\$\$</sup>                |
| • Akshyata Kirtania <sup>\$</sup> | • K K Naja <sup>\$</sup>           |  |
| • Mahima Dutta                    | • V P Fathima Rana <sup>\$</sup>   |  |
| • Muhammad Ijas M                 | • K M Hanoona <sup>\$</sup>        | <sup>\$</sup> Students from other institutions |
| • Nafeesa Farsana <sup>\$</sup>   | • Jewel Elsa Josan <sup>\$</sup>   |  |
| • Neha Nazeer <sup>\$</sup>       | • N Nafeeha <sup>\$</sup>          | <sup>\$\$</sup> International students         |
| • Manish Mukherjee <sup>\$</sup>  | • K S Aswathi <sup>\$</sup>        |  |
| • Parveen Kumar <sup>\$</sup>     | • V Sneha <sup>\$</sup>            |  |
|                                   | • S Radhika Bharathi <sup>\$</sup> |  |

### Project Technicians

- Balamurugan
- K. Banupriya
- C. Meyyarasan

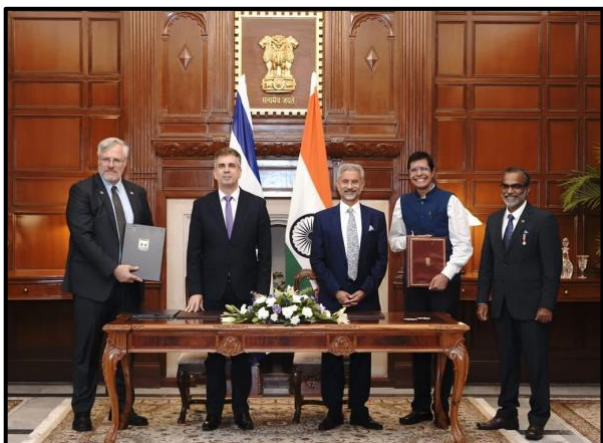
### Centre of Excellence (CoE) on Molecular Materials and Functions CoE Fellows

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

## What's Inside

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## Glimpses of 2023



A letter of Intent was signed for India-Israel Center of water technology at IIT Madras by Mr. Manoj Joshi, Secretary, MoHUA, Govt. of India, in presence of Shri. S. Jaishankar and Mr. Naor Gilon, Hon'ble Ministers of External Affairs of India and Israel, respectively and the Director, IITM, on May 9, 2023.



The book, "Empowering India" co-authored by Prof. T. Pradeep and Mr. Krishnan Narayanan was released by the Minister of Education in presence of the Director, IITM at Bharat Mandapam, New Delhi on July 30, 2023.



CoE Winter School on Molecular Materials and Functions, IIT Madras, December 11-15, 2023.



Book launch event at Infosys Science Foundation, Bengaluru on August 20, 2023, the authors are with Mr. N. R. Narayana Murthy, Co-founder, Infosys and Prof. Umesh Waghmare, President, Indian Academy of Sciences.



International Conference on Molecular Matter - Emerging Directions for Sustainability, IIT Madras, December 16-18, 2023.

## Awards and Honours



Prof. T. Pradeep was bestowed with the 'IISc Distinguished Alumni Award' of 2021. He received the honour from the Director of IISc. on December 2, 2023.



Prof. T. Pradeep has received the 'SASTRA-CNR Rao Award' in Chemistry and Materials Science for the year 2023. The award was presented by Dr. Charan Gurumurthy, Tata Electronics to all the awardees, Prof. T. Pradeep, Prof. M.S. Valiathan, Prof. Sriram Ramaswamy, Prof. Samir Maji and Prof. S. Natarajan, on February 28, 2023.



Prof. T. Pradeep receiving the first 'International Excellence Award of Karlsruhe Institute of Technology, Germany and Fellowship of SCHROFF Foundation', on November 27, 2023.



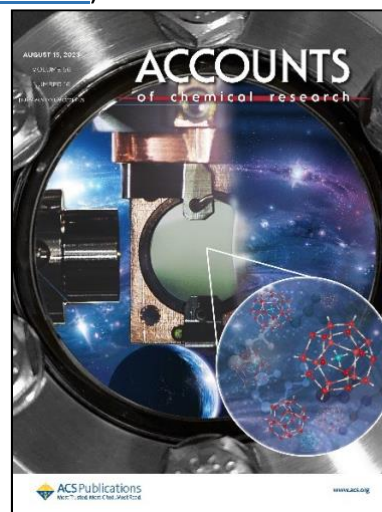
Prof. T. Pradeep receiving the prestigious Eni Award 2023 from Sergio Mattarella, President of the Republic of Italy at the Quirinal Palace, Rome, on October 16, 2023. Eni Award has come to India for the second time.

Prof. T. Pradeep has received the 'International Medal for Materials Science and Technology' of the Materials Research Society of India, on December 12, 2023, at IIT-BHU, Varanasi. This is the highest award of MRSI.

Prof. T. Pradeep has received the 'Careers360 2<sup>nd</sup> Faculty Research Award' for the most outstanding researcher in the country in the field of Materials Science, on October 6, 2023.

## Publications

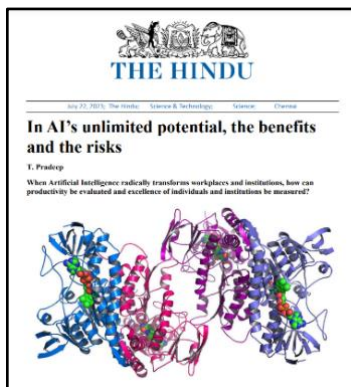
1. Vacuum ultraviolet photolysis of condensed methyl chloride in interstellar model conditions and trapping of intermediates at inter-grain interfaces, Bijesh Malla, Gaurav Vishwakarma, Soham Chowdhury, and Thalappil Pradeep, *J. Phys. Chem. C*, 127(2023), 24149-24157 (DOI: [10.1021/acs.jpcc.3c05889](https://doi.org/10.1021/acs.jpcc.3c05889)).
2. A concise guide to chemical reactions of atomically precise noble metal nanoclusters, Paulami Bose, Krishnadas Kumaranchira Ramankutty, Papri Chakraborty, Esma Khatun, and Thalappil Pradeep, *Nanoscale*, (2023) (Just accepted) (DOI: [10.1039/D3NR05128E](https://doi.org/10.1039/D3NR05128E)).
3. Structure and electrocatalytic performance of co-crystallized ternary molybdenum oxo-sulfide clusters for efficient water splitting, Biswajit Mondal, Arijit Jana, Jayoti Roy, Astrid Campos Mata, Akhil S. Nair, Ananthu Mahendranath, Soumyabrata Roy, Biswarup Pathak, Pulickel M. Ajayan, and Thalappil Pradeep, *ACS Mater. Lett.*, 5 (2023), 3306–3315 (DOI: [10.1021/acsmaterialslett.3c00957](https://doi.org/10.1021/acsmaterialslett.3c00957)).
4. Observing real-time adhesion of microparticles on glass surfaces, Pillalamarri Srikrishnarka, Dhivyaraja Kumaran, Amoghavarsha Ramachandra Kini, Vishal Kumar, Ankit Nagar, Md Rabiul Islam, Ramamurthy Nagarajan, and Thalappil Pradeep, *Langmuir*, 39(2023), 17071-17079 (DOI: [10.1021/acs.langmuir.3c01856](https://doi.org/10.1021/acs.langmuir.3c01856)).
5. Photoconversion of Ag<sub>31</sub> to Ag<sub>42</sub>, Initiated by solvated electrons, Arijit Jana, Wakeel Ahmed Dar, Sourav Kanti Jana, Ajay Poonia, Vivek Yadav, Jayoti Roy, Sourov Chandra, Kumaran Nair Valsala Devi Adarsh, Robin Ras, and Thalappil Pradeep, *Chem. Mater.*, 35 (2023), 7020-7031 (DOI: [10.1021/acs.chemmater.3c01293](https://doi.org/10.1021/acs.chemmater.3c01293)).
6. Macropolyhedral syn-B<sub>18</sub>H<sub>22</sub>, the “forgotten” isomer, Deepak Patel, B. S. Sooraj, Kaplan Kirakci, Jan Machacek, Monika Kučeráková, Jonathan Bould, Michal Dusek, Martha Frey, Christof Neumann, Sundargopal Ghosh, Andrey Turchanin, and Thalappil Pradeep, *J. Am. Chem. Soc.*, 145 (2023) 17975-17986 (DOI: <https://doi.org/10.1021/jacs.3c05530>).
7. Formation and transformation of clathrate hydrates under interstellar conditions, Jyotirmoy Ghosh, Gaurav Vishwakarma, Rajnish Kumar, and Thalappil Pradeep, *Acc. Chem. Res.*, 56 (2023), 2241–2252 (DOI: <https://doi.org/10.1021/acs.accounts.3c00317>).
8. Secondary ligand-induced orthogonal self-assembly of silver nanoclusters into superstructures with enhanced NIR emission, Korath Shivan Sugi, Amritha P Sandra, Nonappa, Debasmita Ghosh, Jyoti Sarita Mohanty, Murugesan Paulthangam Kannan, B. S. Sooraj, Pillalamarri Srikrishnarka, Jayoti Roy, Wakeel Ahmed Dar, and Thalappil Pradeep, *Nanoscale*, 15 (2023) 11927-11934 (DOI: <https://doi.org/10.1039/D3NR02561F>).
9. Existence of acetaldehyde clathrate hydrate and its dissociation leading to cubic ice under ultrahigh vacuum and cryogenic conditions, Gaurav Vishwakarma, Bijesh K. Malla, Soham Chowdhury, Sakshi Pradip Khandare and Thalappil Pradeep, *J. Phys.*



- Chem. Lett., 14 (2023) 5328–5334 (DOI: <https://doi.org/10.1021/acs.jpcllett.3c01181>).
10. Endangered indigenous rice varieties as a source of B vitamins for the undernourished population, Priyabrata Roy, Debal Deb, Arunan Suganya, Brindaban Roy, Thalappil Pradeep, and Tanima Saha, Cereal Chem., 100 (2023) 887-894 (DOI: [10.1002/cche.10668](https://doi.org/10.1002/cche.10668)).
  11. Atomically precise clusters: Chemical evolution of molecular matter at the nanoscale, Arijit Jana, Amoghavarsha Ramachandra Kini, and Thalappil Pradeep, AsiaChem, 3 (2023) 56-65 (DOI: <https://doi.org/10.51167/acm00040>).
  12. Dissociative reactions of  $[\text{Au}_{25}(\text{SR})_{18}]^-$  at copper oxide nanoparticles and formation of aggregated nanostructures, Jayoti Roy, Biswajit Mondal, Gaurav Vishwakarma, Nishanthi Vasanthi Sridharan, Pattabiraman Krishnamurthi, Nonappa, and Thalappil Pradeep, Nanoscale, 15 (2023) 8225-8234 (DOI: [10.1039/D3NR00897E](https://doi.org/10.1039/D3NR00897E)).
  13. A luminescent  $\text{Cu}_4$  cluster film grown by electrospray deposition: A nitroaromatic vapour sensor, Arijit Jana, B. K. Spoorthi, Akhil S. Nair, Ankit Nagar, Biswarup Pathak, Tomas Base, and Thalappil Pradeep, Nanoscale, 15 (2023) 8141-8147 (DOI: [10.1039/d3nr00416c](https://doi.org/10.1039/d3nr00416c)).
  14. Induced migration of  $\text{CO}_2$  from hydrate cages to amorphous solid water under ultrahigh vacuum and cryogenic conditions, Gaurav Vishwakarma, Bijesh Malla, Karri Sesha Surya Vara Prasad Reddy, Jyotirmoy Ghosh, Soham Chowdhury, Sharma S. R. K. C. Yamijala, Sandeep Kumar Reddy, Rajnish Kumar, and Thalappil Pradeep, J. Phy. Chem. Lett., 14 (2023) 2823-29 (DOI: [10.1021/acs.jpcllett.3c00373](https://doi.org/10.1021/acs.jpcllett.3c00373)).
  15. Vertically aligned nanoplates of atomically precise  $\text{Co}_6\text{S}_8$  cluster for practical arsenic sensing, Anagha Jose, Arijit Jana, Tanvi Gupte, Akhil Nair, Keerthana Unni, Ankit Nagar, Amoghavarsha Kini, B. K. Spoorthi, Sourav Jana, Biswarup Pathak, and Thalappil Pradeep, ACS Mater. Lett., 5 (2023) 893–899 (DOI: [10.1021/acsmaterialslett.3c00085](https://doi.org/10.1021/acsmaterialslett.3c00085)).
  16. Gold  $\text{Au}(\text{I})_6$  clusters with ligand-derived atomic steric locking: Multifunctional optoelectrical properties and quantum coherence, Sourov Chandra, Alice Sciortino, Susobhan Das, Faisal Ahmed, Arijit Jana, Jayoti Roy, Diao Li, Ville Liljeström, Hua Jiang, Leena-Sisko Johansson, Xi Chen, Nonappa, Marco Cannas, Thalappil Pradeep, Bo Peng, Robin H. A. Ras, Zhipei Sun, Olli Ikkala, and Fabrizio Messina, Adv. Opt. Mater., (2023) 2202649 (DOI: [10.1002/adom.202202649](https://doi.org/10.1002/adom.202202649)).
  17. The frontiers of water and sanitation, Anna M. Michalak, Jun Xia, Damir Brdjanovic, Aimée-Noël Mbiyozo, David Sedlak, Thalappil Pradeep, Upmanu Lall, Nitya Rao, and Joyeeta Gupta, Nat. Water., 1 (2023) 10–18 (DOI: [10.1038/s44221-022-00020-1](https://doi.org/10.1038/s44221-022-00020-1)).
  18. Tunable reactivity of silver nanoclusters: Facile route to synthesize a range of bimetallic nanostructures, Amrita Chakraborty, Megha Maria Stanley, Biswajit Mondal, Nonappa, Md Bodiuzzaman, Papri Chakraborty, M. P. Kannan, and Thalappil Pradeep, Nanoscale, 15 (2023) 2690-2699 (DOI: [10.1039/D2NR06350F](https://doi.org/10.1039/D2NR06350F)).

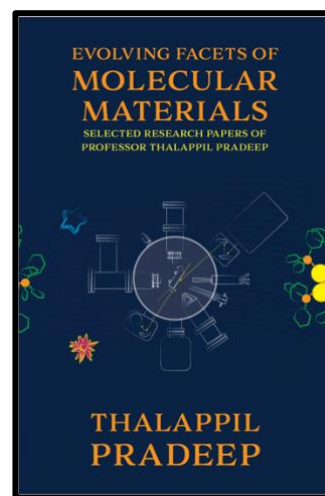
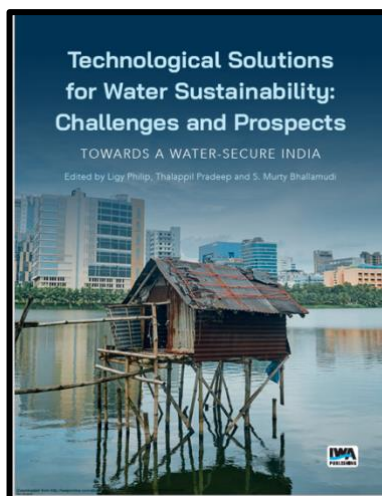
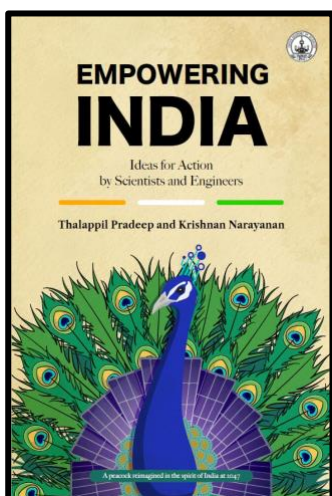
## Popular Science

1. The AI's unlimited potential, the benefits and the risks, Thalappil Pradeep, published in The Hindu, July 20, 2023.



## Books

1. Empowering India: Ideas For Action By Scientists and Engineers, Thalappil Pradeep and Krishnan Narayanan, published by Indian Academy of Sciences, 2023.
2. Technological solutions for water sustainability challenges and prospects, Ligy Philip, Thalappil Pradeep, and S. Murty Bhallamudi (Eds.), published by IWA Publishing House, 2023.
3. Evolving facets of molecular materials, Thalappil Pradeep, published by Pradeep Research Group for private circulation, 2023.



## Patents Granted

1. A selective and efficient process for the extraction of noble metal ions from complex mixtures, Thalappil Pradeep, Md Rabiul Islam and Tanmayaa Nayak, application no. 202241026274, May 5, 2022, issued as patent no. 417781, dated January 12, 2023.
2. Method for colocalization of plasmonic nanoparticles and biomolecules with plasmonic and Raman scattering microspectroscopy, T. Pradeep and Kamalesh Choudhari, application no. 1864/CHE/2015, dated April 09, 2015, issued as patent no. 419154, dated January 24, 2023.
3. Method of fabricating a conducting cloth based breath humidity sensor and applications thereof, T. Pradeep, Pillalamarri Srikrishnarka, Dasi Raaga Madhuri, Sourav Kanti Jana and Bobby George, application no. 202241008331, dated February 17, 2022, issued as patent no. 480519, dated December 12, 2023.
4. Method for accumulation of silver by rice and possible metal extraction by agriculture, T. Pradeep, Soujit Sengupta, Ananya Baksi and Debal Deb, application no. 6846/CHE/2014, dated December 31, 2014; full specification filed on December 28, 2015, issued as patent no. 416654, dated January 3, 2023.
5. A method for facile, rapid and industrially scalable preparation of metal hydroxide composition, Hydromaterials Private Limited & Indian Institute of Technology Madras (IIT Madras), application no. 201941054546, dated December 30, 2019, issued as patent no. 429730 dated April 24, 2023.
6. Methods for selective visual detection of TNT, T. Pradeep, Ammu Mathew and P. R. Sajanalal, application no. 3150/CHE/2012, dated August 1, 2012, issued as patent no. 442508, dated August 2, 2023.
7. An electrode system based on differential oxidant response for the detection of free chlorine, Thalappil Pradeep, Kamalesh Chaudhari, Tullio Servida, Vishnu Kannan and Spoorthi Bhat, application no. 202141031970, TEMP/E-1/42985/2021-CHE, dated July 15, 2021, issued as patent no. 443964, dated August 9, 2023.
8. Reactivation of silver metal particle-based antimicrobial compositions, T. Pradeep, Sahaja Aigal, Amrita Chaudhary, M. Udhaya Sankar and Anshup, application no. 4300/CHE/2011, dated December 9, 2011, issued as patent no. 462074, dated October 26, 2023.
9. A compact, modular and scalable continuous-flow greywater sink for potable and non-potable uses, Pradeep and Ankit Nagar, application no. 202141054715, dated November 26, 2021, issued as patent no. 462091, dated October 26, 2023.
10. Vertically aligned nanoplates of atomically precise  $\text{Co}_6\text{S}_8$  cluster for practical arsenic sensing, T. Pradeep, Anagha Jose, Arijit Jana, Tanvi Gupte, Keerthana Unni, Ankit Nagar, Amoghavarsha R. Kini and B.K. Spoorthi, application no. 202241076581, dated December 29, 2022, issued as patent no. 465466, dated November 3, 2023.
11. A method for environmental arsenic detection and public awareness using human cells, Thalappil Pradeep and Tanvi Gupte, application no. 202241049077, dated August 28, 2022, issued as patent no. 484281, dated December 18, 2023.

12. A point-of-care (POC) amperometric device for selective arsenic sensing, Thalappil Pradeep, Sourav Kanti Jana and Kamalesh Choudhuri, application no. 202041023576, dated June 5, 2020, issued as patent no. 490895, dated December 28, 2023.

### Patents Applied

1. A method of identifying authenticity of ayurvedic preparations using hand-held Raman spectroscopy, Thalappil Pradeep, Ajaya Kumar Barik, Mithun N, Anish R Nath, Jijo Lukose and Santhosh Chidangil, Application no: 202341048917, dated July 20, 2023.

### PCT Applied

1. A selective and efficient process for the extraction of noble metal ions from complex mixtures, Thalappil Pradeep, Md Rabiul Islam and Tanmayaa Nayak, application no. PCT/IN2023/050401, dated April 24, 2023.
2. A method to transform crystalline minerals to nanoparticles by microdroplets, Thalappil Pradeep, B. K. Spoorthi and Pallab Basuri, application no. PCT/IN2023/050649, dated July 4, 2023.
3. Material and method for sustainable and affordable atmospheric water harvesting, Thalappil Pradeep, Ankit Nagar and Sonali Seth, application no. PCT/IN2023/050808, dated August 27, 2023.
4. Vertically aligned nanoplates of atomically precise  $\text{Co}_6\text{S}_8$  cluster for practical arsenic sensing, Thalappil Pradeep, Anagha Jose, Arijit Jana, Tanvi Gupte, Keerthana Unni, Ankit Nagar, Amoghavarsha R. Kini and B. K. Spoorthi. Application no. PCT/IN2023/050856, dated September 12, 2023.

### Degree Holders

1. Dr. Ankit Nagar, Department of Chemistry, IIT Madras, 2023, "Engineered nanomaterials and devices for water and energy sustainability".
2. Dr. Arijit Jana, Department of Chemistry, IIT Madras, 2023, "Atomically precise clusters of silver and copper: Diversity in structure and properties".
3. Dr. Srikrishnarka Pillalamarri, Department of Chemistry, IIT Madras, 2023, "Investigations into the understanding and remediation of air-pollution".
4. Dr. Gaurav Vishwakarma, Department of Chemistry, IIT Madras, 2023, "Photochemical and thermal evolution of clathrate hydrates in interstellar ice mimics".



Dr. Ankit Nagar



Dr. Arijit Jana



Dr. Srikrishnarka  
Pillalamarri



Dr. Gaurav  
Vishwakarma

## Lectures Delivered

1. Inaugural lecture on “Affordable clean water using advanced materials” in Nanomaterials and Sustainable Applications NanoSa-2023, Institute of Chemical Technology, Mumbai, Marathwada Campus, Jalna, January 9-11, 2023.
2. “Atomically precise clusters for applications” in Emerging Frontiers in Chemical Sciences, EFCS-2022, Farook College, Kerala, January 19-20, 2023.
3. “Global science for global well-being” National Science day celebration, IIT Tirupati, February 25, 2023.
4. “Global science for global well-being” IIT Madras, February 27, 2023.
5. “Atomically precise noble nanoclusters” SASTRA Deemed University, Thanjavur, February 28, 2023.
6. “Affordable clean water using advanced materials” in New Developments in Polymeric Materials, DPM-2023, Kerala Arts and Craft Village, Kovalam, Thiruvananthapuram, March 2, 2023.
7. “Affordable clean water using advanced materials” in SS Bhatnagar memorial lecture, INST Mohali, March 15, 2023.
8. “Affordable clean water using advanced materials” in 7<sup>th</sup> Pran Nath Vohra oration, Department of Chemistry, Panjab University, Chandigarh, March 16, 2023.
9. “Atomically precise matter” in International Conference on Science and Technology of Advanced Materials STAM 23, Mar Athanasius College (autonomous), Kerala, April 17, 2023.
10. “Affordable clean water using advanced materials” in H H Sree Visakham Thirunal Endowment lecture, ICAR-CTCRI, Thiruvananthapuram, Kerala, June 5, 2023.
11. “Affordable clean water using advanced materials” in INAE NATFOE symposium, Birla Institute of Technology Mesra, Ranchi, June 25, 2023.
12. Plenary talk “Atomically precise metal clusters” in International Conference on Thin Films and Nanotechnology: Knowledge, Leadership and Commercialization, Department of Physics, IIT Madras, July 7, 2023.
13. “Affordable clean water using advanced materials” in International Conference on Sustainable and applied Nanotechnology for Agriculture and Health SANATH, IIT Madras, July 20, 2023.
14. “Our universities” Lecture in the session ‘VISION 2035’ in the Freedom Fest 2023 event, Thiruvananthapuram, August 13, 2023.
15. “Affordable clean water using advanced materials” in Residential Filtration Innovation Summit, Marmon Water Research Center, Bangalore, September 27, 2023.
16. “Clathrate hydrates under UHV” in Materials, Methods and Devices for Futuristic Technologies, MDFT conference, September 30, 2023.
17. “Metal nanoclusters: synthesis, characterization, surface functionalization and properties” in Indo-France seminar under CEFIPRA, INST Mohali, Panjab, India, October 2, 2023.
18. “Affordable clean water using advanced materials” in the first International conference on Water Security and Climate Adaption WSCA 2023, IIT Madras, October 6, 2023.

19. "Quantum dots-Seeds of Nanoscience" Tamil Nadu Science Forum, Chennai, October 21, 2023.
20. "Quantum dots-Seeds of Nanoscience" Department of Chemistry, IIT Madras, October 25, 2023.
21. "Higher education and knowledge economy" Panellist and Commentator in the session "Higher education in Kerala" in Keraleeyam 2023, Thiruvananthapuram, October 25, 2023.
22. "From molecular acorns to institutional oaks" in Karlsruhe Institute of Technology, Germany, November 27, 2023.
23. "From molecular acorns to institutional oaks" in Science Salon, Hotel Fitzgerald, Vítkova 151/26, 186 00 Praha-Karlín, Czech Republic, November 28, 2023.
24. "Atomically precise metal clusters and gas hydrate cages" in IRIS 2.0 webinar series: Centre of Excellence in Molecular Materials and Functions, IIT Madras, December 1, 2023.
25. "Atomically precise metal clusters" in International Winter School 2023 and Recent Advances in Materials, RAM-90 in JNCASR, Bangalore, December 4, 2023.
26. "Atomically precise clusters of noble metals" in Centre of Excellence Winter School on Molecular Materials and Functions, IIT Madras, December 11, 2023.
27. "Atomically precise metal clusters" in Materials Research Society of India, Annual Conference, IIT BHU, Varanasi, December 13, 2023.



Prof. T. Pradeep during the inaugural event of the conference, "Emerging Frontiers in Chemical Sciences", in Farook college, Kerala on December 19, 2023 along with the inaugural speaker, Prof. Francesco Stellacci.

30. "Affordable clean water using advanced materials" in International Conference on Advanced Materials for Sustainability ICAMS 2023, University of Calicut, Kerala, December 21-23, 2023.

28. "Surface science of water ice" in the International Conference on Molecular Matter, ICM 2023, IIT Madras, December 18, 2023.
29. "Atomically precise matter" in Emerging Frontiers in Chemical Sciences, EFCS-2023, Farook College, Kerala, December 19-20, 2023.



With the participants of the International Conference on Advanced Materials for Sustainability ICAMS 2023, in Calicut University Conference hall after Prof. T. Pradeep's talk, December 22, 2023.

## Students' Activities

1. Ms. Jayoti Roy visited Ohio to work with Prof. Vicki Wysocki at Biomedical Research tower, Ohio State University. Picture is dated January 15-April 2, 2023.
2. Ms. Anagha Jose has presented a poster on "Vertically aligned nanoplates of atomically precise  $\text{Co}_6\text{S}_8$  cluster for practical arsenic sensing" as part of the PMRF symposium held at IIT Madras, February 17-18, 2023.
3. Ms. Jayoti Roy presented a poster on "Dissociative reactions of  $\text{Au}_{25}(\text{SR})_{18}$  at copper oxide nanoparticles and formation of aggregated nanostructures" as part of the 16th International Conference on Materials Chemistry MC16 held in Dublin, Ireland, July 3-6, 2023.



Ms. Jayoti Roy with Prof. Vicki Wysocki during her visit to Ohio State University, January 15, 2023.



Dr. Gaurav Vishwakarma with Prof. Praveen Linga during his visit to NUS, Singapore, July 9, 2023.

4. Dr. Gaurav Vishwakarma has given oral presentation on "Existence of acetaldehyde clathrate hydrate and its dissociation leading to cubic ice under ultrahigh vacuum and cryogenic conditions" as part of the International Conference on Gas Hydrate held at National University of Singapore, Singapore, July 09-14, 2023.
5. Mr. Gaurav Vishwakarma visited Prof. Praveen Linga's lab at the Department of Chemical and Biomolecular Engineering, National University of Singapore, March 15-July 15, 2023.
6. Mr. Deepak Kumar Patel visited Czech Academy of Science, Czech Republic to work with Dr. Tomas Base as a visiting research fellow, March 22-June 18, 2023.
7. Ms. Spoorthi Bhat presented a poster on "Ambient microdroplet annealing of nanoparticles" as part of the 16th International Conference on Materials Chemistry MC 16 Theme Materials for Life (Green Chemistry), in Dublin, Ireland, July 3-6, 2023.
8. Mr. Bijesh Kumar Malla has presented a poster on "Vacuum ultraviolet photolysis of condensed methyl chloride in interstellar conditions and trapping of intermediates at inter-grain interfaces" as part of the Chemistry In-House Symposium CiHS-2023 organised by IIT Madras, August 23, 2023.
9. Mr. Amoghavarsha R. Kini has presented a poster on "Nanomechanical investigations on crystals of tetranuclear copper clusters protected by isomeric carborane-thiols" as



Mr. Deepak Patel with Dr. Tomas Base during his visit to Czech Republic, March 22, 2023.

- part of the Chemistry In-House Symposium CiHS-2023 organised by IIT Madras, August 23, 2023.
10. Mr. Deepak Kumar Patel has presented a poster on “ Macropolyhedral syn-  $B_{18}H_{22}$  the Forgotten isomer” as part of the Chemistry In-House Symposium CiHS-2023 organised by IIT Madras, August 23, 2023.
  11. Ms. Swetashree Acharya has presented a poster on “ Dissociative dimerization occurs during the reactions of atomically precise  $(M_{Ag_{24}}(DMBT)_{18})^{-}$  and  $Ag_{29}(BDT)^{3-}$  clusters forming their 16  $e^{-}$  super atomic adducts as part of the Chemistry In-House Symposium CiHS-2023 organised by IIT Madras, August 23, 2023.
  12. Ms. S. Jenifer has given a flash talk on “ Exploring the microdroplet world: analyte aggregation unveiled” as part of Royal Society of Chemistry-Water at interfaces Faraday Discussion held in London, United Kingdom, September 20, 2023.
  13. Ms. Anagha Jose has presented a poster on “ Vertically aligned nanoplates of atomically precise  $Co_6S_8$  cluster for practical arsenic sensing” as part of the 8th International Conference on Advanced Nanomaterials and Nanotechnology ICANN 2023 held at IIT Guwahati, November 29-December 1, 2023.
  14. Mr. Amoghavarsha R. Kini has presented a poster on "Nanomechanical investigations on crystals of tetranuclear copper clusters protected by isomeric carborane-thiols" as part of the 8th International Conference on Advanced Nanomaterials and Nanotechnology ICANN 2023 held at IIT Guwahati, November 29-December 1, 2023.
  15. Ms. Swetashree Acharya presented a poster on “Formation of molybdenum-oxo clusters via soft chemistry; its tungsten doping and optical sensing of Arsenic” as part of the 8th International Conference on Advanced Nanomaterials and Nanotechnology ICANN 2023 held at IIT Guwahati, November 29-December 1, 2023.
  16. Mr. Subrata Duary presented a poster on “A new  $Cu_8$  nanomolecule: Engineering luminescence and vapor sensing” as part of the 8th International Conference on Advanced Nanomaterials and Nanotechnology ICANN 2023 held at IIT Guwahati, November 29-December 1, 2023.
  17. Ms. Anagha Jose has given oral presentation on “Vertically aligned nanoplates of atomically precise  $Co_6S_8$  cluster for practical arsenic sensing” as part of the 8th International Conference on Advanced Nanomaterials and Nanotechnology ICANN 2023 held at IIT Guwahati, November 29-December 1, 2023.
  18. Mr. Sujan Manna presented a poster on “Surface-enhanced Raman spectroscopy of atomically precise nanoclusters” as part of the International Winter School 2023 and Recent Advances in Materials RAM-90 held at JNCASR, Bangalore, December 4-9, 2023.
  19. Ms. Tanmayaa Nayak has given oral presentation on “Sustainable cellulose-derived nanomaterials for adsorptive removal of uranium from wastewater with rapid kinetics” as part of the 3<sup>rd</sup> International Conference on Water Technologies ICWT 2023 held at IIT Bombay, December 4-7, 2023.
  20. Ms. S. Jenifer has given oral presentation on “Antibacterial spheroids of  $Cu_{17}$  nanocluster, protected by cysteine for arsenic detection” as part of the 8th International Conference on Advanced Nanomaterials and Nanotechnology ICANN 2023 held at IIT Guwahati, November 29-December 1, 2023.

21. Mr. Vivek Yadav visited Karlsruhe Institute of Technology, Karlsruhe, Germany to work with Prof. Manfred Kappes as a visiting research fellow during August 2023. Picture is dated August 20, 2023.
22. Mr. Vivek Yadav visited Czech Academy of Science, Czech Republic to work with Dr. Tomas Base as a visiting research fellow during September 2023.
23. Mr. Vivek Yadav visited the lab of Prof. Mukundan Thelakkat, University of Bayreuth, Germany to initiate a collaboration on October 15, 2023.



Mr. Vivek Yadav with Prof. Manfred Kappes during his visit to KIT, Germany, August 20, 2023.



Mr. Vivek Yadav with Prof. Paul Weiss and Dr. Tomas Base in Science Salon organised by Dr. Tomas Base in Prague, Czech Republic in September, 2023.

24. Mr. Vivek Yadav visited University of Bayreuth, Germany to work with Prof. Josef Breu as a visiting research fellow, during October 2023.
25. Mr. Deepak Kumar Patel presented a poster on "Macropolyhedral  $\text{syn-B}_{18}\text{H}_{22}$  the Cinderella Isomer" as part of the International Conference on Molecular Matter ICMM 2023 held at IIT Madras, December 16-18, 2023.
26. Mr. Sujan Manna presented a poster on "Surface-enhanced Raman spectroscopy of atomically precise nanoclusters" as part of the International Conference on Molecular Matter ICMM 2023 held at IIT Madras, December 16-18, 2023.
27. Ms. Spoorthi Bhat gave a talk "Molecules and materials in microdroplets" as part of the International Conference on Molecular Matter ICMM 2023 held at IIT Madras, December 16-18, 2023.
28. Mr. Soham Chowdhury presented a poster on "Formation of composition-dependent clathrate hydrates of trimethylene oxide in ultrahigh vacuum and their varying consequences in dissociation-induced crystallization of ice" as part of the International Conference on Molecular Matter ICMM 2023, held at IIT Madras, December 16-18, 2023.

## Students' Recognitions

1. Dr. Arijit Jana has received the Keshav Ranganath Award and Institute Research Award in recognition of his excellent Ph.D. work.
2. Ms. Anagha Jose has received the International Immersion Experience(IIE) travel award 2023, funded by IIT Madras.
3. Mr. Bijesh Kumar Malla has received the International Immersion Experience(IIE) travel award 2023, funded by IIT Madras.



4. Mr. Subrata Duary has received the International Immersion Experience(IIE) travel award 2023, funded by IIT Madras.
5. Ms. Anagha Jose has received the best poster award for "Vertically aligned nanoplates of atomically precise  $\text{Co}_6\text{S}_8$  cluster for practical arsenic sensing" as part of the 8th International Conference on Advanced Nanomaterials and Nanotechnology ICANN 2023 held at IIT Guwahati, November 29-December 1, 2023.
6. Mr. Deepak Kumar Patel received the V R S Rao prize for the best academic performance in year 2023.
7. Ms. Swetashree Acharya has received the best poster award for "Formation of molybdenum-oxo clusters via soft chemistry; its tungsten doping and optical sensing of Arsenic" as part of the 8th International Conference on Advanced Nanomaterials and Nanotechnology ICANN 2023 held at IIT Guwahati, November 29-December 1, 2023.
8. Ms. S. Jenifer has received the best poster award for "Antibacterial spheroids of  $\text{Cu}_{17}$  nanocluster, protected by cysteine for arsenic detection" as part of the 8th International Conference on Advanced Nanomaterials and Nanotechnology ICANN 2023 held at IIT Guwahati, November 29-December 1, 2023.
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10. Mr. Deepak Kumar Patel has received the best poster award for "Macropolyhedral syn- $\text{B}_{18}\text{H}_{22}$  the Cinderella Isomer" as part of the International Conference on Molecular Matter ICMM 2023 held at IIT Madras, December 16-18, 2023.
11. Mr. Sujan Manna has received the best poster award for "Surface-enhanced raman spectroscopy of atomically precise nanoclusters" as part of the International Conference on Molecular Matter ICMM 2023 held at IIT Madras, December 16-18, 2023.

Dr. Arijit Jana received the Keshav Ranganath Award and Institute Research Award in recognition of his excellent research work on April 13, 2023.

## Alumni News

1. Dr. Rahul Narayanan was appointed as an Assistant Professor at SRM Institute of Science and Technology, Chennai, India.
2. Dr. K. R. Krishnadas was appointed as a Ramanujan Fellow at IISER Thiruvananthapuram, India.
3. Dr. Depanjan Sarkar has joined IIT Madras, India as a CoE Fellow.
4. Dr. K. S. Sugi has joined Aix-Marseille University, France as a Postdoc.
5. Ms. Paulami Bose has joined Tampere university, Finland as a Postdoc.
6. Dr. Srikrishnarka Pillalamarri has joined Tampere university, Finland as a Postdoc.
7. Dr. Biswajit Mondal has joined University of Barcelona, Spain as a Postdoc.
8. Dr. Ankit Nagar has joined Columbia University, USA as a Postdoc.
9. Dr. Pallab Basuri has joined ETH Zurich, Switzerland as a Postdoc.
10. Dr. Tripti Ahuja has joined IIT Kanpur, India as a Postdoc.
11. Dr. Amrita Chakraborty has joined University of Texas at Dallas, USA as a Postdoc.
12. Dr. Debasmita Ghosh has joined Weizmann Institute of Science, Israel as a Postdoc.
13. Dr. Arijit Jana has joined Karlsruhe Institute of Technology, Germany as a Postdoc.

## Research Grants

### Ongoing Projects

1. National facility of cryo-electron microscopy: Remotely operable, 24x7 for academia and industry, SERB Rs. 28.6 crores principal investigator with IIT Tirupati, IIT Palakkad, RGCB Thiruvananthapuram, Sastra Thanjavur, VIT Vellore and MRF Chennai.
2. JC Bose fellowship, Department of Science and Technology, 98 lakhs (principal investigator), renewed.
3. Fingerprinting authenticity of ayurvedic preparations using ambient electrospray deposition Taman spectroscopy (AERS), a home-grown method for rapid analysis, DST, Rs. 93 lakhs (principal investigator), along with Santhosh Chidangil, Manipal Academy of Higher Education(co-principal investigator).
4. Sustainable ion exchange resin-based technology for rare earth extraction, Ministry of Mines, Rs. 52 lakhs (principal investigator).
5. Atomically precise naked clusters assemblies from ligand-stabilized clusters new materials for catalysis, Department of Science and Technology, DST-DFG grant with Manfred Kappes, KIT, Rs. 72 lakhs (principal investigator).
6. Carborane-protected metal nanoclusters: A new family of materials with atomic precision-DST/Czech 37 lakhs (principal investigator).
7. Understanding surface properties of atomically engineered cluster-assembled solids, SPARC project with Prof. Robin Ras and Prof. Olli Ikkala, Aalto University, Finland with Prof. Tiju Thomas, IITM, Rs. 66.3 lakhs (principal investigator).
8. Atomically precise materials for sustainable water and energy harvesting, SERB Rs. 75.32 lakhs (principal investigator).

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9. SUTRAM for EASY water, DST, Rs 890 lakhs (co-principal investigator with Prof. Ligy Philip).
10. p-CoE on molecular Materials and Functions, IIT Madras, Rs. 5.80 crores (principal investigator) with colleagues from IITM and other institutions.

### Consultancy

1. Steel-Rubber adhesion improvement-Phase 2, MRF Ltd., 2019-2023, Rs. 48.8 lakhs(principal investigator).
2. Affordable smart mask for online health monitoring, Venus Safety and Health Private Ltd., 2023-2024, Rs. 11.97 lakhs.
3. Exploring the Ullmann cyclization reaction in microdroplets, Ambernath Organics Private Ltd., 2023-2024, Rs. 10.44 lakhs.

### Implementation Project

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

## Visitors

1. Mr. Siddarth Krishna Kumar (Son of Krishnakumar Natarajan of Mindtree), January 7, 2023.
2. Prof. Horst Hahn, KIT distinguished senior fellow and Thirumalai Venkatesan, Director, Center of Quantum Research and Technology, University of Oklahoma, January 12, 2023.



Prof. T. Pradeep with Prof. Horst Hahn and Prof. T. Venkatesan, The University of Oklahoma, January 12, 2023.



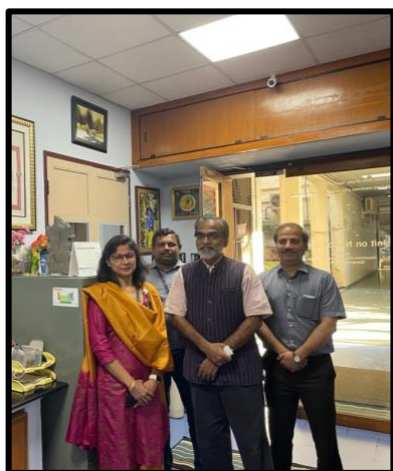
Prof. T. Pradeep with Mr. Irfan Malik and Ms. Jodi McKay, National Chair of the Australia -India Business Council along with IITM Director, Prof. V. Kamakoti, January 13, 2023.

5. Dr. Lior Asaf, Water Attaché, Embassy of Israel, New Delhi and Neeraj Gahlawat, Senior Water Resources Specialist, Embassy of Israel, New Delhi, India, January 17, 2023.
6. Prof. Kuruvilla Jacob, Prof. Subrahmanian Moosath K.S., Ph.D. Professor, Prof. Lekshmi V. Nair, and Dr. K Rajeev, Director SPL, February 8, 2023.
7. Mr. Gopinath, Nanocomps R&D India Private Ltd., February 9, 2023.
8. Dr. T. Thangaradjou Scientist-F , Dr. Dipti Thurkal, Scientist-G (Program Coordinator), Dr. AV. Balachandar, Scientist-F, DST, February 17, 2023.
9. Dr. Jothibasu Seetharaman, Senior Research Scientist, Buckman Laboratories Pvt. Ltd., India and Ms. Liu Lili, Manager, Technology, Buckman Laboratories (Asia) Pte Ltd., Singapore, February 21, 2023.

3. Mr. Irfan Malik, National Associate Chair & President, New South Wales, Australia India Business Council Ltd. (AIBC), and Ms. Jodi McKay, National Chair, Australia India Business Council Ltd. (AIBC), January 13, 2023.
4. Turki Mana and Abdullah Alshammrari, Master's graduates from Prof. Khayyat's lab, KACST, Saudi Arabia, January 16, 2023.



Prof. T. Pradeep with Dr. Lior Asaf, Water Attache, Israel Embassy, New Delhi and Neeraj Gahlawat, January 17, 2023.



Prof. T. Pradeep with Dr. T. Thangaradjou, Dr. Dipti Thukral, and Dr. A. V. Balachandar, SERB, February 17, 2023.



Prof. T. Pradeep, Dr. Jothibasu Seetharaman and Ms. Liu Lili, Buckman Laboratories along with colleagues from ICCW, February 21, 2023.

10. Mr. Vinod Aachi, Cleanedge Water, Singapore, March 8, 2023.
11. Students of Farook College, Kerala, March 10, 2023.
12. Dr. Soumyabrata Roy, Research Scientist, Ajayan Research Group, Material Science and Nanoengineering, Rice University, March 10, 2023.
13. Prof. Sushanta Mitra, University of Waterloo, March 13, 2023.
14. Dr. Debabrata Rautaray, Chief Product Development and Innovation officer and Mr. Raj Kapoor, DCM Shriram Innovation Centre, Vadodara, Gujarat, March 20, 2023.
15. Dr. N. Gomathi, Professor, Department of Chemistry, Indian Institute of Space Science and Technology, Thiruvananthapuram, March 29, 2023.
16. Prof. Radha Boya, FRSC and Dr. Ashok Keerthi, University of Manchester, March 31, 2023.
17. Dr. Jothibas Seetharaman, Senior Research Scientist, Buckman Laboratories Pvt. Ltd., India, April 21, 2023.
18. Mr. Ramasubramanian Oruganti, Director, Samanvaya social Ventures, April 28, 2023.
19. Prof. Kartik Chandran, Columbia University, May 1, 2023.
20. Mr. Krishna Kant, CSR Manager for Skillsbuild-South/West India leader for Volunteerism, IBM, India, May 16, 2023.
21. Dr. Kanniks Kannikeswaran, musician, composer, and music educator, IITM Distinguished Alumnus, May 24, 2023.
22. Mr. Girish Agarwal and Ms. Pooja Agarwal, Crypto relief, May 26, 2023.



Prof. T. Pradeep with Prof. Radha Boya and Dr. Ashok Keerthi, March 31, 2023.



Prof. T. Pradeep along with Mr. Girish Agarwal and Ms. Pooja Agarwal, Crypto relief, May 26, 2023.

25. Prof. Bommanna Loganathan, Department of Chemistry, Murray State University, June 6, 2023.
26. Ms. D. Thara, IAS, Mission Director, AMRUT, June 9, 2023.

23. Mr. Anurag, ONGC official, Executive director, ASSET manager, May 30, 2023.
24. Mr. Chetan Savla, Chief human resource officer and head ,sustainability and Mr. Himanshu Nivsarkar, Senior EVP and head, CSR and Mr. Amit Dhalwade, AVP CSR, Kotak Mahindra Bank, June 2, 2023.



Prof. T. Pradeep with Ms. D Thara. IAS, Mission Director, AMRUT, June 9, 2023.



Prof. T. Pradeep with Ms. Tammy Ben-Haim, Consul General of Israel, and Prof. V. Kamakoti, Director, IITM, June 15, 2023.

27. Ms. Tammy Ben-Haim, Consul general of Israel. Discussion along with director of IIT Madras Prof. V. Kamakoti on India-Israel Center of Water Technology, June 15, 2023.

28. Dr. Mithieux Gilles, director, INSERM unit for nutrition, diabetes and brain, University of Lyon, and Dr. G. Velmurugan, June 17, 2023.

29. Dr. Dillip Kumar Singh, assistant professor, Birla Institute of Technology, Mesra, Ranchi, July 7, 2023.

30. Dr. Akshaya K. Samal, Associate Professor, Centre of nano and Material Science, Jain University, July 9, 2023. Prof. Hadas Mamane, Head of Environmental Engineering program, School of Mechanical Engineering, Faculty of Engineering, Tel-Aviv University, Israel, June 18, 2023.

31. Dr. D. H. Nagaraju, Professor, Department of Chemistry, Reva University, Bengaluru along with his students, July 20, 2023.

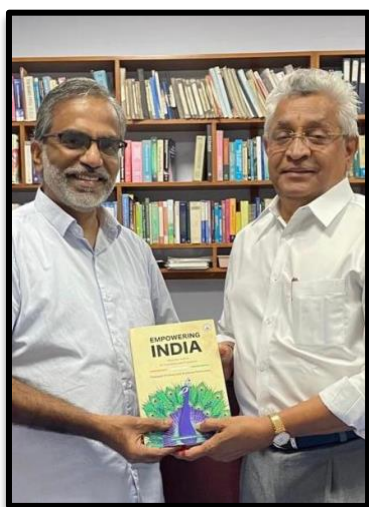
32. Prof. Vinod Kumar Singh, IIT Kanpur, July 23, 2023.

33. Dr. Saji George, Associate Professor, Department of Food Science and Agricultural Chemistry, McGill University, July 26, 2023.

34. Water ambassadors-Prof Ram Fishman, Tel-Aviv University of Public Policy, and Prof. Hadas Mamane, August 1, 2023.



Prof. T. Pradeep with Prof. Vinod K Singh, July 23, 2023.



Prof. T. Pradeep with Dr. Varaprasad Reddy, September 14, 2023.

35. Dr. Satish Satyarthi, Chief Innovation and R&D officer at EFL, and Dr. Swathy, EFL, September 4, 2023.

36. Mr. Suman Bery, Vice Chairman of Niti Aayog, September 5, 2023.

37. Padma Bhushan Dr. Varaprasad Reddy, Sept 14, 2023.

38. Dr. Baskaran R, Institute of Mathematical Science, Chennai, September 14, 2023.

39. Dr. Bosco Emmanuel, Chief Scientist (Retired), CSIR - Central Electrochemical Research Institute, September 14, 2023.

40. Mr. Anuj Khandelwal, Vice President, Premji Invest, September 23, 2023.

41. Dr. Pawan Labhasetwar, Chief Scientist & Head, CSIR-National Environmental Engineering Research Institute, September 26, 2023.

42. Mr. S Sivakumar, ITC Leadership, Agri & IT Businesses October 7, 2023.
43. Mr. Chandru Raman Chandrasekar, Sustein Ltd., October 23, 2023.
44. Dr. Michael Willer, Global Water R&D Director, Buckman International Private Ltd., October 24, 2023.
45. Dr. Venugopal Vijayakrishnan and Dr. Gayathri Subramanyam, Senior Scientist, October 31, 2023.
46. Prof. Bryan Brooks, Baylor University, USA, Editor in Chief, ES&T Letters Baylor University, Department of Environmental Science, Waco, Texas, Dr. Maggie Mills, Managing Editor, ACS Publications, ACS International Ltd. Oxford OX2 0QS, UK and Dr. Ashesh Mahto Development Editor, ACS Publications, ACS International India, and Dr. Ajay Jha, Lead, Global Editorial Strategy, ACS Publications, ACS International India, November 13, 2023.
47. Dr. M.K. Padmanabhan, Director Virginia Tech India, Center for Advanced Research and Education, IITRP, November 20, 2023.
48. Prof. Hanu Hakkinen, Prof. Francesco Stellacci, Dr. Tomas Base, Prof. Sukhendu Mandal, December 12, 2023.
49. Prof. Biswarup Pathak, Prof. Tatsuya Tsukuda, December 13, 2023.
50. Prof. Horst Hahn, Prof. Nonappa, Prof. Richard Zare, December 14, 2023.
51. Prof. Paul Weiss, Prof. Bala Subramaniam, Prof. G.V. Pavan Kumar, Prof. Jaydeb Chakrabarti, Prof. Vivek Polshettiwar, Prof. E.S. Shibu, Prof. M.S. Bootharaju, Prof. Vasudevan Biju, Prof. Venkataraman Mahalingam, Prof. Suresh Valiyaveetil visited during ICMM 2023, December 16, 2023.
52. Prof. Rahul Nair, Prof. Umesh Waghmare, Prof. Kuruvilla Joseph, Prof. Thomas Thundat, Prof. Rahul Banerjee, Prof. Chandrabhas Narayana, Prof. R. Murugavel, Prof. G.U. Kulkarni, Prof. Ajayaghosh Ayyappanpillai, Prof. B.L.V. Prasad, Prof. Tanusri Saha Dasgupta, Dr. Indranath Chakraborty, Prof. Samir K. Pal visited during ICMM 2023, December 17, 2023.
53. Prof. Kanishka Biswas, Prof. Subi George, Prof. Sebastian Peter, Prof. Ananya Bakshi visited during ICMM 2023, December 18, 2023.



Prof. Pradeep along with Prof. Bryan Brooks, Dr. Maggie Mills, Dr. Ashesh Mahto, Dr. Ajay Jha and Prof. Ramesh Gardas, November 13, 2023.

## Visits

1. ICT, Mumbai, Institute of Chemical Technology, Mumbai, Marathwada Campus, Jalna, 2<sup>nd</sup> International Conference on “Nanomaterials and Sustainable Applications” NanoSa-2023, January 9-11, 2023.
2. Farook College, Kerala, National Conference on Emerging Frontiers in Chemical Sciences, EFCS-2022, January 19-20, 2023.
3. Mathrubhumi International Festival of Letters-MBIFL, Thiruvananthapuram, February 3, 2023.
4. IIT Tirupati, National Science Day celebration, February 25, 2023. Also chief guest for the flag-off function of the Ek Bharat Shreshtha Bharat (EBSB) event.
5. Received Sastra-CNR Rao award, SASTRA Deemed University, Thanjavur, February 28, 2023.
6. Kerala Arts and Craft College, Kovalam, Thiruvananthapuram, National Conference on New Developments in Polymeric Materials, DPM-2023, March 2, 2023.
7. NIST, Mohali, SS Bhatnagar Memorial lecture, March 15, 2023.
8. Meeting with Sh. Dhirendra Kumar Tiwari, IAS, Principal Secretary, Govt. Of Punjab, Department of Water Supply and Sanitation and Smt. Jaspreet Talwar, IAS, Principal Secretary, Department of Higher Education, March 16, 2023.
9. Department of Chemistry, Panjab University, Chandigarh, 7<sup>th</sup> Pran Nath Vohra oration, March 16, 2023.
10. Plaksha University and group meeting with the faculties of Centre of Water Security, Plaksha University, March 16, 2023.
11. INST, Mohali, Board of Governors(BOG) 16<sup>th</sup> meeting, March 17, 2023.
12. SUTRAM Meeting, IIT Madras, March 18, 2023.
13. Mar Athanasius College, Kerala, International Conference on Science and Technology of Advanced Materials, STAM-2023, April 18-23, 2023.
14. Meeting with Prof. C.N.R. Rao, April 23, 2023.
15. IIT Madras Alumni Association meet in Bangalore along with Prof. Mahesh V. Panchagnula, Krishnan Narayanan, and Kaviraj Nair, April 23, 2023.
16. India-Israel center of water technology at IIT Madras. A letter of intent was signed in New Delhi by Mr. Manoj Joshi, Secretary, Ministry of Housing and Urban Affairs (MoHUA), Government of India, Prof. V. Kamakoti, Director, IIT Madras and Mr. Naor Gilon, Ambassador of Israel to India, in presence of Shri. S. Jaishankar, and Mr. Eli Cohen, Hon’ble External Affairs Ministers of India and Israel, respectively in presence of Prof. T. Pradeep, Institute Professor, IIT Madras, May 9, 2023.
17. Madras Christian College, Meeting of the appointment committee, May 18, 2023.



Visit to Panjab University, Chandigarh. March 16, 2023, with Prof. Arun Kumar Grover, former Vice Chancellor.

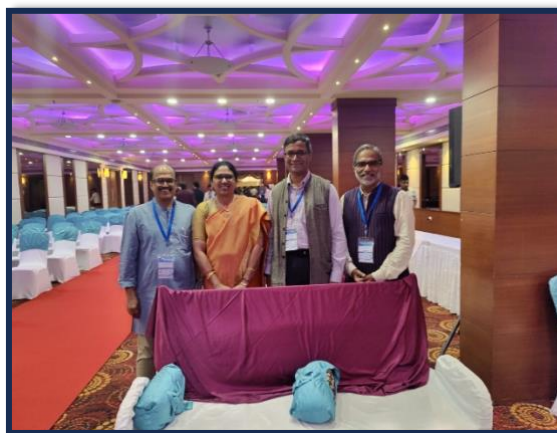
18. Indian Institute of Technology, Palakkad. Chief guest and VVIP for the flag-off function of the Ek Bharat Shreshtha Bharat (EBSB) event and to address the youth, May 23, 2023.
19. ICAR-CTCRI, Thiruvananthapuram, Kerala. Delivered lecture in H H Sree Visakham Thirunal Endowment Lecture by eminent scientists, June 5, 2023.
20. INAE NATFOE symposium at Birla Institute of Technology Mesra, Ranchi, June 25, 2023.
21. International Conference on Thin Films and Nanotechnology: Knowledge, Leadership and Commercialization, Plenary talk, Department of Physics, IIT Madras, July 7, 2023.
22. 8<sup>th</sup> online meeting of technical committee hosted by Jal Jeevan Mission, July 13, 2023.
23. The 3rd Anniversary of National Education Policy (NEP) 2020 was being celebrated at Pragati Maidan Delhi in the presence of Honourable Prime Minister / Shiksha Mantri. As part of the celebrations, we arranged a stall to showcase the Institute of Eminence - Centres of Excellence (IoE-CoEs), IITM, July 29, 2023.



Meeting at the Freedom Fest 2023, Thiruvananthapuram, August 13, 2023.

24. “Empowering India” book release along with Director, IITM, and Hon. Education Minister in Delhi, July 30, 2023.
25. Thiruvananthapuram, ‘Freedom Fest 2023’ an event celebrating Knowledge, Technology and Innovation. Delivered a lecture in the session “Vision 2035”, August 13, 2023. Also distributed the book, “Empowering India”.
26. INST Mohali, 18<sup>th</sup> Board of Governors (BOG) meeting, August 18, 2023.
27. Book launch event at Infosys Science Foundation, Bengaluru. The Indian Academy of Sciences and IIT Madras Alumni Association in collaboration with Bangalore International Centre and Infosys Science Foundation for the release of the book “Empowering India- Ideas for Action by Scientists and Engineers” by Thalappil Pradeep and Krishnan Narayanan, August 20, 2023.

28. Visit to the Satsang Ashram which has been awarded the National Water Award 2019 by the Government of India in recognition of the massive Rain Water Harvesting Project initiated by Satsang which has significantly alleviated shortage of water in Satsang Nagar, Deoghar, Jharkhand, August 26, 2023.
29. Marmon Water Research Center (MWRC), Bangalore. Talk at the residential innovation council held in Ritz Carlton, Bangalore, September 23, 2023.



Prof. Pradeep along with Prof. DD Sharma, Prof. BLV Prasad and his wife during MDFT Conference, September 30, 2023.

30. Methods and Devices for Futuristic Technologies, MDFT, Prof. Giridhar U. Kulkarni's 60<sup>th</sup> birthday Conference, KSHEA, Dharwad, September 29-30, 2023.
31. Institute of Nano Science and Technology (INST), Mohali, Punjab, India, Indo-France Seminar under CEFIPRA, October 2-5, 2023.
32. Visited Delhi to receive 'Careers360 2<sup>nd</sup> Faculty Research Award' for the Most Outstanding Researcher in the country in the field of Materials Science, October 6, 2023.
33. Visit to Nallampatti Village for People's Water Project, Coimbatore, October 8, 2023.
34. Visit to Rome, Italy, to receive the Eni award, October 14-17, 2023.
35. Tamil Nadu Science Forum, Chennai to deliver a lecture, October 21, 2023.
36. Visit Thiruvananthapuram, Kerala, October 25, 2023.
37. Visit to Germany to receive the "International Excellence Award of KIT" and "Fellowship of Schroff Foundation", November 27, 2023.
38. Visit to IISc to receive "IISc Distinguished Alumni Award", December 2, 2023.
39. JNCASR, Bengaluru to International Winter School 2023 and Recent Advances in Materials, RAM-90, JNCASR, Bangalore, December 4, 2023.
40. IIT BHU, Varanasi to receive MRSI International medal for Materials Science and Technology 2023, December 12, 2023.
41. Farook College, Kerala, International Conference on Emerging Frontiers in Chemical Sciences, EFCS – 2023, December 19-20, 2023.
42. University of Calicut, Kerala, International Conference on Advanced Materials for Sustainability ICAMS 2023, December 21-23, 2023.

## Services

- Vice President, Indian Society for Mass Spectrometry, 2014-
- Member, Executive Committee, Neutron Scattering Society of India, 2011-
- Member of the Council of Materials Research Society of India, 2011 –
- Member, Board of Studies, Manipal University, 2012-
- Associate Editor of the journal, ACS Sustainable Chemistry & Engineering, 2014-
- Chairman, Emerging Frontiers in Chemical Sciences Conference series, Farook College, Kozhikode, Kerala, 2017-
- Member, Industry Relevant R &D Expert Committee, DST, 2018-2021.
- Member, Governing Council, Technology Information, Forecasting & Assessment Council (TIFAC), 2019-
- Member, Research Advisory Council, Manipal Academy of Higher Education, Manipal Member, 2018-
- Research Advisory Board, Pandit Deendayal Petroleum University, 2019-
- Member, Research Advisory Committee, IIT Ropar, 2019-
- Co-opted Member, Program Advisory Committee of SERB-SUPRA, 2019-
- Member, Technical Committee for examination and use of innovations and technologies in drinking water and sanitation sector, Department of Drinking Water and Sanitation, Ministry of Jal Shakti, 2019- 2024.

- Member, Program Advisory Committee on Exponential Technologies, DST, 2020-
- Convener, Commission for the Reforms in Higher Education System, Government of Kerala, 2021-
- Chairman, Board of Governors, Institute of Nano Science and Technology, Mohali, 2021.
- Member, Editorial Board of the journals; Chemistry of Materials, ACS Nano, Analytical Chemistry, Nanoscale, ACS Environmental Science & Technology, Particle, Surface Innovations, International Journal of Water and Wastewater Treatment, Nanoscale Advances, and Chemical Communications.

## Upcoming Facilities

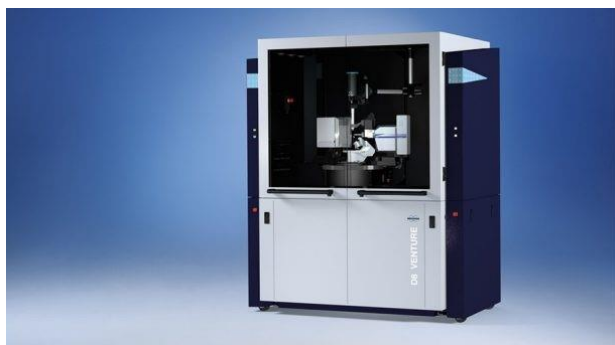
### Mass Photometer



A facility of mass photometer with a wide mass range (30 kDa to 5 MDa), high mass precision and high resolution will be coming up at IIT Madras to obtain accurate mass imaging of single particles, nanoaggregates and biomolecules in

their true native state using light scattering approach. Mass Photometry will measure masses of bigger aggregates of metallic, non-metallic nanoclusters in their native condensed phase. It can measure the proteins on lipid bilayers and membrane-mimetic systems as well. We have placed the purchase orders for the Refeyn Two<sup>MP</sup> mass photometer instrument, along with accessories. The facility will be housed in the Thematic Unit of Excellence, IIT Madras.

### D8 Venture Single Crystal X-Ray Diffractometer



A facility of Bruker Single Crystal X-ray Diffractometer (SCXRD), D8 Venture with Photon III C14 detector will be used to determine three dimensional crystal structures. It will be equipped with two micro-focus X-ray sources (Cu and Mo radiation) providing a choice of two wavelengths , for

measuring patterns in very small crystals. Powder diffraction of capillary samples can also be obtained. Different cooling systems are available, enabling low temperatures such as 100K.

## Incubation

- Hydromaterials have installed village water treatment units, altogether supplying arsenic and iron free water to over 900,000 people. In many places, we have addressed uranium contamination as well. Altogether, there are around 1200 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.



AIRP treatment plant



Installation in Birbhum, West Bengal.

- InnoDi expanded its reach, it has installed more than 150 units across 10 states serving clean water to over 100,000 people and saving over 100 million litres of water every year which otherwise would have gone down the drain. One of the latest installations at Birbhum, West Bengal is shown in the left.

- Vayujal Technologies has installed a solar and power operated 2000 litres per day (LPD) atmospheric water harvesting unit at Engineers India Limited, Gurugram, Haryana. They now have 40, 140, 450, 1100, and 2200 LPD units in production. Vayujal now have 104 machines in 29 states in India and Europe, catering to more than 4800 people with drinking water from air. Highlights include : Awarded as Top-50 Fast Growing Indian Companies by US-India SME council, November 4, 2023 ; Awarded as Company with Best Sustainable Water Management Practices at Sustainability Conclave and awards, November 2, 2023 ; Awarded as Mentor for Blue Ocean Awards at Umanage Chennai, March 2023 (Blue Ocean awards is from INSEAD Business School-Paris). Shown on the right is the view of the factory.



- **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 bottle, called the 'blue bottle'. Also, the company has developed a rolling water purifier called 'roll pure' that helps in reducing the effort in water transportation and provides clean water, when the water reaches the point of use.
- **EyeNetAqua Solutions Private Limited** is a start-up company incubated at ICCW to develop and commercialize IoT-based sensing technologies for water quality monitoring. In the past EyeNetAqua has demonstrated inline measurements of pH, TDS, residual chlorine, nitrate, pressure and volume of flow for source water quality monitoring. EyeNetAqua has made its recent installations at Waddepally water filter bed in Warangal, Telangana. These installations are made as a part of 'India Water Pitch-Pilot-Scale Start-up Challenge' under AMRUT 2.0 by the Ministry of Housing and Urban Affairs (MoHUA), Govt. of India. Followed by this, EyeNetAqua has qualified in a Cohort-4 of the Akamai Accelerator Program for Early Stage Innovations in Water. Funding support from Akamai will be provided for the development and pilot studies with the product for mobile water quality mapping unit. Apart from this, EyeNetAqua is actively working towards the lab-to-field translation of low-cost, colorimetric online and portable devices for multiparametric water quality testing.



Water quality monitoring unit by EyeNetAqua at Waddepally water filter bed in Warangal, Telangana, Hyderabad.

- A new initiative of IIT Madras, the **International Centre for Clean Water** made tremendous progress in all its activities. We have initiated research, implementation, outreach and incubation activities. Major highlights include: 33 CDI-based Water ATMs have been commissioned over the past 5 years. ICCW was the first Challenge Owner for the 3<sup>rd</sup> edition of the AIM-ICDK Challenge, held in Denmark. ICCW also signed an MOU with Feng China University, Taiwan to sustainable water solutions in India. Key to these initiatives is the support of all our well-wishers, well-meaning individuals, Companies well as institutions. All are co-owned by IIT Madras.



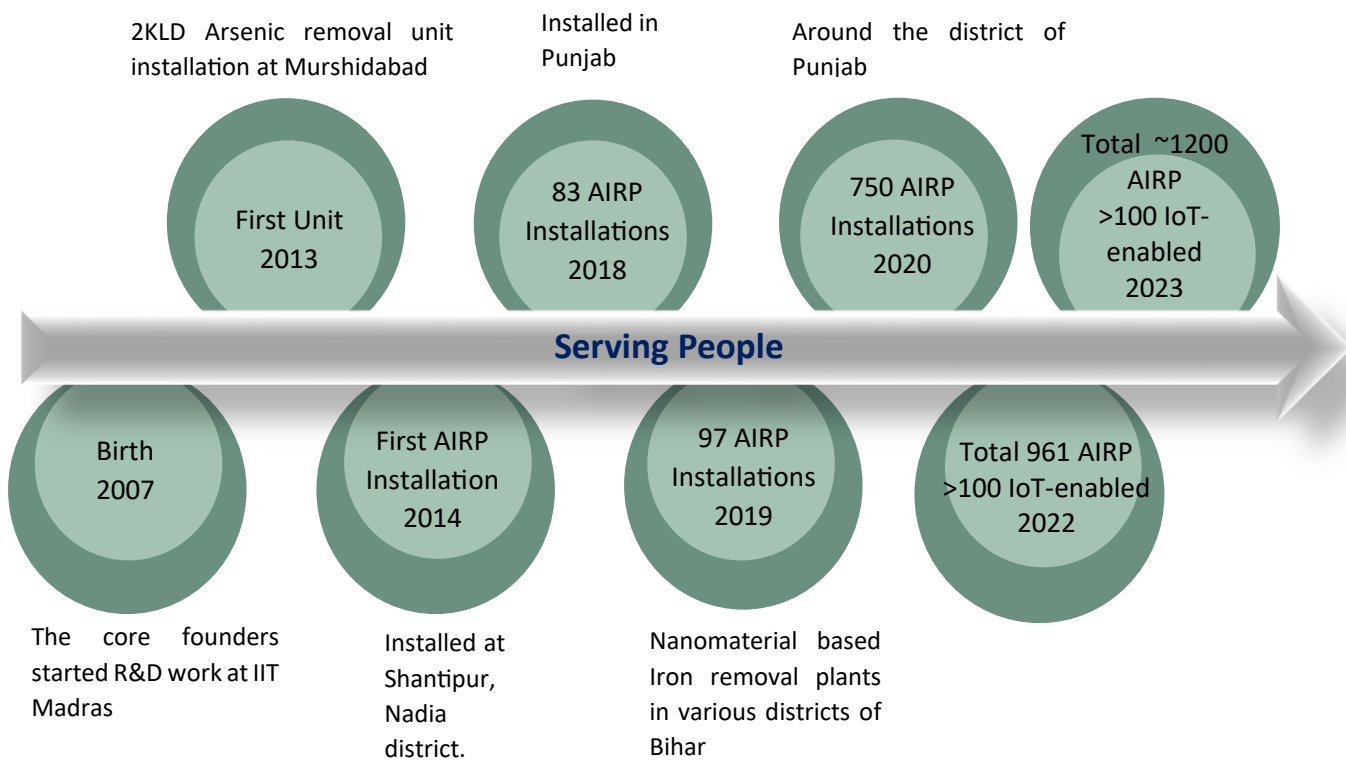
Our initiatives and companies

## Reach of some of our Technologies

### VayuJal

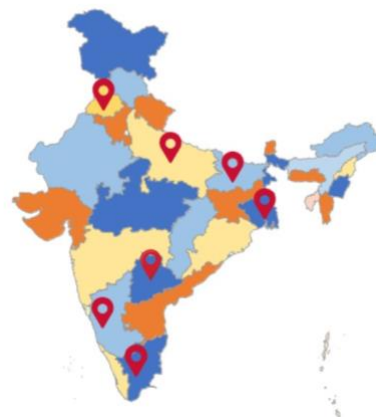


### AMRIT-Anion and Metal Removal by Indian Technology



\* AIRP-Arsenic and Iron Removal Plant

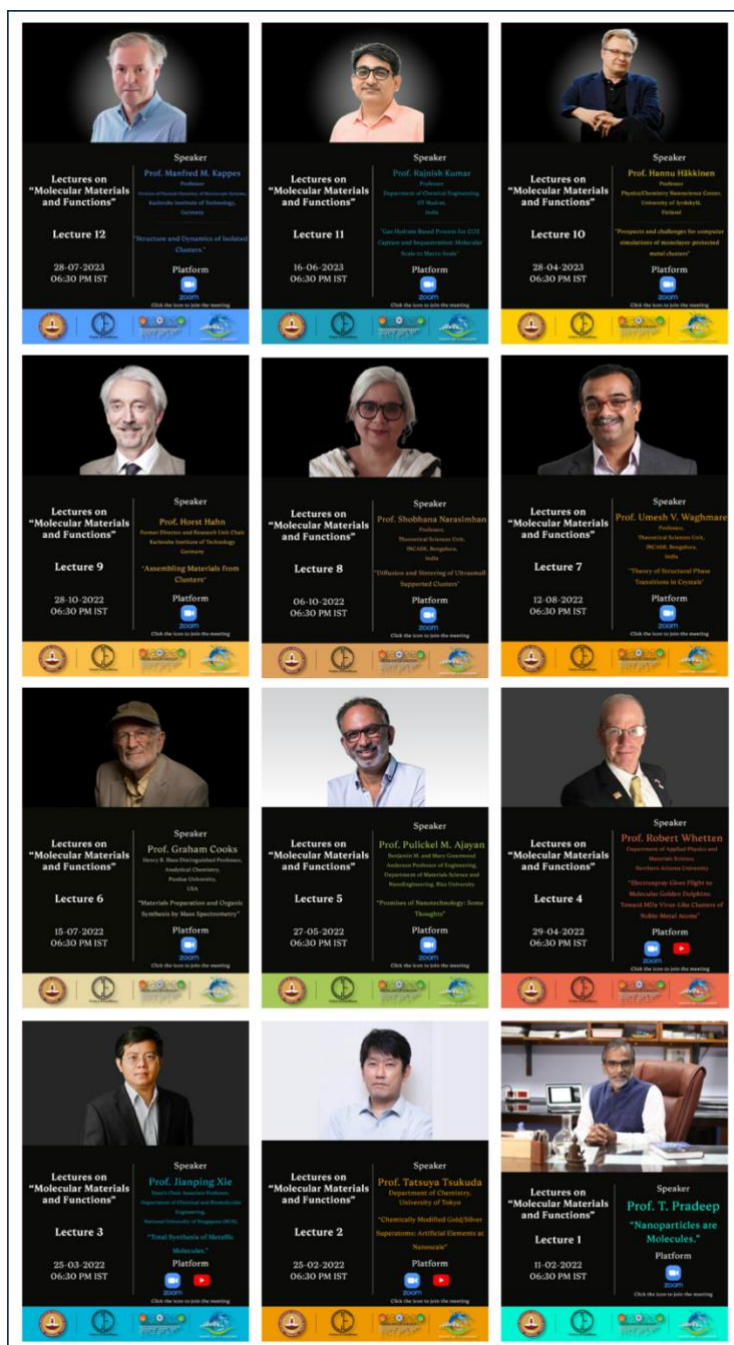
Installations across India



## Activities of Centre of Excellence on Molecular Materials and Functions

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

### 1. p-CoE on molecular Materials and Functions lecture series



To watch the lectures please visit our [Youtube channel](#).

## 2. CoE Winter School on Molecular Materials & Functions

The Winter School details are available at  
<https://molmatter.org/coe-winter-school-2023/>.

 <p>CoE Winter School on Molecular Materials &amp; Functions December 11-15, 2023</p> <p>THEMATIC UNIT OF EXCELLENCE, IIT MADRAS, Chennai, Tamil Nadu-600036</p> <p>Co-ordinators</p> <p>Prof. T. Pradeep Institute Professor Deepak Parekh Institute Chair Professor Department of Chemistry IIT Madras</p> <p>Prof. Rajnish Kumar Professor Department of Chemical Engineering IIT Madras</p>	<p>Day 1 - Monday, December 11, 2023</p> <p><b>Session 1</b></p> <p>09:00 AM - 10:30 AM Prof. T. Pradeep, IIT Madras Atomically Precise Clusters of Noble Metals</p> <p>10:30 AM - 10:45 AM Tea Break</p> <p><b>Session 2</b></p> <p>10:45 AM - 12:15 PM Prof. Tju Thomas, IIT Madras Materials Design and Development for Energy and Environmental Solutions</p> <p>12:15 PM - 02:00 PM Lunch Break</p> <p><b>Session 3</b></p> <p>02:00 PM - 03:30 PM Prof. Piyush Ghosh, IIT Madras Fundamentals of Nanosynthesis &amp; its Application to Molecular Crystals</p> <p>03:30 PM - 03:45 PM Tea Break</p> <p><b>Session 4</b></p> <p>03:45 PM - 05:15 PM Prof. Dilip Kumar Chand, IIT Madras Single-Cavity and Multi-Cavity Coordination Architectures</p>	<p>Day 2 - Tuesday, December 12, 2023</p> <p><b>Session 1</b></p> <p>09:00 AM - 10:30 AM Prof. Hannu Hakkinen, University of Jyväskylä</p> <p>10:30 AM - 10:45 AM Tea Break</p> <p><b>Session 2</b></p> <p>10:45 AM - 12:15 PM Prof. Francesco Stellacci Eco-Polymeric Nanoparticles de Luxe: Amphiphilic Nanoparticles: Basic Science and Applications in Biology</p> <p>12:15 PM - 02:00 PM Lunch Break</p> <p><b>Session 3</b></p> <p>02:00 PM - 03:30 PM Dr. Tomáš Baile, The Czech Academy of Sciences Boron Clusters, Versatile Molecular Constituents for 2D Materials</p> <p>03:30 PM - 03:45 PM Tea Break</p> <p><b>Session 4</b></p> <p>03:45 PM - 05:15 PM Prof. Sukhendu Mandal ISER Thiruvananthapuram Recent Advances in Silver and Copper Nanoclusters</p>
<p>Day 3 - Wednesday, December 13, 2023</p> <p><b>Session 1</b></p> <p>09:00 AM - 10:30 AM Prof. Biswanup Pathak, IIT Indore Computational Modelling of Nanoclusters</p> <p>10:30 AM - 10:45 AM Tea Break</p> <p><b>Session 2</b></p> <p>10:45 AM - 12:15 PM Prof. Manfred Koppers Karlsruhe Institute of Technology What can be Learned by Studying Atomically Precise Clusters in Gas Phase?</p> <p>12:15 PM - 02:00 PM Lunch Break</p> <p><b>Session 3</b></p> <p>02:00 PM - 03:30 PM Prof. Tatsuya Tsukuda, The University of Tokyo Atomically Precise Synthesis and Characterization of Gold Clusters</p> <p>03:30 PM - 03:45 PM Tea Break</p> <p><b>Session 4</b></p> <p>03:45 PM - 05:15 PM Prof. Kunnikuruvan Sooraj, IIT Madras Quantum Chemical Calculations and Microkinetic Analysis for Catalysis and Polymer Structure Prediction</p>	<p>Day 4 - Thursday, December 14, 2023</p> <p><b>Session 1</b></p> <p>09:00 AM - 10:30 AM Prof. Horst Hahn, The University of Oklahoma Structural and Chemical Disorder Towards Advanced Materials</p> <p>10:30 AM - 10:45 AM Tea Break</p> <p><b>Session 2</b></p> <p>10:45 AM - 12:15 PM Prof. S. R. K. Chaitanya Sharma Yamijala, IIT Madras Simulating 2D Anode Materials and Solid-Electrolyte Interphase Using Ab Initio Methods</p> <p>12:15 PM - 02:00 PM Lunch Break</p> <p><b>Session 3</b></p> <p>02:00 PM - 03:30 PM Prof. Yuichi Negishi, Tokyo University of Science Covalent Organic Framework: Basics and Application</p> <p>03:30 PM - 03:45 PM Tea Break</p> <p><b>Session 4</b></p> <p>03:45 PM - 05:15 PM Prof. Nonappa, Tampere University 3D Electron Microscopy of Colloidal Superstructures</p>	<p>Day 5 - Friday, December 15, 2023</p> <p><b>Session 1</b></p> <p>09:00 AM - 10:30 AM Prof. P Venkatakrishnan, IIT Madras Organic Functional Materials for Lighting</p> <p>10:30 AM - 10:45 AM Tea Break</p> <p><b>Session 2</b></p> <p>10:45 AM - 12:15 PM Prof. Ramesh L. Gardas, IIT Madras Ionic Liquids: Revolutionizing Sustainable Chemistry</p> <p>12:15 PM - 02:00 PM Lunch Break</p> <p><b>Session 3</b></p> <p>02:00 PM - 03:30 PM Prof. Thangavelu Palaniselvam, IIT Madras All-Solid State Batteries and Their Future</p> <p>03:30 PM - 03:45 PM Tea Break</p> <p><b>Session 4</b></p> <p>03:45 PM - 05:15 PM Prof. Rajnish Kumar, IIT Madras Gas Hydrates: Basics and Application</p>

### 3. International Conference on Molecular Matter (ICMM 2023)-Emerging Directions for Sustainability

The conference details are available at  
<https://www.chem.iitb.ac.in/ICMM/speakers.html>



**International Conference on Molecular Matter - Emerging Directions for Sustainability**  
 December 16-18, 2023  
 T. T. Jagannathan Auditorium,  
 Industrial Consultancy and Sponsored Research (IC&SR),  
 IIT Madras,  
 Chennai,  
 Tamil Nadu-600 036



**Day 1 - Saturday, December 16, 2023**

**Venue: T. T. Jagannathan Auditorium, IC&SR, IIT Madras**

08:00 AM - 09:00 AM Registration  
 09:00 AM - 09:15 AM Inauguration and welcome remarks

**Session 1** **Chair: Prof. Venkataramanan Mahalingam, IC&SR, IIT Madras**  
 09:15 AM - 09:40 AM Prof. Horst Hahn, The University of Oklahoma  
 Clusters as building blocks for advanced materials  
 09:40 AM - 10:05 AM Prof. Tatsuya Tsukuda, The University of Tokyo  
 Electronic structures and optical properties of chemically-modified gold superatoms  
 10:05 AM - 10:30 AM Prof. Rajnish Kumar, IIT Madras  
 How sustainable is carbon capture, utilization and sequestration?  
 10:30 AM - 10:55 AM Dr. M. S. Bootharaja, Sree Narayana College  
 Gold-silver core-shell nanoclusters for enhanced solar hydrogen production  
 10:55 AM - 11:30 AM Tea Break

**Session 2** **Chair: Prof. Suresh Vaidyanathan, IIT Madras**  
 11:30 AM - 11:55 AM Prof. Paul Weiss, UCLA  
 Advancing sustainability through control of charge, heat, and spin at atomically precise interfaces

**Day 1 - Saturday, December 16, 2023**

11:55 AM - 12:20 PM Prof. Bala Subramaniam, University of Kansas  
 Sustainable polyolefins recycling with acidic polyoxometalates  
 12:20 PM - 12:45 PM Prof. G.V. Pavan Kumar, IC&SR, IIT Madras  
 Gold nanoparticle-driven optothermal tweezers  
 12:45 PM - 01:10 PM Prof. Jaydeb Chakrabarti, S. N. Bose National Centre for Basic Sciences  
 Ordering in driven thermo-responsive colloids  
 01:10 PM - 02:00 PM Lunch and Poster Session  
 02:00 PM - 03:00 PM Poster Session  
 03:00 PM - 03:45 PM Panel Discussion  
 Dr. G. Raghuvaran, IIT Madras  
 Dr. Kamallesh Chaudhary, IC&SR, IIT Madras  
 Dr. Rishabh Chandra, IC&SR, IIT Madras  
 Mr. Satish Satpati, IIT Madras

**Session 3** **Chair: Prof. Arvind K. Chandra, IIT Madras**  
 03:45 PM - 04:10 PM Prof. Ligy Phillips, IIT Madras  
 Sustainable wastewater management adopting circularity principles  
 04:10 PM - 04:35 PM Prof. Hannu Häkkinen, University of Jyväskylä  
 DNA-stabilized silver clusters: Electronic structure and photophysics

**Day 1 - Saturday, December 16, 2023**

04:35 PM - 05:00 PM Prof. Vivek Polshettiwar, TIFR Mumbai  
 Utilizing plasmonic effects: hot electrons for solar-driven catalysis  
 05:00 PM - 05:25 PM Tea Break  
**Session 4** **Chair: Prof. Edamana Prasad, IIT Madras**  
 05:25 PM - 05:50 PM Prof. Vasudevan Biju, Hokkaido University  
 Excitons and free carriers in quantum dots  
 05:50 PM - 06:15 PM Prof. G. Ranga Rao, IIT Madras  
 Materials for green hydrogen generation  
 06:15 PM - 06:40 PM Prof. E. S. Shibu, University of Calicut  
 Light-induced self-assembly in precision noble metal nanoclusters: New directions and application

**Day 2 - Sunday, December 17, 2023**

**Venue: T. T. Jagannathan Auditorium, IC&SR, IIT Madras**

**Session 5** **Chair: Prof. Samir K. Pal, SNBNCIS**  
 09:00 AM - 09:25 AM Dr. Tomáš Bažel, The Czech Academy of Sciences  
 Carbaborane clusters in self-assembled nanomaterials: symmetry and reactivity

**Day 2 - Sunday, December 17, 2023**

09:25 AM - 09:50 AM Prof. Rahul Nair, University of Manchester  
 Molecular transport through self-adaptive nano capillaries  
 09:50 AM - 10:15 AM Prof. Umesh Waghmare, IC&SR  
 Metal-organic frameworks of unusual properties of group IV chalcogenide crystals  
 10:15 AM - 10:40 AM Prof. Kuruvilla Joseph, Indian Institute of Space Science and Technology  
 Surface engineered nanosystems for bio-medical and space applications  
 10:40 AM - 11:00 AM Xylem  
 Mr. Siva Natarajan  
 DPM - Channel Management - Sales Support  
 Mr. Naran Madhavan  
 Innovation Manager - Emerging Markets - Technical Management - IIT Madras  
 11:00 AM - 11:30 AM Tea Break

**Session 6** **Chair: Prof. Indranath Chakraborty, IIT Kharagpur**  
 11:30 AM - 11:55 AM Prof. Thomas Thundat, University at Buffalo  
 Light-matter interaction at nanoscale for chemical sensing  
 11:55 AM - 12:20 PM Prof. Rahul Banerjee, IC&SR, IIT Madras  
 Porous covalent organic nanotubes (CONTs): reticular chemistry in one-dimension

**Day 2 - Sunday, December 17, 2023**

12:20 PM - 12:45 PM Prof. Chandrabhas Narayana, Raju Gandhi Centre for Biotechnology  
 Materials science and raman spectroscopy an ideal jugal bundi  
 12:45 PM - 01:10 PM Prof. R. Murugavel, IIT Bombay  
 Phosphate materials for sustainability  
 01:10 PM - 02:00 PM Lunch and Poster Session  
**Session 7** **Chair: Prof. B. L. V. Prasad, IIT Madras**  
 02:00 PM - 02:25 PM Prof. G. U. Kulkarni, IC&SR  
 Stabilizing gold in non-cubic crystal structures  
 02:25 PM - 02:50 PM Prof. Ajayashree Ayyappanpillai, CSIR-NIST  
 Ionic covalent organic frameworks for bacterial deactivation  
 02:50 PM - 03:15 PM Prof. Tanvi Saha Dasgupta, S. N. Bose National Centre for Basic Sciences  
 Pressure-tuned valence transition, insulator-metal transition in van der Waals antiferromagnet CrPS<sub>2</sub>  
 03:15 PM - 03:40 PM Group photo session  
 03:40 PM - 04:10 PM Tea Break

**Day 2 - Sunday, December 17, 2023**

**Session 8** **Chair: Prof. Ramesh Gardas, IIT Madras**  
 04:10 PM - 04:35 PM Prof. Richard Zare, Stanford University  
 Using water microdroplets to make molecules  
 04:35 PM - 05:00 PM Ms. Spoorthi B. K., IIT Madras  
 Molecules and materials in microdroplets  
 05:00 PM - 05:25 PM Dr. Udhaya Shankar, Hydromaterials Pvt. Ltd.  
 05:25 PM - 06:20 PM Felicitation  
 07:30 PM onwards Conference banquet dinner  
 Venue: Holiday Inn, Velachery

**Day 3 - Monday, December 18, 2023**

**Venue: Central Lecture Theatre, IIT Madras**

**Session 9** **Chair: Prof. Ananya Baksi, Jadavpur University**  
 09:00 AM - 09:25 AM Prof. Nonappa, Tampere University  
 Seeing nanoscale assemblies in 3D  
 09:25 AM - 09:50 AM Prof. Kanishka Biswas, IC&SR  
 Enhanced atomic ordering leads to ultra-high thermoelectric performance

**Day 3 - Monday, December 18, 2023**

09:50 AM - 10:15 AM Prof. Subi George, IC&SR  
 Secondary nucleation triggered supramolecular polymerization  
 10:15 AM - 10:40 AM Prof. Sebastian Peter, IC&SR  
 Substitutional effects in materials to design efficient catalysts for CO<sub>2</sub> reduction, hydrogen production and fuel cell operation  
 10:40 AM - 11:05 AM Prof. Francesco Stellacci, Ecole Polytechnique Fédérale de Lausanne  
 Supramolecular antivirals  
 11:05 AM - 11:30 PM Tea Break

**Session 10** **Chair: Mr. Vivek Yadav, IIT Madras**  
 11:30 AM - 11:55 AM Prof. C. Subramaniam, IIT Bombay  
 What's hot in solar for sustainability?  
 11:55 AM - 12:30 PM Prof. T. Pradeep, IIT Madras  
 Surface science of water ice  
 12:30 PM - 01:00 PM Concluding remarks and poster-prize distribution  
 01:00 PM onwards Lunch and departure

**Abstract Book**



**Contacts**

C. Subramaniam +91 97 6992 7194  
 Jobin Dnyan +91 94 9521 9200  
 Venkataramanan Mahalingam +91 90 0760 3474  
 Indranath Chakraborty +91 94 4542 0226  
 Vivek Yadav +91 99 9740 0978  
 Priya K +91 44 2257 5329

4. IRIS 2.0 Webinar Series on Centre of Excellence in Molecular Materials and Functions



The banner features the IIT Madras logo on the left. The title 'Indian Institute of Technology Madras' is at the top, followed by 'IRIS 2.0 WEBINAR SERIES' in large bold letters, and 'Centre of Excellence in Molecular Materials and Functions' below it. Three topics are listed with numbered icons: 1. Explore the realm of molecular materials, emphasizing the shift from atoms to molecules as fundamental building blocks. 2. Engage in groundbreaking research on two key molecular material families - atomically precise metallic clusters and gas hydrate cages. 3. Investigate the unique properties of large metallic clusters and molecular cages, highlight these studies in both fundamental understanding and practical applications. Below each topic is a portrait of a speaker: Prof. Rajnish Kumar, Prof. Thalappil Pradeep, and Prof. Manfred Kappes. Their titles and affiliations are listed below their names. The date and time '01 December 2023, 4:00 pm IST' are shown with a clock icon. A QR code is provided for registration, with the text 'Scan to Register for Free'. At the bottom, the website 'https://ge.iitm.ac.in/iris-2-0/' and email 'ioe.liaison@ge.iitm.ac.in' are listed.

**Indian Institute of Technology Madras**

**IRIS 2.0 WEBINAR SERIES**

**Centre of Excellence  
in  
Molecular Materials and Functions**

**1** Explore the realm of molecular materials, emphasizing the shift from atoms to molecules as fundamental building blocks.

**2** Engage in groundbreaking research on two key molecular material families - atomically precise metallic clusters and gas hydrate cages.

**3** Investigate the unique properties of large metallic clusters and molecular cages, highlight these studies in both fundamental understanding and practical applications.

**Prof. Rajnish Kumar**  
Co-PI, Molecular Materials and Functions  
Professor, Chemical Engineering  
IIT Madras

**Prof. Thalappil Pradeep**  
PI, Molecular Materials and Functions  
Professor, Chemistry  
IIT Madras

**Prof. Manfred Kappes**  
Moderator  
Professor  
Karlsruhe Institute of Technology  
Germany

**Date and Time**  
**01** December  
2023  
4:00 pm IST

**Scan to Register  
for Free**

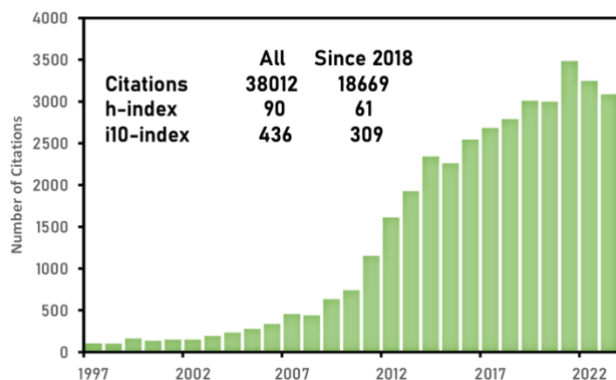
<https://ge.iitm.ac.in/iris-2-0/> [ioe.liaison@ge.iitm.ac.in](mailto:ioe.liaison@ge.iitm.ac.in)

To watch the lecture please visit our [Youtube](#) channel.



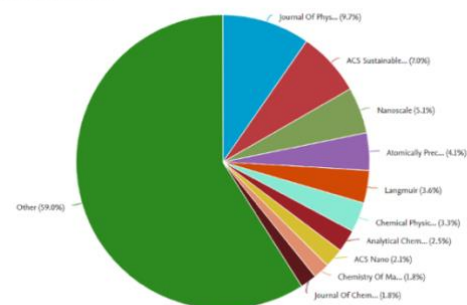
## Publication Analysis

### Google Scholar



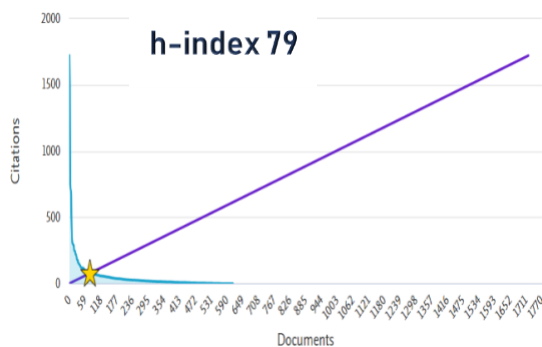
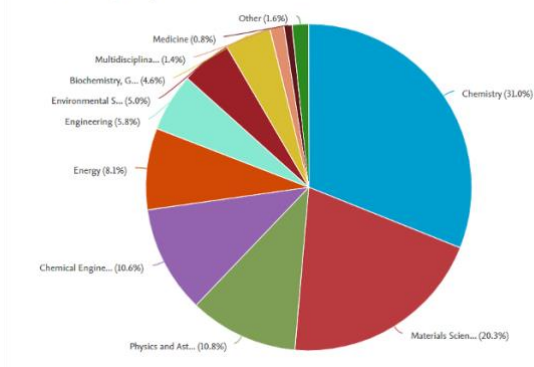
### By type-Scopus

Documents by source



### Scopus

Documents by subject area



### Sources

1. Scopus visited on December 30, 2023.
2. Google Scholar visited on December 30, 2023.

## Abstracts at a glance

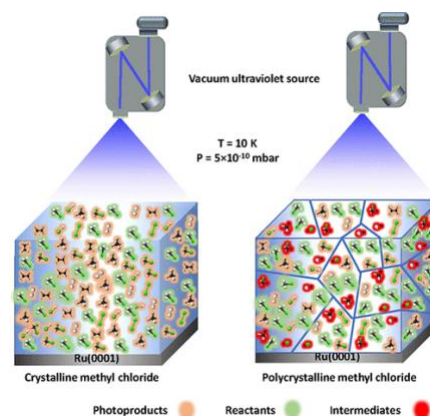
### Vacuum Ultraviolet Photolysis of Condensed Methyl Chloride in Interstellar Model Conditions and Trapping of Intermediates at Intergrain Interfaces

Bijesh Malla, Gaurav Vishwakarma, Soham Chowdhury, and Thalappil Pradeep

J. Phys. Chem. C, 2023. (Just accepted) (DOI: 10.1021/acs.jpcc.3c05889)

Photochemistry can generate chemical complexity in an interstellar space. This may occur due to photolysis and associated events that can happen in condensed molecular solids under the prevailing temperature and pressure conditions. In the present study, using reflection absorption infrared spectroscopy (RAIRS), three different condensed phases of methyl chloride ice, namely, amorphous, crystalline, and polycrystalline, were detected in ultrahigh vacuum (UHV) ( $p = 5 \times 10^{-10}$  mbar) and cryogenic conditions ( $T = 10\text{--}90$  K). Upon vacuum ultraviolet (VUV) photoirradiation, crystalline methyl chloride formed more photoproducts than amorphous and polycrystalline forms. This unusual finding is attributed to the rapid diffusion and reaction of photochemical intermediates in a crystalline matrix, whereas the intermediates are trapped at grain boundaries in the polycrystalline solid. Normally, the intermediate diffusion is

high in the case of the amorphous phase as resulting in enhancement in the case of the amorphous phase as resulting in enhancement in the formation of photoproducts in the matrix, which was observed by the intensified desorption of photoproducts in temperature-programme desorption mass spectrometry (TPD-MS). Further, all major and minor neutral photoproducts were detected by highly surface-sensitive Cs<sup>+</sup> ion-based secondary ion mass spectrometry (SIMS).



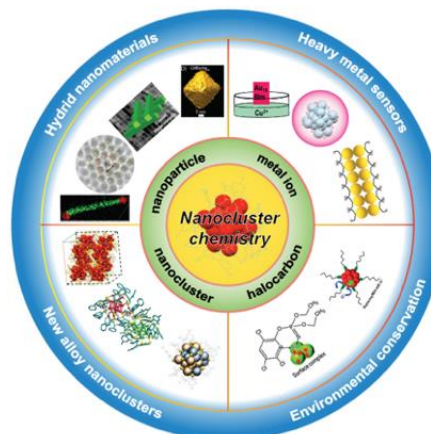
### A concise guide to chemical reactions of atomically precise noble metal nanoclusters

Paulami Bose, Krishnadas Kumaranchira Ramankutty, Papri Chakraborty, Esma Khatun, Thalappil Pradeep

Nanoscale, 2023. (Just accepted) (DOI:10.1039/D3NR05128E)

Nanoparticles (NPs) with atomic precision, known as nanoclusters (NCs), are an emerging field in materials science in view of their fascinating structure-property relationships. Ultrasmall noble metal NPs have molecule-like properties that make them fundamentally unique compared to their plasmonic counterparts and bulk materials. In this review, we present a comprehensive account of the chemistry of monolayer-protected atomically precise noble metal nanoclusters with a focus on the chemical reactions, their diversity, associated kinetics, and implications. To begin with, we briefly review the history of the evolution of such precision materials. Then the review explores the diverse chemistry of noble metal nanoclusters, including ligand exchange reactions, ligand-induced structural transformations, and reactions with metal ions, metal thiolates, and halocarbons. Just as

molecules, these precision materials also undergo intercluster reactions in solution.



Supramolecular forces between these systems facilitate the creation of well-defined hierarchical assemblies, composites, and hybrid materials. We conclude the review with a future perspective and scope of such chemistry.

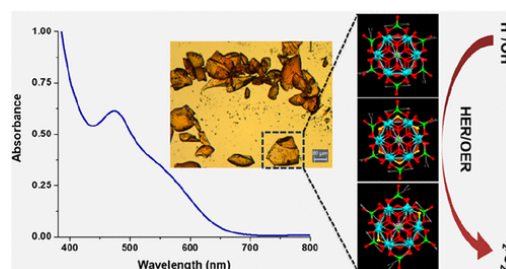
### Structure and electrocatalytic performance of co-crystallized ternary molybdenum oxo-sulfide clusters for efficient water splitting

Biswajit Mondal, Arijit Jana, Jayoti Roy, Astrid Campos Mata, Akhil S. Nair, Ananthu Mahendranath, Soumyabrata Roy, Biswarup Pathak, Pulickel M. Ajayan, and Thalappil Pradeep

ACS Materials Lett., 5, 2023, 3306–3315. (DOI: 10.1021/acsmaterialslett.3c00957 )

Polyoxometalates (POMs) belong to a class of metal oxoanion clusters that hold enormous promise for a wide range of catalytic reactions, due to their structural diversity and the presence of redox-active metal centers and heteroatomic sites within the framework. In this study, we successfully determined the structures of the first cocrystallized ternary molybdenum oxo-sulfide clusters:  $\text{Mo}_{12}\text{NaO}_{54}\text{P}_8\text{C}_{48}\text{H}_{40}$ ,  $\text{Mo}_{12}\text{NaS}_2\text{O}_{52}\text{P}_8\text{C}_{48}\text{H}_{40}$ , and  $\text{Mo}_{12}\text{NaS}_6\text{O}_{48}\text{P}_8\text{C}_{48}\text{H}_{40}$ , which are abbreviated as  $\text{Mo}_{12}$ ,  $\text{Mo}_{12}@\text{S}_2$ , and  $\text{Mo}_{12}@\text{S}_6$ , respectively. Together, they are referred to as  $\text{Mo}_{12}$ -TC. These clusters

exhibit nearly identical exterior structures, making them indistinguishable, leading to their cocrystallization in a single unit cell



with 50%, 25%, and 25% occupancy for  $\text{Mo}_{12}$ ,  $\text{Mo}_{12}@\text{S}_2$ , and  $\text{Mo}_{12}@\text{S}_6$ , respectively, and could not be separated easily. To confirm their molecular formulae and occupancy within a crystal,

we conducted single-crystal X-ray diffraction (SCXRD) and high-resolution electrospray ionization–mass spectrometry (ESI-MS) studies. The clusters exhibit a dumbbell-like shape, with each terminal of the dumbbell comprising a hexagonal Mo<sub>6</sub> basal plane shielded by multiple oxo, and oxosulfide moieties for Mo<sub>12</sub> and Mo<sub>12</sub>@S<sub>2</sub>/Mo<sub>12</sub>@S<sub>6</sub> clusters, respectively. Additionally, the clusters are protected by a ligand shell consisting of vertically aligned phenylphosphonic acid (PPA). Mo<sub>12</sub>-TC demonstrates promising activity

for electrochemical hydrogen and oxygen evolution reactions (HER and OER). Mo<sub>12</sub>-TC exhibits overpotentials of 0.262 and 0.413 V vs RHE to reach HER current densities (in H<sub>2</sub>SO<sub>4</sub>) of 10 and 100 mA cm<sup>-2</sup>, respectively, and overpotentials of 0.45 and 0.787 V vs RHE to reach OER current densities (in KOH) of 10 and 100 mA cm<sup>-2</sup>, respectively, stable up to 5000 cycles. Density functional theory (DFT) calculations further elucidate their electrocatalytic potential, revealing the presence of active sites within these molecular frameworks.

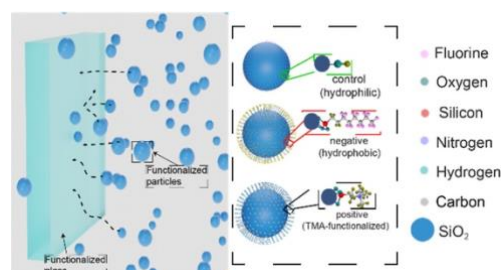
### Observing real-time adhesion of microparticles on glass surfaces

Pillalamarri Srikrishnarka, Dhivyaraja Kumaran, Amoghavarsha Ramachandra Kini, Vishal Kumar, Ankit Nagar, Md Rabiul Islam, Ramamurthy Nagarajan, Thalappil Pradeep

Langmuir, 2023. (DOI:10.1021/acs.langmuir.3c01856)

Fouling on glass surfaces reduces the solar panel efficiency and increases water consumption for cleaning. Superhydrophobic coatings on glass enable self-cleaning by allowing water droplets to carry away dirt particles. Observing the interaction between charged particles and surfaces provides insights into effective cleaning. Using a high-speed camera and a long-distance objective, we analyzed the *in situ* deposition of variously functionalized and charged silica dust microparticles on chemically treated glass. The ambient charges for the control, hydrophobic, and positively charged particles were approximately -0.5, -0.13, and +0.5 nC, respectively. We found that a positively

charged particle of 2.3 ± 1.2 μm diameter adhered to hydroxylated glass in ~0.054 s, compared to 0.40 and 0.45 s for quaternary ammonium- and fluorosilane-functionalized hydrophobic glass.



Experiments suggest that quaternary ammonium-functionalized glass surfaces are about 77.8% more resistant to soiling than bare surface.

Photoconversion of Ag<sub>31</sub> to Ag<sub>42</sub>, initiated by solvated electrons

Arijit Jana, Wakeel Ahmed Dar, Sourav Kanti Jana, Ajay Poonia, Vivek Yadav, Jayoti Roy, Sourov Chandra, Kumaran Nair Valsala Devi Adarsh, Robin Ras, and Thalappil Pradeep

Chem. Mater., 2023. (DOI: 10.1021/acs.chemmater.3c01293)

Light-matter interactions, especially in atomically precise nanomaterials, belong to an unexplored realm of research with potential benefits for the synthesis of materials. Here, we present an interesting light-activated expansion process of an Ag<sub>31</sub> nanocluster to an Ag<sub>42</sub> analogue, both clusters being protected with 6-(dibutylamino)-1,3,5-triazine-2, 4-dithiol (shortly, TRZ-H<sub>2</sub>) ligands. The conversion process was initially monitored through UV-vis, revealing that the violet-colored Ag<sub>31</sub> got converted to greenish Ag<sub>42</sub>, exhibiting their characteristic absorption features. High-resolution mass spectrometric studies confirmed that the as-synthesized [Ag<sub>31</sub>(TRZ)<sub>10</sub>] with coexisting di- and monoanionic charged species in dichloromethane solution got converted to [Ag<sub>42</sub>(TRZ)<sub>13</sub>] with a dipositive charge state. Electrochemical studies revealed the photoresponsive



nature of Ag<sub>31</sub>, and light illumination resulted in transient intermediate clusters covered with solvated electrons, which contributed to the core expansion. Ag<sub>31</sub> is NIR-emitting, while Ag<sub>42</sub> is red-emitting. The ultrafast transient absorption studies reveal that Ag<sub>42</sub> has strikingly short excited-state carrier dynamics than Ag<sub>31</sub>. The stable excited-state carriers for Ag<sub>31</sub> upon photoexcitation also underline the unique electronic characteristics responsible for such light-activated structural evolution.

## Formation and Transformation of Clathrate Hydrates under Interstellar Conditions

Jyotirmoy Ghosh, Gaurav Vishwakarma, Rajnish Kumar, and Thalappil Pradeep

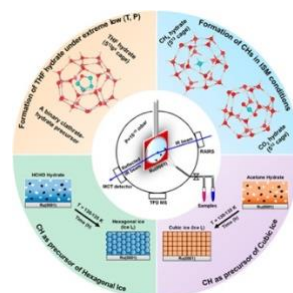
Acc. Chem. Res., 56, 2023, 2241–2252. (DOI: 10.1021/acs.accounts.3c00317)

This Account discusses our effort to discover clathrate hydrates (CHs) of several molecules and their structural varieties, transformations, and kinetics in a simulated interstellar environment. CHs are nonstoichiometric crystalline host-guest complexes in which water molecules form cages of different sizes to entrap guest molecules. CHs are abundant on earth and require moderate temperatures

and high pressures for their formation. Our focus has been to form CHs at extremely low pressure and temperature as in the ISM, although their existence under such conditions has been a long-standing question since water and guest molecules (CH<sub>4</sub>, CO<sub>2</sub>, CO, etc.) exist in space. In multiple studies conducted at ~10<sup>-10</sup> mbar, we showed that CH<sub>4</sub>, CO<sub>2</sub>, and C<sub>2</sub>H<sub>6</sub> hydrates could be formed at 30,

10, and 60 K, respectively. Well-defined IR spectroscopic features supported by quantum chemical simulations and temperature-programmed desorption mass spectrometric analyses confirmed the existence of the  $5^{12}$  (for  $\text{CH}_4$  and  $\text{CO}_2$ ) and  $5^{12}6^2$  (for  $\text{C}_2\text{H}_6$ ) CH cages. Mild thermal activation for long periods under ultrahigh vacuum (UHV) allowed efficient molecular diffusion, which is crucial for forming CHs. We also explored the formation of THF hydrate (a promoter/stabilizer for binary CHs), and a spontaneous method was found for its formation under UHV. In a subsequent study, we observed a binary THF- $\text{CO}_2$  hydrate and its thermal processing at 130 K leading to the transportation of  $\text{CO}_2$  from the hydrate cages to the matrix of amorphous water. The findings imply that such systems possess a dynamic

setting that facilitates the movement of molecules, potentially accounting for the chemical changes observed in the ISM.



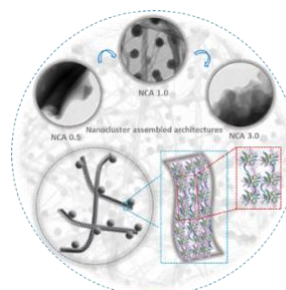
Furthermore, an intriguing fundamental phenomenon is the consequences of these CHs and their dynamics. We showed that preformed acetone and formaldehyde hydrates dissociate to form cubic ( $\text{I}_c$ ) and hexagonal ( $\text{I}_h$ ) ices at 130–135 K, respectively. These unique processes could be the mechanistic routes for the formation of various ices in astrophysical environments.

### Secondary ligand-induced orthogonal self-assembly of silver nanoclusters into superstructures with enhanced NIR emission

Korath Shivan Sugi, Amritha P Sandra, Nonappa, Debasmita Ghosh, Jyoti Sarita Mohanty, Murugesan Paulthangam Kannan, B. S. Sooraj, Pillalamarri Srikrishnarka, Jayoti Roy, Wakeel Ahmed Dar, and Thalappil Pradeep

Nanoscale, 15, 2023, 11927-11934. (DOI: 10.1039/D3NR02561F)

Orthogonal self-assembly is one of the crucial strategies for forming complex and hierarchical structures in biological systems. However, creating such ordered complex structures using synthetic nanoparticles is a challenging task and requires a high degree of control over structure and multiple non-covalent interactions. In this context, nanoarchitectonics serves as an emerging tool to fabricate complex functional materials. Here, we present a secondary ligand-induced orthogonal self-assembly



of atomically precise silver nanoclusters into complex superstructures. Specifically, we use  $\text{Ag}_{14}\text{NCs}$  protected with naphthalene thiol and 1,6-bis(diphenylphosphino)hexane ligands.

Controlled addition of 1,6-bis(diphenylphosphino)hexane, the secondary ligand resulted in a self-assembled supracolloidal structure including helical fibers, spheres, and nanosheets. The self-assembly process is tunable by controlling the molar ratio of the ligand. The resulting superstructures

exhibit enhanced NIR emission due to restricted intramolecular motion. This demonstrates that by tuning supramolecular interactions, hierarchical nanostructures with desired properties similar to biomolecules can be obtained from atomically precise building blocks

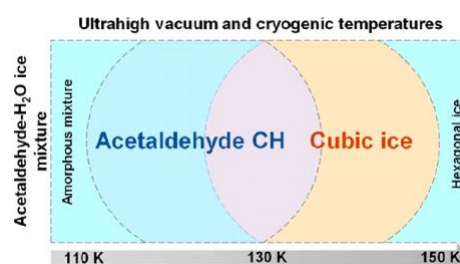
### Existence of acetaldehyde clathrate hydrate and its dissociation leading to cubic ice under ultrahigh vacuum and cryogenic conditions

Gaurav Vishwakarma, Bijesh K. Malla, Soham Chowdhury, Sakshi Pradip Khandare, and Thalappil Pradeep

J. Phys. Chem. Lett., 14, 2023, 5328–5334. (DOI: 10.1021/acs.jpcllett.3c01181)

Acetaldehyde in a dilute aqueous solution gets hydrated to produce a geminal diol under atmospheric conditions. The acetaldehyde–water ice system under high pressure also converts to a geminal diol, and therefore, its stable clathrate hydrate (CH) phase, which in most systems forms at high pressures, is unknown. In the present study, we showed that acetaldehyde CH exists in ultrahigh vacuum ( $10^{-10}$  mbar) under cryogenic conditions (below 140 K) and continues to exist at 115 K for periods well over 1 day. Decomposition of acetaldehyde CH at 130–135 K produces water ice in its cubic crystalline form. The mechanism and

kinetics involved in the process have also been studied. Reflection absorption infrared spectroscopy and temperature-programmed desorption mass spectrometry were utilized to confirm the CH formation. Our study establishes the possibility of a stable CH phase for acetaldehyde in interstellar and cometary environments.



### Endangered indigenous rice varieties as a source of B vitamins for the undernourished population

Priyabrata Roy, Debal Deb, Arunan Suganya, Brindaban Roy, Thalappil Pradeep, and Tanimu Saha

Cereal Chemistry, 2023. (DOI: 10.1002/cche.10668)

**Background and Objectives:** Rice is a staple food for half of the world's population and plays an important role

to deliver several micronutrients including B vitamins to humans. The present investigation was carried out to

detect some B vitamins and estimate their concentrations in 309 traditional indica rice landraces, compared with three modern rice varieties predominantly available in the Indian market.

**Findings:** Liquid chromatographic examination of the rice samples demonstrated that a large number of traditional rice landraces contained considerable amounts of different B vitamins. In the landraces examined, vitamin B1(thiamine) was recorded to be present in the range of 0.01–10.55mg/100 g, vitamin B2 (riboflavin) 0.01–2.63mg/100 g, vitamin B3 (niacin) 0.20–4.52mg/100 g, vitamin B5 (pantothenic acid) 0.01–18.55mg/100 g, vitamin B6 (pyridoxine) 0.01–0.86

mg/100 g, and vitamin B7 (biotin) 0.01–5.90mg/100 g in different rice landraces.

**Conclusion:** Compared with traditional rice, modern rice cultivars seem to have substantially lower B vitamin levels. It appears that these vitamin-rich traditional rice landraces if incorporated into daily diet, may serve to attain nutritional security of the poor.

**Significance and Novelty:** Our results show that many traditional rice landraces are nutritionally superior to any modern rice cultivar, even though traditional rice landraces are normally not in priority for agronomic research and development. This study shows how native rice landraces may be leveraged to constitute novel nutritious diet that could enhance human health.

### Atomically precise clusters: Chemical evolution of molecular matter at the nanoscale

Arijit Jana, Amoghavarsha Ramachandra Kini, and Thalappil Pradeep

AsiaChem, 3, 2023, 56-65. (DOI: 10.51167/acm00040)

The chemistry of nanoparticles with atomic precision has become a subject of interest due to the unique physical and chemical properties of these systems in comparison to their bulk counterparts. Nanoparticles typically contain thousands of atoms, arranged in a specific fashion. There is a need to bridge the gap between single atoms and nanoparticles to understand the size evolution of matter. This regime, composed of a few atoms, is called nanoclusters having size in the range of 1 to 3 nm, with a precise number of atoms, with well-defined structure and properties. Most of studied materials in this class are composed of noble metals. Various techniques, including



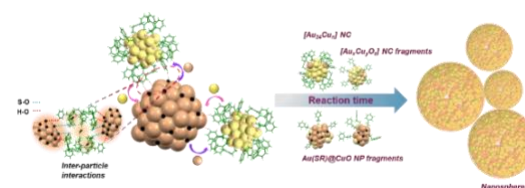
UV/vis spectroscopy, mass spectrometry, and single crystal XRD, reveal their molecular nature. Their unique electronic properties can be used for applications like catalysis, sensing, magnetism, medicine, bio-imaging, etc. This article touches upon the basics of nanoclusters, their synthesis, characterization, atomic structures, and supramolecular arrangements. We hope that this work provides a brief understanding of

nanoclusters and inspires young scientists to conduct research in the chemistry of clusters.

### Dissociative reactions of $[\text{Au}_{25}(\text{SR})_{18}]^-$ at copper oxide nanoparticles and formation of aggregated nanostructures

Jayoti Roy, Biswajit Mondal, Gaurav Vishwakarma, Nishanthi Vasanthi Sridharan, Pattabiraman Krishnamurthi, Nonappa, and Thalappil Pradeep *Nanoscale*, 15, 2023, 8225-8234. (DOI: 10.1039/D3NR00897E)

Reactions between nanoclusters (NCs) have been studied widely in the recent past, but such processes between NCs and metal-oxide nanoparticles (NPs), belonging to two different size ranges, have not been explored earlier. For the first time, we demonstrate the spontaneous reactions between an atomically precise NC,  $[\text{Au}_{25}(\text{PET})_{18}]^-$  (PET = 2-phenylethanethiolate), and polydispersed copper oxide nanoparticles with an average diameter of 50 nm under ambient conditions. These interparticle reactions result in the formation of alloy NCs and copper-doped NC fragments, which assemble to form nanospheres at the end of the reaction. High-resolution electrospray



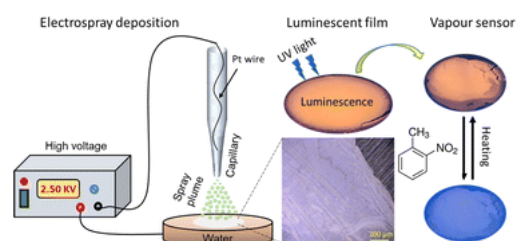
ionization mass spectrometry (ESI MS), transmission electron microscopy (HR-TEM), electron tomography, and X-ray photoelectron spectroscopy (XPS) studies were performed to understand the structures formed. The results from our study show that interparticle reactions can be extended to a range of chemical systems, leading to diverse alloy NCs and self-assembled colloidal superstructures.

### A luminescent $\text{Cu}_4$ cluster film grown by electrospray deposition: A nitroaromatic vapour sensor

Arijit Jana, B. K. Spoorthi, Akhil S. Nair, Ankit Nagar, Biswarup Pathak, Tomas Base, and Thalappil Pradeep *Nanoscale*, 15, 2023, 8141-8147. (DOI:10.1039/D3NR00416C)

We present the fabrication and use of a film of a carborane-thiolprotected tetranuclear copper cluster with characteristic orange luminescence using ambient electrospray deposition (ESD). Charged microdroplets of the clusters produced by an electrospray tip deposit the clusters at an air-water interface to form a film. Different microscopic and

spectroscopic techniques characterized the porous surface structure of the film.



Visible and rapid quenching of the emission of the film upon exposure to 2-nitrotoluene (2-NT) vapours under ambient conditions was observed. Density functional theory (DFT) calculations established the favourable binding sites of 2-NT with the cluster. Desorption of 2-NT upon heating recovered the original

luminescence, demonstrating the reusability of the sensor. Stable emission upon exposure to different organic solvents and its quenching upon exposure to 2,4-dinitrotoluene and picric acid showed selectivity of the film to nitroaromatic species.

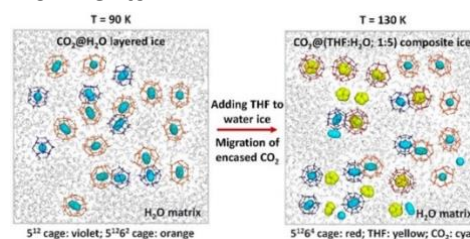
### Induced migration of CO<sub>2</sub> from hydrate cages to amorphous solid water under ultrahigh vacuum and cryogenic conditions

Gaurav Vishwakarma, Bijesh Malla, Karri Sesha Surya Vara Prasad Reddy, Jyotirmoy Ghosh, Soham Chowdhury, Sharma S. R. K. C. Yamijala, Sandeep Kumar Reddy, Rajnish Kumar, and Thalappil Pradeep

J. Phy. Chem. Lett., 14, 2023, 2823–2829. (DOI:10.1021/acs.jpcllett.3c00373)

Restricted migration of reactive species limits chemical transformations within interstellar and cometary ices. We report the migration of CO<sub>2</sub> from clathrate hydrate (CH) cages to amorphous solid water (ASW) in the presence of tetrahydrofuran (THF) under ultrahigh vacuum (UHV) and cryogenic conditions. Thermal annealing of sequentially deposited CO<sub>2</sub> and H<sub>2</sub>O ice, CO<sub>2</sub>@H<sub>2</sub>O, to 90 K resulted in the partitioning of CO<sub>2</sub> in 5<sup>12</sup> and 5<sup>12</sup>6<sup>2</sup> CH cages (CO<sub>2</sub>@5<sup>12</sup>, CO<sub>2</sub>@5<sup>12</sup>6<sup>2</sup>). However, upon preparing a composite ice film composed of CO<sub>2</sub>@5<sup>12</sup>, CO<sub>2</sub>@5<sup>12</sup>6<sup>2</sup> and THF distributed in the water matrix at 90 K, and annealing the

mixture for 6 h at 130 K produced mixed CO<sub>2</sub>–THF CH, where THF occupied the 5<sup>12</sup>6<sup>4</sup> cages (THF@5<sup>12</sup>6<sup>4</sup>) exclusively while CO<sub>2</sub> in 5<sup>12</sup>6<sup>2</sup> cages (CO<sub>2</sub>@5<sup>12</sup>6<sup>2</sup>) got transferred to the ASW matrix and CO<sub>2</sub> in the 5<sup>12</sup> cages (CO<sub>2</sub>@5<sup>12</sup>) remained as is. This cage–matrix exchange may create a more conducive environment for chemical transformations in interstellar environments.



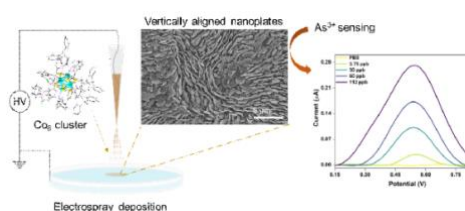
### Vertically aligned nanoplates of atomically precise Co<sub>6</sub>S<sub>8</sub> cluster for practical arsenic sensing

Anagha Jose, Arijit Jana, Tanvi Gupte, Akhil Nair, Keerthana Unni, Ankit Nagar, Amoghavarsha Kini, B. K. Spoorthi, Sourav Jana, Biswarup Pathak, and Thalappil Pradeep

ACS Materials Lett., 5, 2023, 893–899 (DOI: 10.1021/acsmaterialslett.3c00085)

Two-dimensional nanostructures with atomically precise building blocks have potential applications in catalysis and sensing. However, structural instability and surface reactivity limit their practical use. In this work, we demonstrate the formation of vertically aligned nanoplates of  $[\text{Co}_6\text{S}_8\text{DPPE}_6\text{Cl}_6]$  cluster ( $\text{Co}_6$  in short), protected by 1,2-bis(diphenylphosphino)ethane, using ambient electrospray deposition (ESD). Charged microdroplets of  $\text{Co}_6$  formed by ESD on a water surface created such nanostructures. Preferential arrangement of clusters in the nanoplatelets with

enhanced surface area results in sensitive and selective electrochemical response towards arsenite down to 5 parts per billion, in tap water. Density functional

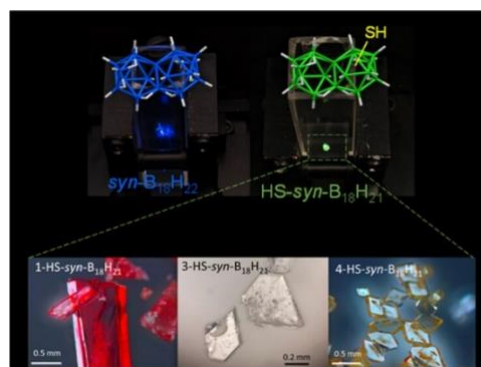


theory calculation reveals the preferential binding of arsenite with  $\text{Co}_6$ . Our work points to a practical application of atomically precise clusters of large societal relevance.

### Macropolyhedral $\text{syn-B}_{18}\text{H}_{22}$ , the “forgotten” isomer

Deepak Patel, B. S. Sooraj, Kaplan Kirakci, Jan Machacek, Monika Kučeráková, Jonathan Bould, Michal Dusek, Martha Frey, Christof Neumann, Sundargopal Ghosh, Andrey Turchanin, Thalappil Pradeep, and Tomas Base  
J. Am. Chem. Soc., 145, 2023, 17975–17986 (DOI: 10.1021/jacs.3c05530)

The chemistry and physics of macropolyhedral  $\text{B}_{18}\text{H}_{22}$  clusters have attracted significant attention due to the interesting photophysical properties of *anti*- $\text{B}_{18}\text{H}_{22}$  (blue emission, laser properties) and related potential applications. We have focused our attention on the “forgotten” *syn*- $\text{B}_{18}\text{H}_{22}$  isomer, which has received very little attention since its discovery compared to its *anti*- $\text{B}_{18}\text{H}_{22}$  isomer, presumably because numerous studies have reported this isomer as nonluminescent. In our study, we show that in crystalline form, *syn*- $\text{B}_{18}\text{H}_{22}$  exhibits blue fluorescence and becomes phosphorescent when substituted at various positions on the cluster, associated with peculiar microstructural-dependent effects. This work is a combined theoretical and experimental investigation that includes the synthesis, separation, structural characterization, and first elucidation of the photophysical properties of three different monothiol-substituted cluster



isomers, [1-HS-*syn*- $\text{B}_{18}\text{H}_{21}$ ] **1**, [3-HS-*syn*- $\text{B}_{18}\text{H}_{21}$ ] **3**, and [4-HS-*syn*- $\text{B}_{18}\text{H}_{21}$ ] **4**, of which isomers **1** and **4** have been proved to exist in two different polymorphic forms. All of these newly substituted macropolyhedral cluster derivatives (**1**, **3**, and **4**) have been fully characterized by NMR spectroscopy, mass spectrometry, single-crystal X-ray diffraction, IR spectroscopy, and luminescence spectroscopy. This study also presents the first report on the mechanochromic shift in the luminescence of a borane cluster and generally enriches the area of rather rare boron-based luminescent materials. In addition, we

present the first results proving that they are useful constituents of carbon-free self-assembled monolayers.

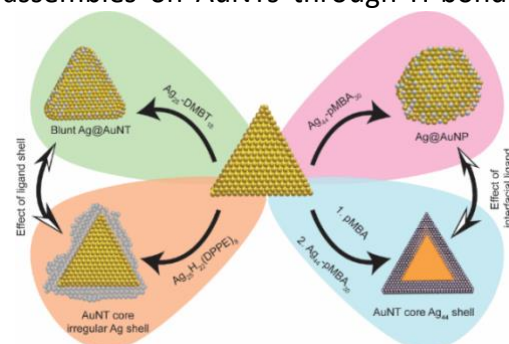
### Tunable reactivity of silver nanoclusters: Facile route to synthesize a range of bimetallic nanostructures

Amrita Chakraborty, Megha Maria Stanley, Biswajit Mondal, Nonappa, Md Bodiuzzaman, Papri Chakraborty, M. P. Kannan, and Thalappil Pradeep

Nanoscale, 15, 2023, 2690-2699 (DOI: 10.1039/D2NR06350F)

Quantized energy levels and unique optoelectronic properties of atomically precise noble metal nanoclusters (NCs) have made them important in materials science, catalysis, sensors, and biomedicine. Recent studies on the profound chemical interactions of such NCs within themselves and with ultrasmall plasmonic nanoparticles (NPs) indicate that depending on the size, shape, and composition of the second reactant, NCs can either take part in colloidal assembly without any chemical modifications or lead to products with atoms exchanged. Anisotropic NPs are a unique class of plasmonic nanomaterials as their sharp edges and protrusions show higher chemical reactivity compared to flat surfaces, often leading to site-specific growth of foreign metals and metal oxide shells. Here, using chemical interactions between gold nanotriangles (AuNTs) and Ag NCs of different compositions, we show for the first time that metal atom etching, alloying/atom exchange, and colloidal assembly can all happen at a particular length scale. Specifically,  $\text{Ag}_{25}(\text{DMBT})_{18}$  NCs (denoted as 1), upon reacting with AuNTs of  $\sim 57$  nm edge length, etch gold atoms from their sharp tips and edges. Simultaneously, the two nanosystems exchange metal atoms, resulting in Ag-doped AuNTs and  $\text{AuAg}_{24-x}(\text{DMBT})_{18}$  ( $x = 1, 2$ ). However, another Ag NC with the same metallic core, but a different ligand shell, namely,  $\text{Ag}_{25}\text{H}_{22}(\text{DPPE})_8$  (denoted as

2), creates dendritic shells made of Ag, surrounding these AuNTs under the same reaction conditions. Furthermore, we show that in the case of a more reactive thiol-protected Ag NC, namely,  $\text{Ag}_{44}(\text{pMBA})_{30}$  (denoted as 3), gold etching is faster from the edges and tips, which drastically alters the identities of both the reactants. Interestingly, when the AuNTs are protected by pMBA, 3 systematically assembles on AuNTs through H-bonding,



resulting in an AuNT core–Ag NC shell nanocomposite. Thus, while shedding light on various factors affecting the reactivity of Ag NCs towards AuNTs, the present study proposes a single strategy to obtain a number of bimetallic nanosystems of targeted morphology and functionality.

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