



# Annual Report 2021

## Pradeep Research Group

Indian Institute of Technology Madras

Chennai 600 036, India

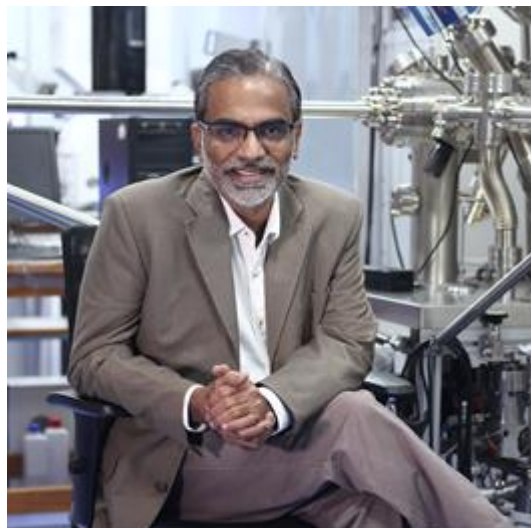


Please visit the links for annual reports of [2014](#), [2015](#), [2016](#), [2017](#), [2018](#), [2019](#) and [2020](#).

## Our Team

### Thalappil Pradeep

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 Deepak Parekh Institute Chair Professor and  
 Professor of Chemistry  
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 Thematic Unit of Excellence  
 Web: <https://pradeepresearch.org/>



### Ph.D. Students

- |                        |                               |                      |
|------------------------|-------------------------------|----------------------|
| ❖ Aishi Mitra          | ❖ Mohd. Azhardin Ganayee      | ❖ Swetashree Acharya |
| ❖ Anil Kumar           | ❖ Pallab Basuri               | ❖ Tanmayaa Nayak     |
| ❖ A. Suganya           | ❖ Paulami Bose                | ❖ Tanvi Gupte*       |
| ❖ Amoghavarsha R. Kini | ❖ S. Jenifer*                 | ❖ Vishal Kumar*      |
| ❖ Anagha Jose          | ❖ Sinchan Mukhhopadhyay       | ❖ Vivek Yadav        |
| ❖ Ankit Nagar*         | ❖ Sonali Seth                 |                      |
| ❖ Arijit Jana          | ❖ Soham Chowdhury             |                      |
| ❖ Bijesh Malla         | ❖ B. S. Sooraj                |                      |
| ❖ Deepak Patel         | ❖ B K Spoorthi                |                      |
| ❖ Gaurav Vishwakarma   | ❖ Srikrishnarka Pillalamarri* |                      |
| ❖ Jayoti Roy           | ❖ Subrata Duary               |                      |
| ❖ Keerthana Unni       | ❖ Sujan Manna                 |                      |

\*Interdisciplinary students, jointly advised with colleagues

### Postdoctoral students/Project associates

- Dr. Angshuman Ray Chowdhury
- Dr. Biswajit Mondal
- Dr. Kartheek Joshua
- Dr. Sourav Kanti Jana
- Dr. Madhuri Jash
- Dr. Md Rabiul Islam
- Mr. Anish R Nath

### M.S. Students

- Ananthu Mahendranath\*
- Ramesh Kumar

### Administrative Officer

- K. Priya

### Project Technicians

- S. Balamurugan



## What's Inside

1. Glimpses of 2021	04
2. Awards & Honours	05
3. Publications	06
4. Editorials of 2021	09
5. General Articles	10
6. Patents	11
7. Degree Holders	13
8. Lectures Delivered	14
9. Students' Recognitions	15
10. Alumni News	16
11. Research Grants	17
12. Visits/Visitors	18
13. Services	19
14. Upcoming Facilities to Lab	20
15. Incubation	22
16. Reach of Some of our Technologies	24
17. Media Reports	25
18. Initiatives	27
19. Publication Analyses	30
20. Abstracts at a Glance	31
21. Acknowledgements	47

## Glimpses of 2021



Prof. T. Pradeep with the Prime Minister of India, November 8, 2021, New Delhi

Indo-Japan virtual workshop  
on  
Cluster science by interdisciplinary  
approach: Emerging materials and  
phenomena

September 3rd, 4th & 5th

Venue :  
Auditorium (Virtual), IIT Madras

Links :  
September 3  
September 4  
September 5

Organized by :  
Centre of Excellence on  
Molecular Materials and  
Functions, IIT Madras

Supported by :  
Government of India  
JSPS

Virtual Indo-Japan workshop,  
September 3-5, 2021

Session - 10

Monthly discussion meeting  
to  
create experiment - theory  
interface

18<sup>th</sup> December 2021  
6 to 8 PM

Lectures :

Prof. Srinivasa Rao Bakshi  
"Reactive Spark Plasma Sintering - Examples and Possibilities"  
from 6:00 PM to 6:30 PM  
Department of Metallurgical and Materials Engineering, IIT Madras

Dr. Pramoda Kumar Nayak  
"Van der Waals Heterostructures"  
from 6:30 PM to 7:00 PM  
Department of Physics, IIT Madras

Prof. Abhijit P. Deshpande  
"Complex fluids viscoelasticity - from "bulk behaviour" to  
"response at small length scales"  
from 7:00 PM to 7:30 PM  
Department of Chemical Engineering, IIT Madras

Announcement of one meeting in this series

## Awards and Honors

Prof. T. Pradeep has been nominated as the **National Representative** for the Analytical Chemistry Division of the International Union of Pure and Applied Chemistry (IUPAC).



Indian Institute of Technology, Madras  
196,851 followers  
1mo • Edited •

Hearty congratulations to Dr. **Thalappil Pradeep**, Deepak Parekh Chair Professor, Department of Chemistry #IITMadras for being conferred with the #PadmaShri award this year. His pioneering contributions in nanotechnology-based water purification are invaluable.

Dr. T. Pradeep has conceptualised and developed the International Centre for Clean Water, an initiative of #IITMadras that provides world-class infrastructure for water research, water quality analysis, product development, incubation and pilot production. The Centre also offers consultancy, training and implementation support to emerging technologies.

#research #awards #recognition #science #ceremony #India #nanotechnology #PadmaAwards2020



Prof. T. Pradeep has been invited to serve as the **convenor** of the Commission for Reforms in the Higher Education Sector constituted by the Government of Kerala.

**CHEMISTRY**  
AN ASIAN JOURNAL

**ACES** Asian Chemical  
Editorial Society

Prof. T. Pradeep has been invited to be the **member** of the International Advisory Board of Chemistry- An Asian Journal, an Asian Chemical Editorial Society (ACES) Journal for the second time.

### IISc Distinguished Alumnus/Alumna Award 2021



Dr Anuradha M Annaswamy  
BE EE '79



Prof Sajal K Das  
ME CSA '85



Prof T Pradeep  
PhD SSCU '91



Prof CS Raghavendra  
BE & ME ECE '76 & '78

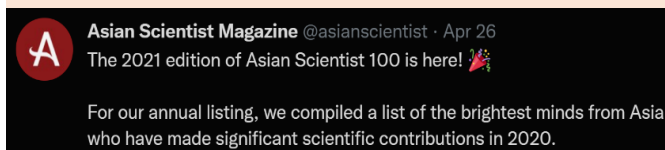


Dr Ritu Shrivastava  
BE & ME ECE '71 & '73

## Awards and Honors

Prof. T. Pradeep has been nominated as the **Chairman**, Board of Governors of Institute of Nano Science and Technology, Mohali.

Prof. T. Pradeep has been chosen for the **Vishwakarma Medal** of the Indian National Science Academy.



Prof. T. Pradeep has won a Silver Medal of the Chemical Research Society of India, 2021.

Prof. T. Pradeep has been chosen for the 2021 Edition of the elite 'Asian Scientist 100 List'. He is in this list for the second time.

## Publications

### Journal publications

1. Gas phase ion chemistry of titanium-oxofullerene with ligated solvents, Jayoti Roy, Papri Chakraborty, Ganesan Paramasivam, Ganapati Natarajan, and Thalappil Pradeep, Phys. Chem. Chem. Phys., 2021 (Just accepted).
2. Assembling atomically precise noble metal nanoclusters using supramolecular interactions, Abhijit Nag, and Thalappil Pradeep, ACS Nanoscience Au, 2021 (Just accepted).
3. Direct imaging of lattice planes in atomically precise noble metal cluster crystals using a conventional transmission electron microscope, Ananthu Mahendranath, Biswajit Mondal, Korath Sivan Sugi, and Thalappil Pradeep, Chem. Commun., (2021) (DOI: 10.1039/D1CC05643C).

4. Desorption-induced evolution of cubic and hexagonal ices in an ultrahigh vacuum and cryogenic temperatures, Gaurav Vishwakarma, Jyotirmoy Ghosh, and Thalappil Pradeep, *Phys. Chem. Chem. Phys.*, 23 (2021) 24052 (DOI: 10.1039/D1CP03872A).
5. Light-activated intercluster conversion of an atomically precise silver nanocluster, Arijit Jana, Madhuri Jash, Ajay Kumar Poonia, Ganesan Paramasivam, Md Rabiul Islam, Papri Chakraborty, Sudhadevi Antharjanam, Jan Machacek, Sundargopal Ghosh, Kumaran Nair Valsala Devi Adarsh, Tomas Base, and Thalappil Pradeep, *ACS Nano*, 15 (2021) 15781–15793 (DOI: 10.1021/acsnano.1c02602).
6. Interference of phosphate in adsorption of arsenate and arsenite over confined metastable two-line ferrihydrite and magnetite, Chennu Sudhakar, Sritama Mukherjee, Avula Anil Kumar, Ganesan Paramasivam, P. Karthigai Meena, Nonappa, and Thalappil Pradeep, *J. Phys. Chem. C*, 125 (2021) 22502–22512 (DOI: 10.1021/acs.jpcc.1c04317).
7. Aminoclay-graphene oxide composite for thin-film composite reverse osmosis membranes with unprecedented water flux and fouling resistance, Md Rabiul Islam, Pratishtha Khurana, Pillalamarri Srikrishnarka, Ankit Nagar, Madhuri Jash, Shantha Kumar Jenifer, Mohd Azhardin Ganayee, Mathava Kumar, and Thalappil Pradeep, *Adv. Mater. Interfaces*, 8 (2021) 2100533 (DOI: 10.1002/admi.202100533).
8. Cellulosic ternary nanocomposite for affordable and sustainable fluoride removal, Moses Egor, Avula Anil Kumar, Tripti Ahuja, Sritama Mukherjee, Amrita Chakraborty, Chennu Sudhakar, Pillalamarri Srikrishnarka, Sandeep Bose, Swathy Jakka Ravindran, and Thalappil Pradeep, *ACS Sustainable Chem. Eng.*, 9 (2021) 12788–12799 (DOI: 10.1021/acssuschemeng.1c03272).
9. Isotopic exchange of atomically precise nanoclusters with materials of varying dimensions: From nanoscale to bulk, Papri Chakraborty, Paulami Bose, Jayoti Roy, Abhijit Nag, Biswajit Mondal, Amrita Chakraborty, and Thalappil Pradeep, *J. Phys. Chem. C*, 125 (2021) 16110–16117 (DOI: 10.1021/acs.jpcc.1c02264).
10. Triboelectric generators for sustainable reduction leading to nanoparticles and nanoclusters, Vishal Kumar, Pillalamarri Srikrishnarka, Jyoti Sarita Mohanty, Murugesan Kannan, Ramamurthy Nagarajan, and Thalappil Pradeep, *ACS Sustainable Chem. Eng.*, 9 (2021) 7431–7436 (DOI: 10.1021/acssuschemeng.1c01586).
11. Gold cluster-loaded dendritic nanosilica: single particle luminescence and catalytic properties in the bulk, Jyoti Sarita Mohanty, Ayan Maity, Tripti Ahuja, Kamalesh Chaudhari, Pillalamarri Srikrishnarka, Vivek Polshettiwar, and Thalappil Pradeep, *Nanoscale*, 13 (2021) 9788–9797 (DOI: 10.1039/d1nr00619c).
12. Transformation of nanodiamonds to onion-like carbons by ambient electrospray deposition, Deeksha Satyabola, Tripti Ahuja, Sandeep Bose, Biswajit Mondal, Pillalamarri Srikrishnarka, Murugesan Kannan, B. Krishnamurthy Spoorthi, and Thalappil Pradeep, *J. Phys. Chem. C*, (2021) (DOI: 10.1021/acs.jpcc.1c00166).
13. Ambient microdroplet annealing of nanoparticles, Angshuman Ray Chowdhuri, B. K. Spoorthi, Biswajit Mondal, Paulami Bose, Sandeep Bose, and Thalappil Pradeep, *Chem. Sci.*, 12 (2021) 6370–6377 (DOI: 10.1039/d1sc00112d).
14. Molecular materials through microdroplets: Synthesis of protein-protected luminescent clusters of noble metals, Sandeep Bose, Amit Chatterjee, Shantha Kumar Jenifer, Biswajit Mondal, Pillalamarri Srikrishnarka, Debasmita Ghosh, Angshuman Ray Chowdhuri, M. P. Kannan, Sailaja Elchuri, and Thalappil Pradeep, *ACS Sustainable Chem. Eng.*, 9 (2021) 4554–4563 (DOI: 10.1021/acssuschemeng.0c09145).
15. Facile crystallization of ice I<sub>h</sub> via formaldehyde hydrate in ultrahigh vacuum under cryogenic conditions, Jyotirmoy Ghosh, Gaurav Vishwakarma, Subhadip Das, and Thalappil Pradeep, *J. Phys. Chem. C*, 125 (2021) 4532–4539 (DOI: 10.1021/acs.jpcc.0c10367).



16. 2D-Molybdenum disulfide-derived ion source for mass spectrometry, Pallab Basuri, Sourav Jana, Biswajit Mondal, Tripti Ahuja, Keerthana Unni, Md Rabiul Islam, Subhashree Das, Jaydeb Chakrabarti, and Thalappil Pradeep, ACS Nano, 15 (2021) 523-531 (DOI: 10.1021/acsnano.0c09985).
17. Scalable drop-to-film condensation on a nanostructured hierarchical surface for enhanced humidity harvesting, Ankit Nagar, Ramesh Kumar, Pillalamarri Srikrishnarka, Tiju Thomas, and Thalappil Pradeep, ACS Appl. Nano Mater., 4 (2021) 1540-1550 (DOI: 10.1021/acsanm.0c03032).
18. Toward vibrational tomography of citrate on dynamically changing individual silver nanoparticles, Tripti Ahuja, Kamalesh Chaudhari, Ganesan Paramasivam, Gopi Ragupathy, Jyoti Sarita Mohanty, and Thalappil Pradeep, J. Phys. Chem. C, 125 (2021) 3553-3566 (DOI: 10.1021/acs.jpcc.0c09981).
19. Hierarchical assembly of atomically precise metal clusters as a luminescent strain sensor, Debasmita Ghosh, Mohd Azhardin Ganayee, Anirban Som, Pillalamarri Srikrishnarka, Nidhi Murali, Sandeep Bose, Amrita Chakraborty, Biswajit Mondal, Pijush Ghosh, and Thalappil Pradeep, ACS Appl. Mater. Interfaces, 125 (2021) 3256–3267 (DOI: 10.1021/acсами.0c19239).
20. Near-infrared chiral plasmonic microwires through precision assembly of gold nanorods on soft biotemplates, Amrita Chakraborty, Nonappa, Biswajit Mondal, Kamalesh Chaudhari, Heikki Rekola, Ville Hynninen, Mauri Kostainen, Robin Ras, and Thalappil Pradeep, J. Phys. Chem. C, 125 (2021) 3256-3267 (DOI: 10.1021/acs.jpcc.0c11512).
21. Selective extraction of gold by niacin, Abhijit Nag, Md Rabiul Islam, and Thalappil Pradeep, ACS Sustainable Chem. Eng., 9 (2021) 2129–2135 (DOI: 10.1021/acssuschemeng.0c07409).

## Collaborations with other groups

22. Design of a waste paper-derived chemically 'reactive' and durable functional material with tailorable mechanical property following an ambient and sustainable chemical approach, Arpita Shome, Adil Rather, Angana Borbora, Pillalamarri Srikrishnarka, Avijit Baidya, Thalappil Pradeep, and Uttam Manna, Chem. Asian J., 16 (2021) 1988-2001 (DOI: 10.1002/asia.202100475).
23. Kinetics of inter-cluster reactions between atomically precise noble metal clusters  $[Ag_{25}(DMBT)_{18}]^-$  and  $[Au_{25}(PET)_{18}]^-$  in room temperature solutions, Marco Neumaier, Ananya Baksi, Patrick Weis, Erik Schneider, Papri Chakraborty, Horst Hahn, Thalappil Pradeep and Manfred Kappes, J. Am. Chem. Soc., 143 (2021) 6969–6980 (DOI: 10.1021/jacs.1c01140).



## Editorials of 2021

### GUEST EDITORIAL

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www.small-journal.com

## Special Issue on “Nanoclusters”: A Glimpse into the Efforts to Redefine Matter at the Nanoscale

*Thalappil Pradeep*

24. Guest editorial on Special Issue on “Nanoclusters”: A Glimpse into the Efforts to Redefine Matter at the Nanoscale, Thalappil Pradeep, *Small*, 17 (2021) 2102931 (DOI:10.1002/smll.202102931).
25. Expectations for perspectives in ACS Sustainable Chemistry & Engineering, David T. Allen, D. Julie Carrier, Jingwen Chen, Nicholas Gathergood, Jinlong Gong, Hongxian Han, King Kuok (Mimi) Hii, Bing-Joe Hwang, Asha Liza James, Peter Licence, Michael Meier, Audrey Moores, Ryuhei Nakamura, Thalappil Pradeep, Bert Sels, Bala Subramaniam, Michael K. C. Tam, Lin Zhang, Julio F. Serrano, *ACS Sustainable Chem. Eng.*, 9 (2021) 16528–16530 (DOI:10.1021/acssuschemeng.1c07865).
26. Nanotechnology for Sustainability in ACS Sustainable Chemistry & Engineering: Some Pointers, Thalappil Pradeep, Zhenxing Li and Rafael Luque, *ACS Sustainable Chem. Eng.*, 9 (2021) 14327–14329. (DOI:10.1021/acssuschemeng.1c07031).
27. ACS Sustainable Chemistry & Engineering Welcomes Manuscripts on Advanced E-Waste Recycling, Lingen Zhang, Lingen Zhang, More by Lingen Zhang, Thalappil Pradeep, Peter Licence, Bala Subramaniam, and David T. Allen, *ACS Sustainable Chem. Eng.*, 9 (2021) 3624–3625 (DOI: 10.1021/acssuschemeng.1c01344).
28. The Power of the United Nations Sustainable Development Goals in Sustainable Chemistry and Engineering Research, Paul Anastas, Marcelo Nolasco, Francesca Kerton, Mary Kirchhoff, Peter Licence, Thalappil Pradeep, Bala Subramaniam, and Audrey Moores, *ACS Sustainable Chem. Eng.*, 9 (2021) 8015–8017 (DOI: 10.1021/acssuschemeng.1c03762).
29. Lab to Market: Where the Rubber Meets the Road for Sustainable Chemical Technologies, Bala Subramaniam, David Allen, King Kuok (Mimi) Hii, Juan Colberg, and Thalappil Pradeep, *ACS Sustainable Chem. Eng.*, 9 (2021) 2987–2989 (DOI: 10.1021/acssuschemeng.1c00980).



## General Articles

1. Personal news, Sanjay Bajpai (1965–2021), Ashutosh Sharma, Rajiv, K. Tayal Akhilesh Gupta, Neelima Alam, G. V. Raghunath Reddy, Vineet Saini, J. B. V. Reddy, Ranjith Krishna Pai, Ligy Philip, Prasada Raju, and T. Pradeep, Current Science, 120 (2021) 1790-1791.
2. A popular science article: Sritama Mukherjee and T. Pradeep, Water security through advanced materials, Emerging Technology Insight 2021, published by the Commonwealth Security Group, London. Available at: <https://www.commonwealthsecurity.org/emerging-technology-insight-2021>, pages 66-68.
3. Popular science article in Malayalam, *Keralam jnanasamoothathilekku valarumbol*, T. Pradeep, Deshabhimani Weekly, 30 (52) (2021) 8-13, December 5, 2021.

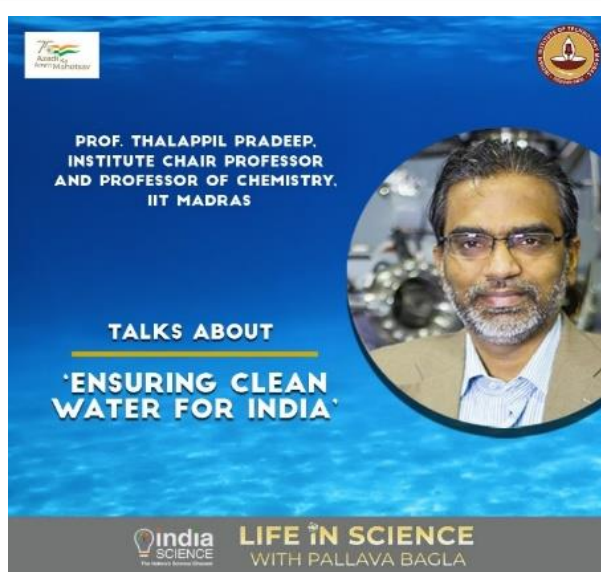


## Interviews



Prof. T. Pradeep has been interviewed by K. L. Jose, during November 2021, and an article based on the same appeared in Vol. 30, Issue 52, of Deshabhimani Weekly, December 5, 2021.

Link to the video:  
<https://www.indiascience.in/video/s/ensuring-clean-water-for-india-e-25-slash-9-slash-2021>



Prof. T. Pradeep has been interviewed by Pallava Bagla on Ensuring clean water for India and the video was shown on Rajyasabha TV in the series, IndiaScience, September 20, 2021.

## Patents

### Indian Patents (Granted)

1. A method of ionization on a 2D-nanostructured surface, T. Pradeep, Pallab Basuri, Sourav Kanti Jana and Biswajit Mondal, application no. 202141004464, dated February 02, 2021, issued as patent no. 383701, dated December 03, 2021.
2. Ambient microdroplet annealing method for converting polydispersed nanoparticles to their monodispersed analogues, T. Pradeep, Angshuman Ray Chowdhuri, B. K. Spoorthi, Biswajit Mondal, Paulami Bose and Sandeep Bose application no. 202041056735, dated December 28, 2020, issued as patent no. 377934, dated September 27, 2021.
3. A green method for preparing robust and sustainable cellulose-polyaniline based nanocomposite for effective removal of fluoride from water and a purifier thereof, T. Pradeep and Sritama Mukherjee, application no. 201941046691, dated November 15, 2019, issued as patent no. 376317, dated September 2, 2021.
4. Patterned metallic nanobrushes for capture of atmospheric humidity, Thalappil Pradeep, Depanjan Sarkar, Anindita Mahapatra, Anirban Som and Avijit Baidya, application no. 201641044759, dated December 29, 2016, issued as patent no. 375956, dated August 31, 2021.
5. Method for selective extraction of gold by niacin, Thalappil Pradeep and Abhijit Nag, application no. 202041047984, dated November 03, 2020, issued as patent no. 374251, dated August 10, 2021.
6. A portable water filtration device for removing impurities from water using contaminant - specific purification cartridges, T. Pradeep, Ramesh Kumar and Anupam Chandra, application no. 201741047404, dated December 30, 2017, issued as patent no. 373947 dated August 5, 2021.
7. A method to make unprotected naked clusters of metals of precise composition in air without mass selection, T. Pradeep, Ananya Baksi, Atanu Ghosh, Md Bodiuzzaman, Papri Chakraborty, Depanjan Sarkar, Pallab Basuri and Madhuri Jash, application no. 201641035574, dated October 18, 2016, issued as patent no. 369127, dated June 11, 2021.
8. Removal of lead from waste water using nanoscale MoS<sub>2</sub>, T. Pradeep, Biswajit Mondal, Ananthu Mahendranath, Anirban Som, Sandeep Bose, Tripti Ahuja, Avula Anil Kumar and Jyotirmoy Ghosh, application no. 201741044447, dated December 11, 2017, issued as patent no. 365164, dated April 22, 2021.
9. A process for low temperature, low pressure synthesis of gas hydrates, T. Pradeep, Jyotirmoy Ghosh, Rabin Rajan J. Methikkalam, Radha Gobinda Bhui, Gopi Ragupathy, Nilesh Choudhary and Rajnish Kumar, application no. 201841049836, dated December 29, 2018, issued as patent no. 356814, dated January 27, 2021.
10. Aqueous composition for durable and extremely efficient water repelling superhydrophobic materials at ambient condition thereof, T. Pradeep, Avijit Baidya, Azhar Ganayee and Jakka Ravindran Swathy, application no. 201741036772, dated October 17, 2017, complete specification filed on October 16, 2018, issued as patent no. 356023, dated January 18, 2021.



11. Method for creating nanopores in MoS<sub>2</sub> nanosheets by chemical drilling for disinfection of water under visible light, T. Pradeep, Depanjan Sarkar, Anirban Som, Biswajit Mondal and Jakka Ravindran Swathy, application no. 201741037148, dated October 20, 2017, issued as patent no. 356015, dated January 18, 2021.
12. Method of making nanoparticles of precise isotopic composition by rapid isotopic exchange, T. Pradeep, Papri Chakraborti and Esma Khatun, application no. 201741037349, dated October 23, 2017, complete specification filed on October 23, 2018, issued as patent no. 355248, dated January 4, 2021.

## **Indian Patents (Applied)**

1. A luminescence-based method of detecting arsenic using atomically precise noble metal nanocluster and phosphine, T. Pradeep and Sritama Mukherjee, application no. 202141038227, dated August 24, 2021.
2. An electrode system for detection of free chlorine with differential oxidant response, T. Pradeep, Kamalesh Chaudhari, Tullio Servida, Vishnu Kannan, and B. K. Spoorthi, application no. 202141031970, dated July 15, 2021.
3. A compact, modular and scalable continuous-flow greywater sink for potable and non-potable uses, T. Pradeep, Ankit Nagar, and Md Rabiul Islam, application no. 202141054715, dated November 26, 2021.
4. Synthesis of copper sulfide nanostructures in brass coated steel cords used in radial tires under ambient conditions, T. Pradeep, A. Sreekumaran Nair, Arijit Jana, and C. M. Cherian, application no. 202141047183, dated December 15, 2021.

## **PCT (Applied)**

1. A point-of-care (poc) amperometric device for selective arsenic, T. Pradeep, Sourav Kanti Jana, Kamalesh Chaudhari, Md Rabiul Islam, application no. PCT/IN2021/050496, dated December 9, 2021.
2. Method for selective extraction of gold by niacin, T. Pradeep, Abhijit Nag, application no. PCT/IN2021/051021, dated October 27, 2021.

## Degree Holders

- ❖ **Dr. Madhuri Jash**, Department of Chemistry, IIT Madras.  
'Investigations of phosphine protected silver clusters and their alloys in the gas phase and in solution'.
- ❖ **Dr. Amrita Chakraborty**, Department of Chemistry, IIT Madras.  
'Chemical interactions between nanoscale systems: Novel structures and emerging properties'.
- ❖ **Dr. Sandeep Bose**, Department of Chemistry, IIT Madras.  
'Electrospray deposition: A route to functional nanomaterials'.
- ❖ **Dr. Sritama Mukharjee**, Department of Chemistry, IIT Madras.  
'Towards sustainable engineered nanomaterials for affordable clean water'.
- ❖ **Dr. K. S. Sugi**, Department of Chemistry, IIT Madras.  
'Atomically precise nanocluster-based materials: Emerging properties'.
- ❖ **Dr. Md Rabiul Islam**, Department of Chemistry, IIT Madras.  
'Graphenic materials for affordable clean water'.
- ❖ **Dr. Sudhakar Chennu**, Department of Chemistry, IIT Madras.  
'Interactions of As(III), As(V), P(III) and P(V) ions with iron oxide-based materials'.



Dr. Madhuri Jash



Dr. Sritama Mukharjee



Dr. Md Rabiul Islam



Dr. Amrita Chakraborty



Dr. K. S. Sugi



Dr. Sudhakar Chennu



Dr. Sandeep Bose

## Lectures Delivered (Mostly Online)

1. Affordable clean water using advanced materials, SUNRISE Symposium, UK Resaerch and Innovation, February 21, 2021.
2. Molecular chemistry of nanoparticles, Savitribhai Phule Pune University and Amity, February 25, 2021.
3. Nanotechnology for clean water, Centre for Water Resources Development and Management, March 1, 2021.
4. Atomically precise clusters, Monthly discussion meeting at IITM, March 20, 2021.
5. Advanced materials for clean water, Science Academies' Lecture Workshop, Kongu Engineering college, Perundurai, April 8, 2021.
6. Affordable clean water - evolving technology landscale, International Advanced Research Centre for Powder Metallurgy and New Materials, April 9, 2021.
7. Affordable clean water using advanced materials, Future of Asia Symposium , Nikkei Asia Award Presentation, May 21, 2021.
8. Clean water using nanotechnology - current statusThe National Academy of Sciences India, Allahabad, June 5, 2021.
9. Affordable clean water using advanced materials, Rajiv Gandhi University of Knowledge Technologies, Nuzvid, June 13, 2021.
10. Molecular chemistry of nanoparticles, B. Borooah College, June 17, 2021.
11. Transforming colleges through reserach, Stella Maris College, June 24, 2021.
12. Water!, Vidyashilp Academy, July 13, 2021.
13. Molecular clusters of noble metals, IIT BHU, July 15, 2021.
14. Nanotechnology for improving availability and quality of water, International Life Sciences Institute, India July 26, 2021.
15. Knowledge society: Third Murali master memorial lecture, August 1, 2021.
16. Nanotechnology for clean water, Charotar University, August 7, 2021.
17. Nanotechnology for cleanwater at IITM, Nanotechnology Research and Innovation Bootcamp 2021, August 11, 2021.
18. Clean water - Challenges and opportunities, IIT Madras Siddhi Lecture, August 13, 2021.
19. Nanomaterials for clean water, Tolani College, Kachchh, August 25, 2021.
20. Nanoparticles are molecules, September 3-5, Indo-Japan virtual workshop on cluster science by interdisciplinary approach Emerging materials and phenomena, September 3, 2021.
21. Molecular clusters of noble metals, Chemical Research Society of India, Kolkata, September 29, 2021.
22. Nanomaterials for clean water - Science & Research Opportunities in India, October 2, 2021.
23. Advanced materials for clean water, Rajiv Gandhi Centre for Biotechnology, October 13, 2021.
24. Nanoparticles are molecules, Bhabha Atomic Research Centre, October 20, 2021.
25. Nanoparticles are molecules, IITD - Ashok Ganguli Symposium, Kasauli, October 26, 2021. (Physical meeting)
26. Microdroplet synthesis, Emerging Frontiers in Chemical Sciences, Farook College, October 29, 2021.
27. Atomically precise clusters of noble metals, International Conference on Advanced Materilas and Mechanical Characterization, December 2, 2021.



28. Advanced materials for clean water AISYWLC'2021 December 18, 2021.

29. Affordable clean water using advanced materials, National Conference on Recent Trends in Materials Science, Indian Institute of Space Science and Technology, Thiruvananthapuram, December 29, 2021.

## Students' Recognitions

1. **Dr. Amrita Chakraborty** received Institute research award in recognition for her excellent Ph.D. work by Indian Institute of Technology Madras for the semester January-May, 2021.
2. **Dr. Tripti Ahuja** received AWSAR award by the Department of Science and Technology (DST) on National Science Day (NSD) on popular science writing for research on March 13, 2021.
3. **Ankit Nagar** and **Dr. Md Rabiul Islam** were awarded SRISTI-GYTI appreciation award 2021 for their work on 'Greywater Sink for Potable and Non-potable Use' on October 18, 2021.
4. **Arijit Jana** received the best poster award for 'A Hexagonal Propeller-shaped Silver Nanomolecule' at RSC Chemical Science Symposium 2021 held by JNCASR, Bengaluru during December 12-15, 2021.
5. **Ankit Nagar** was awarded the best flash talk sponsored by ACS, in ICANN2021 Conference, December 14-17, 2021.

## Students' Activities

1. **Gaurav Vishwakarma** delivered a talk on 'Early crystallization of water in ultrahigh vacuum under cryogenic temperatures' organized by Atomic Molecular and Optical Physics Division, PRL, Ahmedabad, May 13, 2021.
2. **Paulami Bose** presented a flash talk in ICANN2021 on 'Atom transfer between precision nanoclusters and polydispersed nanoparticles: A facile route for monodispersed alloy nanoparticles and their superstructures', December 14-17, 2021.
3. **Tanvi Gupte** presented a poster on 'Highly-sensitive  $\text{As}^{3+}$  detection using electrodeposited nanostructured  $\text{MnO}_x$  and phase evolution of the active material during sensing' in ChemSci 2021: Leaders in the field symposium, December 13-15, 2021.
4. **Arijit Jana** presented a talk on 'Light-triggered interconversion of carborane thiol-protected silver nanoclusters' at the Indo-Japan virtual workshop on cluster science by interdisciplinary approach: Emerging materials and phenomena, September 4, 2021.
5. **Arijit Jana** presented a flash talk in ICANN2021 on 'Carborane thiol protected hexagonal propeller-shaped silver nanomolecule with bidirectional rotational orientation', December 14-17, 2021.
6. **Tanvi Gupte** presented a flash talk in ICANN2021 on 'Highly-sensitive  $\text{As}^{3+}$  detection using electrodeposited nanostructured  $\text{MnO}_x$  and phase evolution of the active material during sensing', December 14-17, 2021.
7. **Jayoti Roy** presented a poster on 'Gas phase ion chemistry of titanium-oxofullerene with ligated solvents' at the "International Conference on Advanced Materials and Mechanical Characterization (ICAMMC-2021)", December 2-4, 2021.
8. **Jayoti Roy** presented a poster on 'Gas phase ion chemistry of titanium-oxofullerene with ligated solvents' at "ChemSci 2021: Leaders in the Field Symposium", December 13-15, 2021.

9. **B. K. Spoorthi** presented a poster on “Ambient microdroplet annealing of nanoparticles” at “ChemSci 2021: Leaders in The Field Symposium”, December 13-15.

## Alumni News

1. **Dr. C. Subramaniam** was awarded a Swarnajayanti Fellowship.
2. **Dr. Indranath Chakraborty** was appointed as an Assistant Professor at the Department of Chemistry, IIT Mandi, Himachal Pradesh, India.
3. **Dr. E. S. Shibu** was appointed as an Assistant Professor at the Department of Nanoscience and Technology, University of Calicut, Kerala, India.
4. **Dr. Sathya Ramalingam** was appointed as Scientist at Department of Leather Process Technology, CSIR - Central Leather Research Institute (CLRI), Chennai, India.
5. **Dr. N. Pugazhenthiran** was appointed as an Assistant Professor at the Department of Chemistry, Federico Santa María Technical University, Valparaíso, Chile, South America.
6. **Dr. Soumabha Bag** was appointed as an Assistant Professor at the Department of Industrial Chemistry, Mizoram University, Mizoram, India.
7. **Dr. Aditi Chandrasekhar** was awarded the IISER Kolkata alumni award.
8. **Prof. Bindhu Alappat** was appointed as the Interim Dean, College of Arts & Sciences, St. Xavier University, Chicago.
9. **Dr. K. R. Krishnadas** joined as a post doc at CIC biomaGUNE, Spain.
10. **Dr. K. S. Sugi** joined as a post doc at the Institute of Physical and Theoretical Chemistry, University of Tuebingen, Germany.
11. **Dr. Rahul Narayanan** joined as a post doc at the Department of Pharmaceutical Sciences, University of Illinois, Chicago, USA.
12. **Dr. Abhijit Nag** joined as a post doc at the Department of Chemistry, University of Edinburgh, UK.
13. **Dr. Mohammad Bodiuzzaman** joined as a post doc at the Department of Chemistry, University of Massachusetts, Massachusetts, USA.
14. **Dr. Tripti Ahuja** joined as a post doc at the Department of Chemistry, IIT Delhi, New Delhi, India.
15. **Dr. Esma Khatun** joined as a post doc at the Department of Chemical & Materials Engineering, University of Alberta, Edmonton, Alberta, Canada.
16. **Dr. Sritama Mukherjee** joined as a post doc at the Department of Bioproducts and Biosystems, Aalto University, Otaranta, Finland.
17. **Dr. Amrita Chakraborty** joined as a post doc at the Department of Chemistry, Rice University, Houston, Texas, USA.
18. **Mr. Sathvik Ajay Iyengar** joined as a PhD student at the Department of Materials Science and Nano Engineering, Rice University, Houston, Texas, USA.

## Research Grants

### Ongoing projects

1. National facility of cryo-electron microscopy: Remotely operable, 24x7 for academia and industry, SERB, Rs. 28.6 crores (principal investigator) with IIT Tirupati, IISER Tirupati, IIT Palakkad, RGCB Thiruvananthapuram, Sastra Thanjavur, VIT Vellore and MRF Chennai.
2. Carborane - protected metal nanoclusters: A new family of materials with atomic precision - DST/Czech 37 lakhs (principal investigator).
3. DST-JSPS joint workshop on cluster science by interdisciplinary approach: Emerging materials and phenomena - DST-JSPS (conference proposal, principal investigator).
4. Identification and investigation of efficacy of potential biochemical molecules for extraction of gold and other noble metals from tailings and waste sources, Ministry of Mines, Rs. 34.64 lakhs (principal investigator).
5. Chemical transformations of clathrate hydrates under ultra-high vacuum, Department of Science and Technology, CRG grant, Rs. 76.5 lakhs (principal investigator).
6. Understanding surface properties of atomically engineered cluster-assembled solids, SPARC project with Robin Ras and Olli Ikkala, Aalto, Finland with Tiju Thomas, IITM, Rs. 66.3 lakhs (principal investigator).
7. SUTRAM for EASY water, DST, Rs. 890 lakhs (co-principal investigator with Prof. Ligy Philip).
8. Cluster composite nanofibre membranes for rapid, ultra-trace detection of waterborne contaminants, India-German Science and Technology Forum, Rs. 191.324 lakhs (principal investigator along with InnoNano Research Pvt. Ltd).
9. VAJRA project with Pulickel M. Ajayan, Rice University, Rs. 9.75 lakhs.
10. Affordable clean water in arsenic affected areas, Millennium Alliance, 2018-2020, Rs. 50 lakhs (principal investigator along with Ramesh Kumar).
11. Dust free glass, Saint-Gobain Research India Ltd. Rs. 36 lakhs (principal investigator with Prof. R. Nagarajan).

### Projects approved this year

1. Fingerprinting authenticity of ayurvedic preparations using ambient electrospray deposition raman spectroscopy (AERS), a home-grown method for rapid analysis, DST, Rs. 93 lakhs (principal investigator), along with Santhosh Chidangil, Manipal Academy of Higher Education (co-principal investigator).
2. Sustainable ion exchange resin-based technology for rare earth extraction, Ministry of Mines, Rs. 52 lakhs (principal investigator).
3. 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).
4. pCoE on Molecular Materials and Functions, IIT Madras, Rs. 5.80 crores (principal investigator) with colleagues from IITM and other institutions (details below).
5. JC Bose Fellowship, Department of Science and Technology, 90 lakhs as (principal investigator), renewed.
6. VAJRA project with Prof. Graham Cooks, Purdue University.



## Consultancy

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

## Implementation Projects

1. Providing, fixing and maintenance of nano material-based household water purifiers for providing in arsenic affected habitations of Punjab, Government of Punjab, Rs. 48.5 crores (principal investigator), undertaken by ICCW.
2. House-hold arsenic removal units for Government of Punjab, Rs. 4.8 crores (principal investigator), undertaken by ICCW.

## Visitors

1. Ms. Nikita Sampath and Mr. Vinayak, Krea University, January 19, 2021.
2. Mr. Thomas Pallushek, founder & principal of the school, Ms. Sathya, Director of Education, Mr. Infant Carmel Reju, March 13, 2021.
3. Mr. A. Jayakumar, Vijnana Bharati and his friend from Amrita University- June 26th, 2021.



Prof. Pradeep with Prof. Pulickel M. Ajayan,  
December 27, 2021.

4. Ms. Shreya and Dr. Tuhin, IISc, Bengaluru, September 10, 2021.
5. Mr. Vipul Mathur and Mr. NP Seetharaman, Hindustan Unilever, September 8, 2021.
6. Prof. Pulickel M. Ajayan, Rice University, December 27, 2021.



Prof. Pradeep with Mr. A. Jayakumar, Vijnana Bharati,  
June 26, 2021.

## Visits

1. Institute of Nano Science and Technology (INST), Chandigarh, October 24, 2021.
2. International hybrid meeting on physics and chemistry of advanced materials (PCAM), Kasauli, October 25, 2021.
3. Visit to Rashtrapati Bhavan, New Delhi to receive the Padma Shri Award, November 8, 2021.
4. Meeting with Chief Minister of Kerala on launching the logo on higher education reforms, Thiruvananthapuram, December 2, 2021.



Logo launch by the Chief Minister and the Higher Education Minister of Kerala, along with members of the reforms commission, Thiruvananthapuram, December 2, 2021.



Receiving Padma Shri award from the President of India, November 8, 2021.

## Services

- ❖ Member, India-Japan Council of the Department of Science and Technology, 2014-
- ❖ Vice President, Indian Society for Mass Spectrometry, 2014-
- ❖ Member, Executive Committee, Neutron Scattering Society of India, 2011-
- ❖ Member of the Council of Materials Research Society of India, 2011 –
- ❖ Member, Board of studies, Manipal University, 2012-
- ❖ Member, Program Advisory Committee of Inorganic and Physical Chemistry, DST, 2018-2021
- ❖ 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-
- ❖ Member, Editorial Board of the journals; Chemistry of Materials, ACS Nano, Analytical Chemistry, Nanoscale, Particle, Surface Innovations, International Journal of Water and Wastewater Treatment, Nanoscale Advances, and Chemical Communications.
- ❖ Associate Editor of the journal, ACS Sustainable Chemistry & Engineering, 2014-

## Upcoming Facilities to Lab

### Centre for Molecular Materials and Functions\*

We aim to create a globally recognized Centre focusing on the synthesis and study of molecular materials, where the fundamental building blocks are molecules, rather than atoms. Initially, we aim at specializing in two exciting and important family of molecular materials; those assembled from metallic clusters and those assembled from gas hydrate cages. However, as additional capabilities are established, we will also expand our activities into other kinds of molecular materials, including supramolecular polymers, energy harvesting assemblies, molecular metals and molecular magnets. Important strides have already been made in atomically precise metal clusters containing tens to hundreds of atoms; the participating groups have been among the leaders in this area.

\*In collaborations with Pulikkel M. Ajayan (Rice University, USA), Tomas Base (Institute of Inorganic Chemistry, Czech Republic), R. G. Cooks (Purdue University, USA), Pijush Ghosh (IIT Madras, India), Sundargopal Ghosh (IIT Madras, India), Horst Hah (KIT, Germany), Hannu Häkkinen (University of Jyväskylä, Finland), Manfred Kappes (KIT, Germany), Rajnish Kumar (IIT Madras, India), Praveen Linga (NUS, Singapore), Shobhana Narsimhan (JNCASR, India), Robin Ras (Aalto University, Finland), Tatsuya Tsukuda (University of Tokyo, Japan), Umesh Waghmare (JNCASR, India), Robert L. Whetten (NAU, USA), Jianping Xie (NUS, Singapore).



Instrument being purchased: Ultra-High-Resolution - Hybrid Quadrupole-Orbitrap Mass Spectrometer of ThermoFisher Scientific



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



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

Instruments being purchased: ThermoFisher Scientific Krios G4 300 kV and Talos 200 kV, ThermoFisher Scientific.

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



Artistic view of the building for housing the Cryo-EM facility.

## Incubation

- Hydromaterials** installed 698 community water treatment units in 2020, each supplying arsenic and iron free water to over 900,000 people. Altogether there are 961 units of this kind operational in the country, supplying clean water to 1.2 million people. This year's highlight is the internet-of-things (IoT) enabled community units. Over 100 units of this kind will be completed soon, many are already functional. A picture of one such unit in Amritsar District of Punjab is shown on the right. There are other types of installations too. Amrit technology has been approved by the Jal Shakti Ministry.



Hydromaterials recognized as the Best Startup with deep social impact for the year 2021. The award was given by FICCI-New Indian express (on the right).



(LPD) atmospheric water harvesting unit at Engineers India Limited, Gurugram, Haryana. They have now 30, 100, 400, and 1000 LPD units in production. Shown on the right is a view of the factory.

- InnoNano Research Private Limited** is an IIT Madras-incubated company which developed AMRIT, acronym for Anion and Metal Removal by Indian Technology. AMRIT is an affordable nanotechnology-based water purifier to dispense safe and affordable drinking water at a cost <5 paise/litre. It was first introduced in the villages of Murshidabad district in West Bengal after the Arsenic Task Force of the Government of West Bengal certified and

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

- Vayujal** Technologies has installed a 2000 litres per day



approved its use. AMRIT is installed in 2000 locations in West Bengal, Uttar Pradesh, Bihar and Karnataka providing arsenic-free drinking water to nearly 8 lakh beneficiaries. The company is not active now.

- **AquEasy Innovations Private Limited** is an Indian company incubated by IIT Madras working in the field of domestic water purification 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. EyeNetAqua works with IIT Madras' consortium on sensors to integrate as well as develop new technologies for water quality monitoring. EyeNetAqua has developed and demonstrated a prototype of an online water quality monitoring unit at ICT Grand Challenge 2020 arranged by MeitY (CDAC, Bangalore). Further, a product is being developed as per JJM specifications for the inline measurements of pH, TDS, Residual chlorine, Nitrate, Fluoride, pressure and water volume of flow. The company is actively working towards the lab-to-field translation of low-cost portable devices for fluoride, free chlorine and arsenic in field conditions.
- A new initiative of IIT Madras, the **International Centre for Clean Water** made tremendous progress in all its activities. We have initiated research, implementation, outreach and incubation activities. An overview of these efforts is available [here](#). Key to these initiatives is the support of all our well-wishers, well-meaning individuals, Companies well as institutions. Annual report of ICCW may be viewed [here](#).

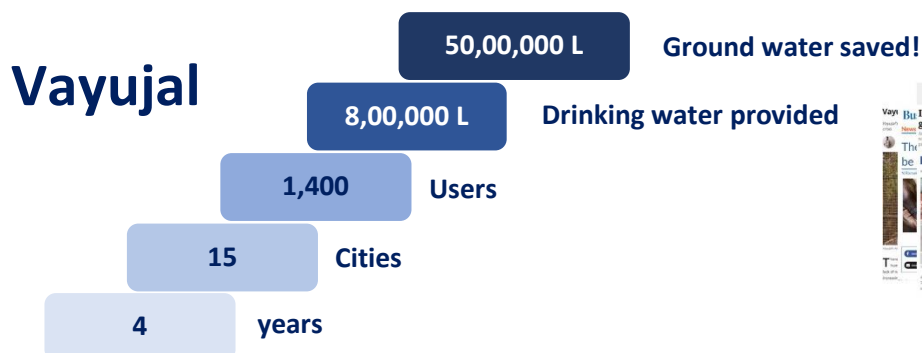


All are co-owned by IIT Madras.



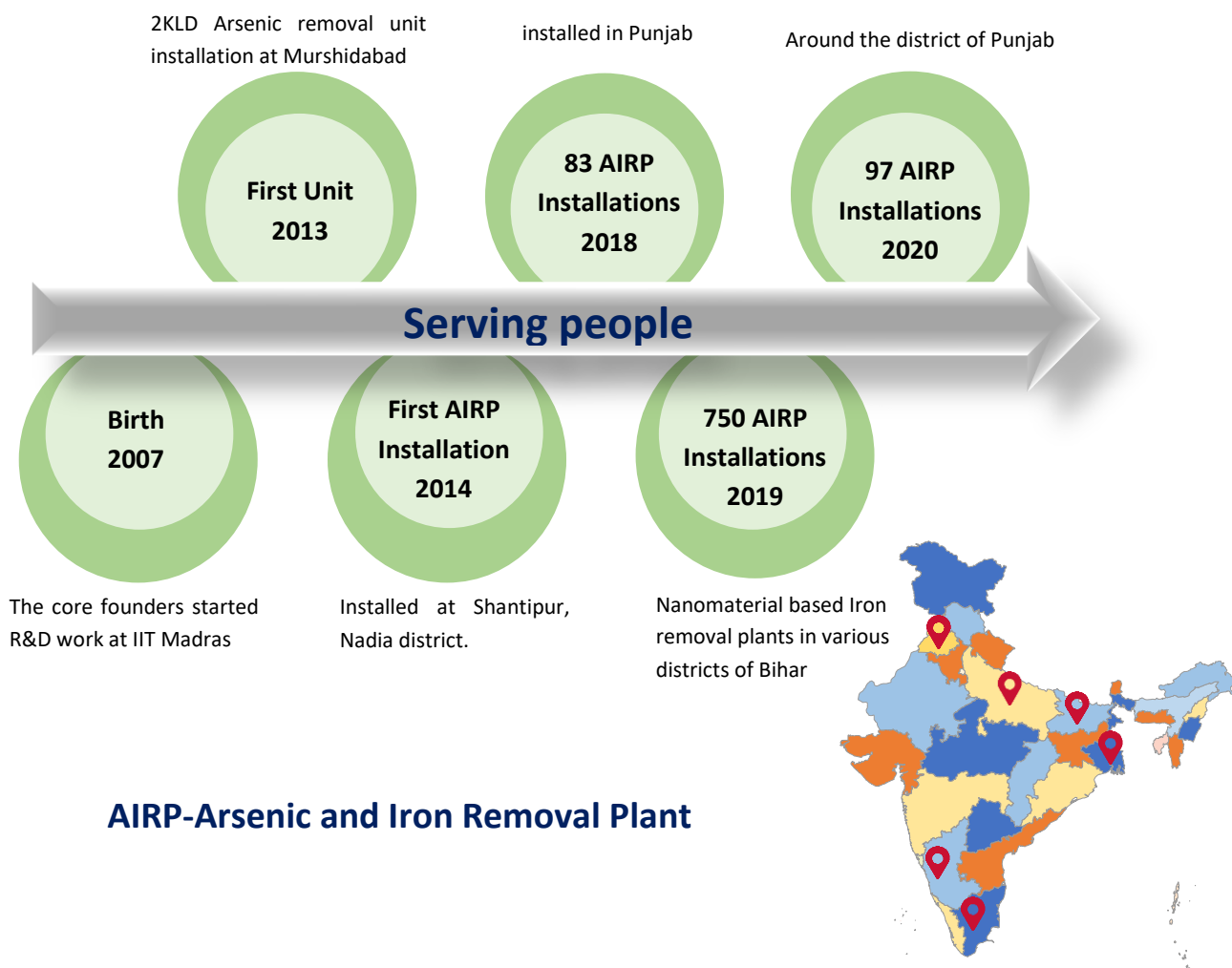


## Reach of some of our Technologies



Media on Vayujal

## AMRIT-Anion and Metal Removal by Indian Technology





# Media Reports

KERALA

## Three panels to overhaul higher education sector



STAFF REPORTER

September 9, 2021

SHARE ARTICLE



To study and bring in reforms that are in tune with the changing times

The Higher Education Department has constituted three commissions in a bid to modernise the sector that has been deemed outdated in several respects.

Shyam B. Menon, former Vice Chancellor, Ambedkar University, New Delhi, will head a seven-member commission to suggest reforms in the field of higher education in the State. The panel will be convened by Shanti Swarup Bhatnagar Prize recipient Pradeep T., professor, IIT Madras; and have noted academics, including Mahatma Gandhi University Vice Chancellor Sabu Thomas; Ayesha Kidwai of Jawaharlal Nehru University; State Planning Board member R. Ramkumar; Kannur University Pro-Vice Chancellor Sabu A.; and M.V. Narayanan of Calicut University.

## From lab to field: IIT-M start-up takes clean water to people

March 30, 2021



Prof. Pradeep Thalappil has enabled clean water technologies to reach people through the VayuJal start-up (Photo courtesy: IIT-M website)

▲ Rahul Kumar Published: 30-03-2021 11:04 AM 5 min read

Clean water initiatives driven by IIT-M are making their way to the people, successfully bring the lab to the field. In a unique collaboration between professors and students, research from the labs is changing people's lives.

One such innovation is the Atmospheric Water Generator (AWG), which has been created using nano-technology.

Prof. K. VijayRaghavan, Principal Scientific Adviser to the Government of India, says: "Safe and readily-available water is the mark of a healthy society and also the primary responsibility of those working in public health. The VayuJal technology is an example by innovators to solve real-world problems."

He adds that scaling up the availability of such water technologies will help improve the health of people.

## INCUBATING DEEP TECH



With 240 startups valued at ₹10.5k or incubated over 8 years, IIT Madras is India's hi-tech haven by **Dia Rekhi & Alnoor Peermohamed**

VAYUJAL TECHNOLOGIES

VayuJal Technologies, a start-up from IIT Madras, has developed a water purifier that can purify water from any source, including tap water, rainwater, and even seawater. The device is called VayuJal and is designed to be used in rural areas where access to clean water is a challenge. It is a portable, solar-powered device that can purify up to 100 litres of water per day. The device is made of stainless steel and is easy to use. It is also very durable and can last for many years. The device is currently being used in several villages in Tamil Nadu and Karnataka. It has helped many people to have access to clean water and has improved their health. The device is also being used in schools and hospitals. It is a great example of how technology can be used to solve real-world problems.



Dia Rekhi and Alnoor Peermohamed

Founders of VayuJal Technologies



EPICURE COMPANY

Founders of Epicure Company

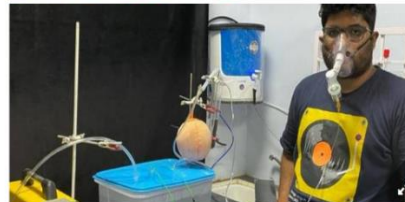
News

OXYGEN INNOVATIONS

April 26, 2021

## Coming, DIY oxygen kits, using off-the-shelf materials

TV Jayan | New Delhi | Updated on April 26, 2021



Pradeep's research student Srikrishnarka Pillalamarri demonstrating the prototype oxygen generator

Researchers at IIT Madras have fabricated a DIY kit that can generate oxygen sufficient for a patient in home care.

As the acute shortage of medical oxygen leaves hospitals across the country gasping, scientists at several

laboratories are trying to put together a kit that can help deliver the live-saving gas for critical patients at home or hospitals.

CHENNAI

## IISc honours IIT Madras professor



SPECIAL CORRESPONDENT

October 14, 2021

SHARE ARTICLE



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The Indian Institute of Science, Bengaluru, has awarded T. Pradeep, institute chair professor and professor of chemistry at the Indian Institute of Technology Madras, the Distinguished Alumnus Award for 2021, according to a post by IIT Madras in LinkedIn.

Mr. Pradeep completed his Ph.D in chemical physics from the IISc in 1991. He conceptualised and developed the International Centre for Clean Water at IIT Madras. He was conferred the Padma Shri in 2020.

THE HINDU

TAMIL NADU

## In Thoothukudi district, swipe a card to get potable water



R. Sujatha

October 14, 2021

SHARE ARTICLE



## Media Reports

**THE HINDU**  
FEBRUARY 25, 2021

## Nanosheets help in the detection of uric acid in urine, alcohol in breath

The device could detect alcohol concentrations of even less than 3% in breath

**ANAND PICHAI**

Simple but effective: Flowing urine over the nanostructured surface and measuring the current, the team detected uric acid in the urine of a healthy individual.

with the flowing liquid on the MoS<sub>2</sub>-coated surface. A volunteer who had consumed 600 ml of beer containing 9% (v/v) alcohol blew over the paper, and the corresponding current was measured. While standard breath analysers detect breath alcohol concentration above 5%, this device could detect even less than 3%.

**Many applications**

The device can find many more applications: check glucose in blood, toxic chemicals in any liquid, pesticide or any contaminants in drinking water. The main plus point is that it can even detect very low levels. The current wet chemical or reagent-based methods are lengthy and require skilled labour. The new method is cost-effective, and all you need is simple paper coated with nanostructures. By just flowing the liquid and studying the spectrum, molecular detection has now been made simple and easy," adds the first author of the paper Pallab Basu, a PhD scholar at the institute.

**Man's old friend**

**Did dogs migrate with humans to the Americas?**

A bone fragment discovered from southwest Alaska has now answered a few questions on dog migration into the Americas. Researchers found that the thigh bone belonged to a dog that lived in the region about 10,150 years ago. Scientists say the remains represent the oldest confirmed remains of a domestic dog in the Americas. Analysis of the mitochondrial genome revealed that the dog belonged to a lineage of dogs that diverged from Siberian dogs. Researchers of the Royal Society B: Biological Sciences say in a release that this study provides not only the timing but also a location for the entry of dogs and people into the Americas.

**Sheet-like structures**

The team used a simple sheet of paper as a support material and coated it with 20-nm-thick MoS<sub>2</sub> nanosheets. The nanosheet generates a micro-high current of 1.3 microampere. The sample is to be tested can be mixed with the liquid and directly

**rat to diversity**

Two were some of the first animals to diversify in this post-mass extinction world, taking advantage of a forest canopy. Mantella

**February 25, 2021**

### Five scientists, engineers get IISc's Distinguished Alumnus Award

Professor C S Raghavendra is known for his significant contributions to the design and analysis of interconnection networks

Akhil Kaddal, DMNS, Bengaluru, OCT 13 2021, 12:37:01 | UPDATED

**October 13, 2021**

**Coffee Sciences**  
@Coffee\_Sciences

## Looking into Ice transformations in the Interstellar medium

[disq.us/t/42coxa4](https://disq.us/t/42coxa4)

Brief outtake from the publication of [@GAURAVV61504672](https://doi.org/10.1038/s41586-021-03404-4). In his recent publication, he recreated interstellar media in the lab and studied various forms of ice.

**October 28, 2021**

### Prof Subramaniam Chandramouli receives the prestigious Swarnajayanti Fellowship for 2021

Tweet Like Retweet Share

Susheela

Read time: 4 mins

Mumbai Dec 8, 2021, (Research Matters):

**December 8, 2021**



**Tweet**

**Coffee Sciences**  
@Coffee\_Sciences

With the successive launch of the JWST, the need for the operation in the IR region is expressed by [@GAURAVV61504672](https://doi.org/10.1038/s41586-021-03404-4). "James Webb space telescope: Deploying IR spectrometer in space" [coffeeandsciences.com/f/james-webb-s...](https://coffeeandsciences.com/f/james-webb-s...) via [@Coffee\\_Sciences](https://twitter.com/Coffee_Sciences)

coffeeandsciences.com

James Webb space telescope: Deploying IR spectrometer in... James Webb space telescope (JWST) is a telescope designed to work in space while performing almost all its observation...

**c&en**  
CHEMICAL & ENGINEERING NEWS

TOPICS MAGAZINE COLLECTIONS VIDEOS JOBS

**MASS SPECTROMETRY**

**February 28, 2021**

## Ionization source for mass spectrometry needs no external power supply

Device could have applications for portable instruments

by Celia Henry Arnaud  
FEBRUARY 28, 2021 | APPEARED IN VOLUME 99, ISSUE 7

A 2D MoS<sub>2</sub>-coated paper can be used as an ionization source for mass spectrometry.

### Please visit the links for full articles

- <https://www.thehindu.com/news/national/kerala/three-panels-to-overhaul-higher-education-sector/article36383763.ece>
- <https://www.thehindubusinessline.com/news/coming-diy-oxygen-kits-using-off-the-shelf-materials/article34408486.ece>
- <https://www.indianarrative.com/india-news/from-lab-to-field-iit-m-start-up-takes-clean-water-to-people-77282.html>
- <https://www.thehindu.com/news/cities/chennai/iisc-honours-iit-madras-professor/article36996226.ece#:~:text=The%20Indian%20Institute%20of%20Science,by%20IIT%20Madras%20in%20LinkedIn>
- <https://www.thehindu.com/news/national/tamil-nadu/in-thoothukudi-district-swipe-a-card-to-get-potable-water/article34214923.ece#:~:text=Two%20village%20panchayats%20in%20Thoothukudi,card%20for%20a%20nominal%20payment>
- <https://binj.in/science/nanosheets-help-in-the-detection-of-uric-acid-in-urine-alcohol-in-breath/>
- <https://researchmatters.in/news/prof-subramaniam-chandramouli-receives-prestigious-swarnajayanti-fellowship-2021>



## Initiatives

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

### 1. Theory-Experiment Interface

#### Session 01 – 20/03/2021

1. **Prof. T. Pradeep**, Department of Chemistry delivered a talk on “Atomically precise clusters”.
2. **Prof. Madhav Ranganathan**, Department of Chemistry delivered a talk on “Modeling shapes of semiconductor nanoparticles using atomistic and continuum approach”.
3. **Prof. Sundargopal Ghosh**, Department of Chemistry delivered a talk on “Molecular cluster: A combined experimental and theoretical approach”.
4. **Dr. Ranjit Kumar Nanda**, Department of Physics delivered a talk on “Atomistic modelling towards materials design through first principles methods”.

#### Session 02 – 17/04/2021

5. **Dr. Manu Jaiswal**, Department of Physics delivered a talk on “Mechanical instabilities and transport phenomena in two-dimensional systems”.
6. **Prof. Arti Dua**, Department of Chemistry delivered a talk on “Transients generate memory and break hyperbolicity in stochastic enzymatic networks”.
7. **Dr. Rajnish Kumar**, Department of Chemical Engineering delivered a talk on “Role of surfaces and additives on nucleation and growth of hydrate crystals”.
8. **Prof. Srinivasa Chakravarthy**, Department of Biotechnology delivered a talk on “Simplifying the Brain”.

#### Session 03– 22/05/2021

9. **Dr. Soumya Dutta**, Department of Electrical Engineering delivered a talk on “Organic Electronics: From Materials to Devices”.
10. **Dr. Ratna Kumar Annabattula**, Department of Mechanical Engineering delivered a talk on “Numerical Modeling of Photoresponsive Liquid Crystal Thin Film Systems as Soft Actuators”.
11. **Dr. Hema Chandra Kotamarthi**, Department of Chemistry delivered a talk on “Probing molecular mechanisms of enzymes, insights from single-molecule tools”.
12. **Dr. Tarak Patra**, Department of Chemical Engineering delivered a talk on “Integrating AI and molecular modelling for accelerating materials design”.

#### Session 04– 19/06/2021

13. **Prof. Sanjib Senapati**, Department of Biotechnology delivered a talk on ‘Biomolecular simulations at different scales from electronic to coarse-graining’.
14. **Prof. Sridharakumar Narasimhan**, Department of Chemical Engineering delivered a talk on “ Networks and experimental design”.
15. **Dr. Sumesh P. Thampi**, Department of Chemical Engineering delivered a talk on “Dilute and dense suspensions of active particles”
16. **Dr. Esma Khatun**, Department of Chemistry delivered a talk on “Atomically precise alloy nanoclusters”.

Session 05– 17/07/2021

17. **Prof. Pijush Ghosh**, Department of Applied Mechanics delivered a talk on “Solvent Triggered Actuation of Polymer Thin Film”.
18. **Prof. Ravindran B**, Department of Computer Science and Engineering delivered a talk on “Learning and inference with complex graph structures”.
19. **Dr. Athi N. Naganathan**, Department of Biotechnology delivered a talk on “Protein Folding, Assembly and Function: Working at the Interface of Physics, Chemistry and Biology”.
20. **Dr. Ethayaraja Mani**, Department of Chemical Engineering delivered a talk on “Self-assembly of colloids”.

Session 06– 21/08/2021

21. **Dr. Chaitanya Sharma Yamijala**, Department of Chemistry talk delivered a talk on “A Few Applications of the Adiabatic and Nonadiabatic Molecular Dynamics Methods”.
22. **Prof. Kannan A**, Department of Chemical Engineering delivered a talk on “Solar and Wind Aided Cross Flow Natural Evaporator for RO Reject Management”.
23. **Prof. Raghunathan Rengasamy**, Department Chemical Engineering delivered a talk on “Droplet microfluidic design through a dialog between computations and experiments”.
24. **Dr. Satyesh Kumar Yadav**, Department of Metallurgical and Materials Engineering delivered a talk on “Atomistic modelling of Materials”.

Session 07– 18/09/2021

25. **Dr. Pradeep K G**, Department of Metallurgical and Materials Engineering delivered a talk on “Cluster analysis at atomic scale”.
26. **Dr. Himanshu Goyal**, Department of Chemical Engineering delivered a talk on “High performance computing for clean energy technologies”.
27. **Dr. Jithin John Varghese**, Department Chemical Engineering delivered a talk on “Atomic Modelling for Catalysis”.
28. **Prof. Prabhu Rajagopal**, Department of Mechanical Engineering delivered a talk on “Phononic Metamaterials”.

Session 08– 23/10/2021

29. **Prof. Sachin S Gunthe**, Department of Civil Engineering delivered a talk on “Atmospheric Aerosols and Trace Gases in Indian Perspective: Impact on regional climate and ecosystem health”.
30. **Prof. Susy Varughese**, Department of Chemical Engineering delivered a talk on “Role of Calcium and Water in the Mechanics of Biomacromolecular Networks”.
31. **Prof. Ravi Kumar N V**, Department of Metallurgical and Materials Engineering delivered a talk on “Architectural Design of Technological Ceramics”.
32. **Dr. Tiju Thomas**, Department of Metallurgical and Materials Engineering delivered a talk on “Theory-Experiment Interface: Case Studies From 'Energy Nanoscience'”.

Session 09– 27/11/2021

33. **Dr. P. Venkatakrishnan**, Department of Chemistry delivered a talk on “Building Bridges and Forging Bonds for Functional Organics”.
34. **Mr. Kamal Kishor**, Department of Mechanical Engineering delivered a talk on “Seismic Metamaterials to Damp Low Frequency Surface Disturbances”.



35. **Dr. Ahana Purushothaman**, Department of Chemical Engineering delivered a talk on “Hydrodynamics of Channel Confined Micro Swimmers”.
36. **Mr. Sourav Kar**, Department of Chemistry delivered a talk on “Polyhedral Metallaborane Clusters in Materials Science”.

#### Session 10– 18/12/2021

37. **Prof. Srinivasa Rao Bakshi**, Department of Metallurgical and Materials Engineering delivered a talk on “Reactive Spark Plasma Sintering - Examples and Possibilities”.
38. **Dr. Pramoda Kumar Nayak**, Department of Physics delivered a talk on “Van der Waals Heterostructures”.
39. **Prof. Abhijit P. Deshpande**, Department of Chemical Engineering delivered a talk on “Complex Fluids Viscoelasticity-From Bulk Behaviour to Response at Small Length Scales”.

2. A book discussion on ‘Method in the Madness’ with the author, Parameswaran Iyer, currently with the World Bank, Washington DC, April 15, 2021.
3. Indo-Japan workshop on Cluster science by interdisciplinary approach: Emerging materials and phenomena, September 3-5, 2021.
4. Technical writing course, IITM, January 19, 2021.
5. Workshop on using Blender; an open-source 3D illustration software on August 5-8, 2021.
6. IITM Research initiative spotlight-Molecular materials and functions-Advanced materials.

Please visit our YouTube channel to access a glimpse of a few events [here](#)

7. A lecture series on Cryo-EM and related techniques, October 13-16, 2020 and December 8-11, 2020.

#### Lecture Series on Cryo-EM and Related Techniques (Season- I) 13-16<sup>th</sup> October



To watch the lecture series please visit our youtube channel:

[Prof. Miguel Jose Yacaman](#)

[Prof. Maia Azubel](#)

[Prof. Richard Palmer](#)

#### Lecture Series on Cryo-EM and Related Techniques (Season- II) 8-11<sup>th</sup> December



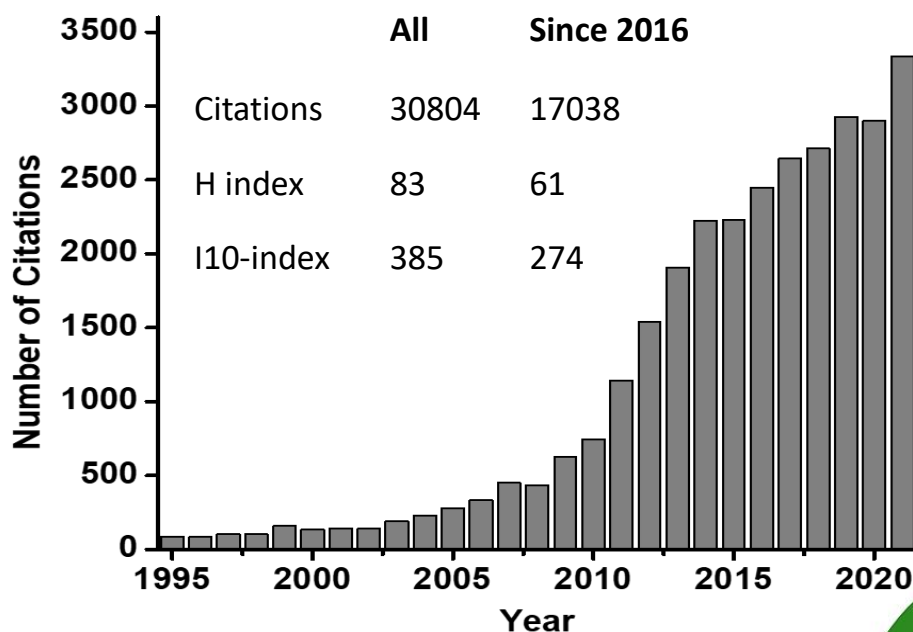
[Prof. Yi Cui](#)

[Prof. Yu Han](#)

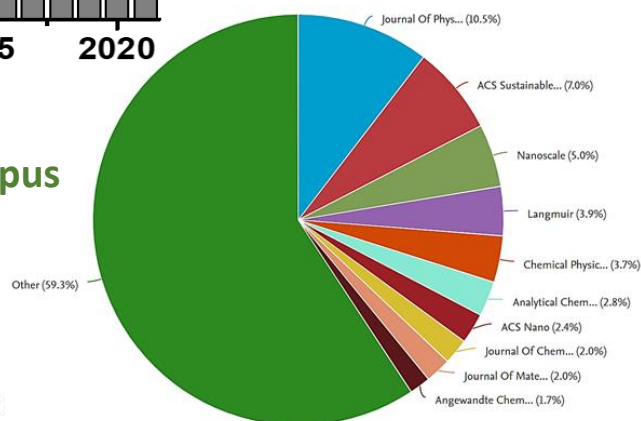
[Prof. Wah Chiu](#)

## Publication Analyses

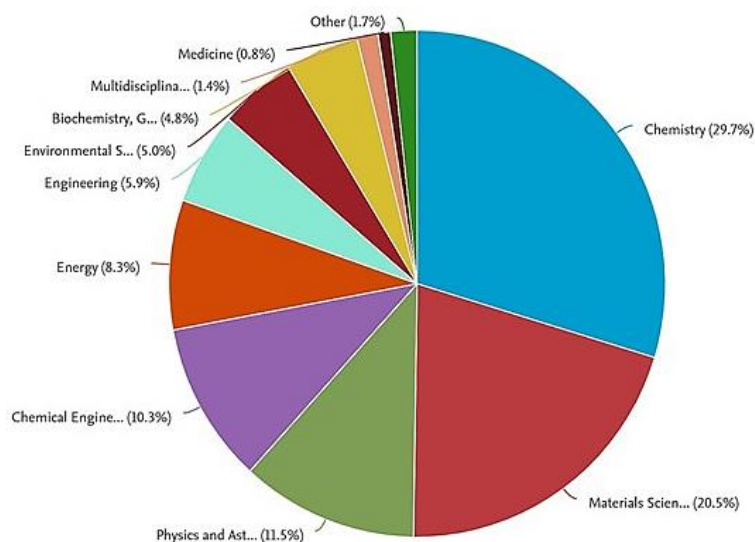
### Google Scholar



### By type - Scopus

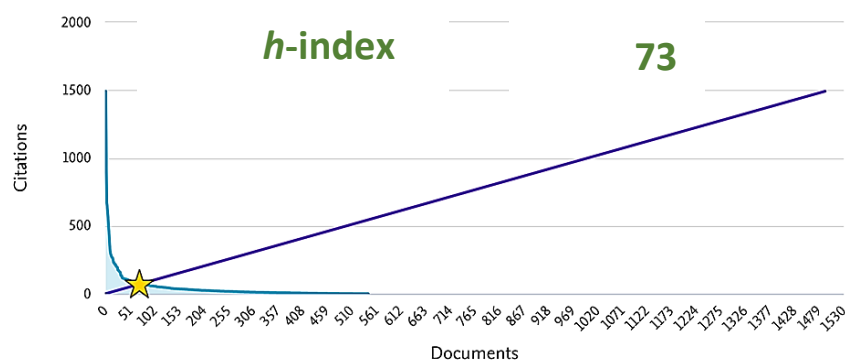


### Documents by subject area - Scopus



### Sources

1. Scopus, visited on December 31, 2021.
2. Google Scholar, visited on December 31, 2021.



## Abstracts at a Glance

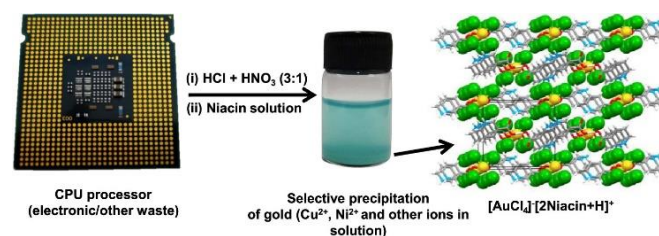
### Selective Extraction of Gold by Niacin

Abhijit Nag, Md Rabiul Islam, and Thalappil Pradeep

ACS Sustainable Chem. Eng. 2021, 9, 5, 2129–2135 (DOI:10.1021/acssuschemeng.0c07409)

**Abstract:** Gold recovery using a sustainable and inexpensive method has tremendous environmental and economic implications. We developed a highly cost-effective and sustainable method of gold extraction in which aqueous  $\text{Au}^{3+}$  is precipitated selectively as it is complex with the biomolecule niacin, having an overall formula,  $[\text{AuCl}_4]^- [2\text{Niacin} + \text{H}]^+$ , abbreviated as I. This selective precipitation occurs from mixtures of  $\text{Au}^{3+}$  with  $\text{Ni}^{2+}$ ,  $\text{Cu}^{2+}$ , and  $\text{Zn}^{2+}$  along with commonly occurring alkali ( $\text{Na}^+/\text{K}^+$ ) and alkaline earth ( $\text{Mg}^{2+}/\text{Ca}^{2+}$ ) metal ions. From single-crystal studies, it was confirmed that electrostatic attraction and supramolecular interactions are the reasons for such co-precipitation, which was also confirmed by spectroscopy. Using the method,

about 96.5% of gold was extracted in 2 min from electronic waste composed of Au, Cu, and Ni. This method was also employed to extract gold from nanomaterial waste generated in laboratories. Niacin, being inexpensive and renewable, costing ~US\$ 6000 per ton in the local market, the method may be used for cost-effective, selective and sustainable extraction of gold from diverse raw materials.



### Near-Infrared Chiral Plasmonic Microwires through Precision Assembly of Gold Nanorods on Soft Biotemplates

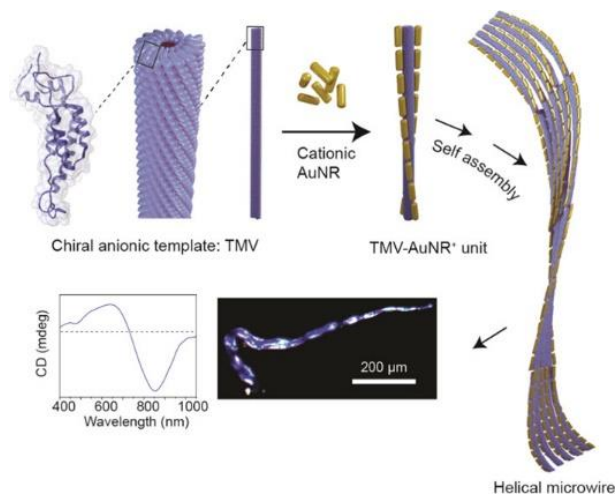
Amrita Chakraborty, Nonappa, Biswajit Mondal, Kamalesh Chaudhari, Heikki Rekola, Ville Hynninen, Mauri A. Kostianen, Robin H. A. Ras, and Thalappil Pradeep

J.Phys. Chem. C 2021, 125, 5, 3256–3267 (DOI: 10.1021/acs.jpcc.0c11512)

**Abstract:** Directing the assembly of plasmonic nanoparticles into chiral superstructures has diverse applications including, chiroptical sensing, nonlinear optics, and biomedicine. Though soft template-mediated assemblies of both spherical and nonspherical gold nanoparticles have made significant progress, most approaches require sophisticated chemical synthesis or advanced methodologies. Besides, reports of structurally precise chiral plasmonic assemblies beyond nanoscale are limited. Here, we propose an efficient yet simple strategy to grow such precision assemblies up to mesoscale, which is beneficial for

a broader community. Briefly, cationic gold nanorods (AuNRs) are allowed to systematically assemble along atomically precise, chiral, rodlike tobacco mosaic virus (TMV) particles via electrostatic attraction under ambient condition. This leads to spontaneous formation of helical hybrid microwires with high structural precision, as evidenced by cryogenic transmission electron microscopy and tomography. Resulting composite superstructures show a strong circular dichroism response at the plasmon wavelength of the AuNRs, which is supported by simulations using discrete dipole approximation. Further, chirality of the

system is investigated at a single-microwire level using polarized dark-field scattering microscopy. An alternative chiral template, negatively charged colloidal cellulose nanocrystals, also arrange AuNRs into similar chiral microstructures. Thus, our report proposes a generic methodology to obtain chiral plasmonic response at the NIR region using inexpensive templates that will encourage the exploration of a wider range of nanoscale templates for creating hybrid mesostructures with emerging optoelectronic properties.

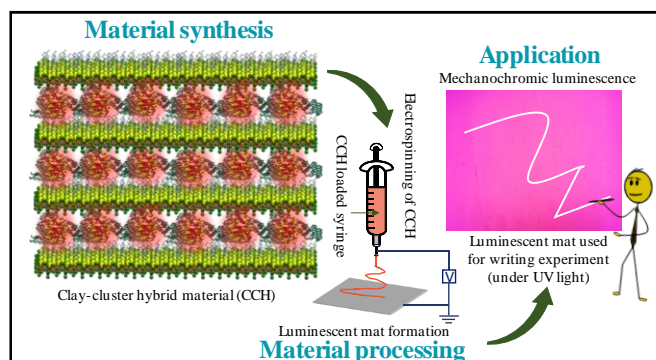


### Hierarchical Assembly of Atomically Precise Metal Clusters as a Luminescent Strain Sensor

Debasmita Ghosh, Mohd Azhardin Ganayee, Anirban Som, Pillalamarri Srikrishnarka, Nidhi Murali, Sandeep Bose, Amrita Chakraborty, Biswajit Mondal, Pijush Ghosh, Thalappil Pradeep  
ACS Appl. Mater. Interfaces 2021, 13, 5, 6496–6504 (DOI.org/10.1021/acsami.0c19239)

**Abstract:** We demonstrate the formation of a versatile luminescent organo-inorganic layered hybrid material, composed of bovine serum albumin (BSA)-protected  $\text{Au}_{30}$  clusters and aminoclay sheets. X-ray diffraction revealed the intercalation of  $\text{Au}_{30}@\text{BSA}$  in the layered superstructure of aminoclay sheets. Coulombic attraction of the clusters and the clay initiates the interaction, and appropriate size of the clusters allowed them to intercalate within the lamellar aminoclay galleries. Electron microscopy measurements confirmed the hierarchical structure of the material and also showed the cluster attached clay sheets. Zeta potential measurement and dynamic light scattering probed the gradual formation of the ordered aggregates in solution. The hybrid material could be stretched up to 300% without fracture. The emergence of a

new peak in the luminescence spectrum was observed during the course of mechanical stretching. This peak was increased in intensity gradually with the degree of elongation or strain of the material. A mechanochromic luminescence response was further demonstrated with a writing experiment on a luminescent mat of the material, made by electrospinning.





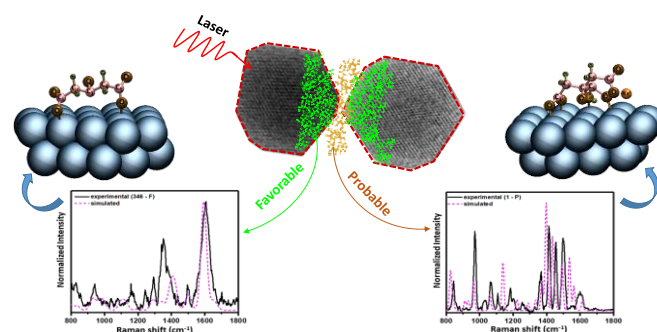
## Toward Vibrational Tomography of Citrate on Dynamically Changing Individual Silver Nanoparticles

Tripti Ahuja, Kamalesh Chaudhari, Ganesan Paramasivam, Gopi Ragupathy, Jyoti Sarita Mohanty, and Thalappil Pradeep

J. Phys. Chem. C 2021, 125, 3553–3566 (DOI: 10.1021/acs.jpcc.0c09981)

**Abstract:** This study explored changes in binding modes of the most common ligand, citrate on silver nanoparticles (AgNPs) using single-particle surface-enhanced Raman scattering (SPSERS). Single AgNPs of  $50 \pm 10$  nm diameter anchored on clean glass slides were monitored using time-dependent SP-SERS with 632.8 nm excitation at 1.3  $\mu$ W incident (0.5  $\mu$ W absorbed) power per nanoparticle. We observed several distinct spectra of citrate during time-dependent SP-SERS. Analysis of 1400 spectra showed the existence of two major groups termed as favorable (F) and probable (P) spectra based on their likelihood of appearance and intensities. These distinct spectra corresponded to a multitude of binding modes, structures, and variants of photocatalyzed products of citrate on the surface of dynamically changing AgNPs. Density functional theory (DFT) simulations were performed to model the structures and binding modes of citrate on an Ag(111) surface, and corresponding Raman spectra were computed and compared with

distinct spectral types. Experiments performed with deuterated (2,2,4,4-d<sub>4</sub>) citrate-capped AgNPs provided additional evidence to understand the shifts in vibrational features obtained in SP-SERS of citrate-capped AgNPs. These systematic analyses of time-dependent SP-SERS spectra may be used for the reconstruction and vibrational tomography (VT) of ligands at the single-particle level. The proposed VT approach is similar to sectioning an object through a multitude of orientations and reconstructing its three-dimensional structure, although the structures reconstructed here are molecular orientations.



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

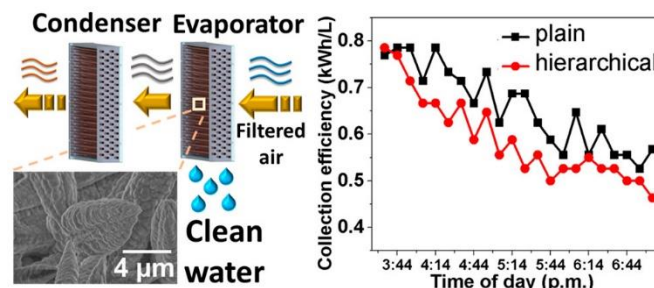
Ankit Nagar, Ramesh Kumar, Pillalamarri Srikrishnarka, Tiju Thomas, and Thalappil Pradeep  
ACS Appl. Nano Mater. 2021, 4, 2, 1540–1550 (DOI: 10.1021/acsanm.0c03032)

**Abstract:** Active cooling-based atmospheric water generators, despite their growing demand, continue to be energy intensive and offer poor collection efficiencies (energy consumption per liter of water production). Despite progress in micro-/ nanofabrication techniques and functional coatings, advanced surfaces have not been successfully scaled onto such harvesters to

accelerate condensation and improve their efficiencies. Here, we present a scalable dual-nanostructured hierarchical surface that comprises sporadically distributed bundles of randomly oriented faceted microcones having facets composed of nanostructures, which are either bumps or ridges. Condensate removal on this surface occurs via drop-to-film coalescence,

followed by film shedding in the form of macrodrops. Compared to a conventional plain metal surface used for condensation, the improvement in latent heat transfer coefficient using a hierarchically textured surface ranged from 19.9% at a subcooling of  $\sim 8^\circ\text{C}$  to 1048.4% at a subcooling of  $\sim 1^\circ\text{C}$  in laboratory scale experiments, subcooling being defined with respect to the dew point. To demonstrate utility at industrial scale and to ensure scalability of the modified surfaces, we create a prototype assembly comprising a tube-fin heat exchanger with hierarchically textured fins, cooled using a standard refrigeration cycle, producing  $\sim 25$  L of

water per day. The prototype containing hierarchically textured fins provides  $\sim 10.8\%$  enhanced water collection at  $\sim 10.4\%$  improved average collection efficiency compared to the traditional water generator when tested in outdoor conditions.



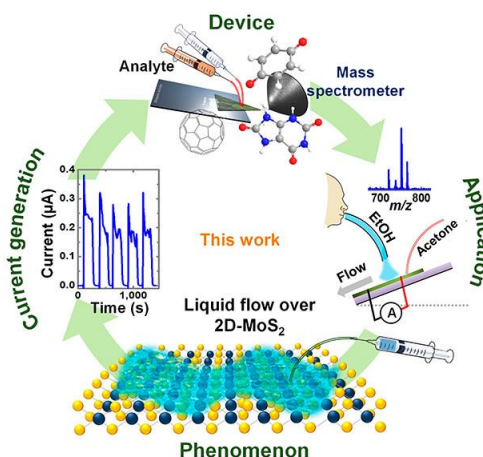
### 2D-Molybdenum disulfide-derived ion source for mass spectrometry

Pallab Basuri, Sourav Jana, Biswajit Mondal, Tripti Ahuja, Keerthana Unni, Md Rabiul Islam, Subhashree Das, Jaydeb Chakrabarti, and Thalappil Pradeep

ACS Nano 2021, 15, 3, 5023–5031 (DOI: 10.1021/acsnano.0c09985)

**Abstract:** Generation of current or potential at nanostructures using appropriate stimuli is one of the futuristic methods of energy generation. We developed an ambient soft ionization method for mass spectrometry using 2D-MoS<sub>2</sub>, termed streaming ionization, which eliminates the use of traditional energy sources needed for ion formation. The ionic dissociation-induced electrokinetic effect at the liquid–solid interface is the reason for energy generation. We report the highest figure of merit of current generation of 1.3 A/m<sup>2</sup> by flowing protic solvents at 22  $\mu\text{L}/\text{min}$  over a  $1 \times 1$  mm<sup>2</sup> surface coated with 2D-MoS<sub>2</sub>, which is adequate to produce continuous ionization of an array of analytes, making mass spectrometry

possible. Weakly bound ion clusters and uric acid in urine have been detected. Further, the methodology was used as a self-energized breath alcohol sensor capable of detecting 3% alcohol in the breath.



### Facile Crystallization of Ice I<sub>h</sub> via Formaldehyde Hydrate in Ultrahigh Vacuum under Cryogenic Conditions

Jyotirmoy Ghosh,<sup>‡</sup> Gaurav Vishwakarma<sup>‡</sup> Subhadip Das, and Thalappil Pradeep

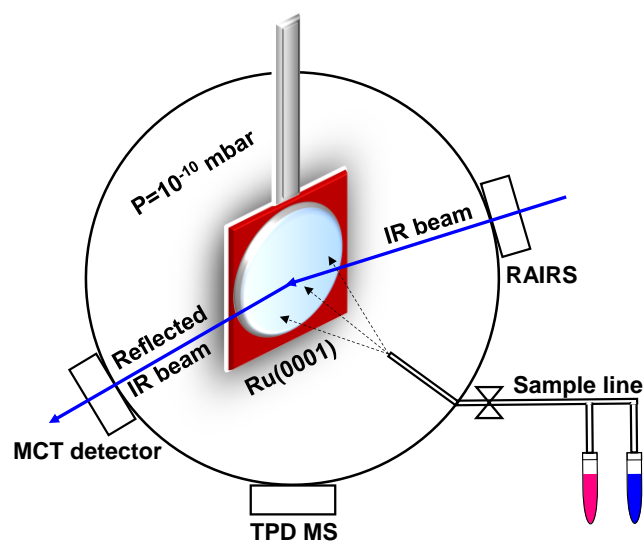
J. Phys. Chem. C 2021, 125, 4532–4539 (DOI: 10.1021/acs.jpcc.0c10367)

**Abstract:** Although hexagonal ice (ice I<sub>h</sub>) is the most common and highly studied crystalline form

of ice, its nucleation from clathrate hydrates is poorly understood. Here, we report the formation

of ice  $I_h$  through the dissociation of formaldehyde hydrate, prepared under ultrahigh vacuum (UHV) in the temperature window of 130–135 K. This unique route for crystallization is highly facile, and it occurs below the usual crystallization temperature of ice  $I_h$  of 155 K in UHV; the associated activation energy is also lower. Time-dependent reflection absorption infrared spectroscopy was used to detect the formaldehyde hydrate and to determine the crystallization kinetics of ice  $I_h$ . The dissociation of formaldehyde hydrate is found to be a diffusion-controlled process, which reduces the activation barrier of crystallization. This study provides evidence that formaldehyde hydrate can exist in extremely low ( $P$ ,  $T$ ) conditions without forming the geminal diol or its polymer in the presence of

water. This new and facile route of crystallization in the context of interstellar environments may have implications for cometary and prebiotic science.



### Molecular Materials through Microdroplets: Synthesis of Protein-Protected Luminescent Clusters of Noble Metals

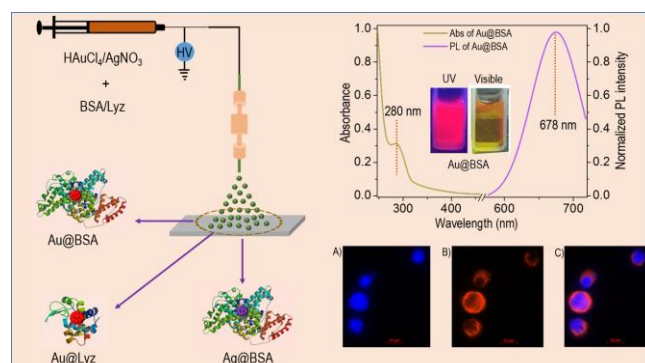
Sandeep Bose, Amit Chatterjee, Shantha Kumar Jenifer, Biswajit Mondal, Pillalamarri

Srikrishnarka, Debasmita Ghosh, Angshuman Ray Chowdhuri, M. P. Kannan, Sailaja V. Elchuri, and Thalappil Pradeep

ACS Sustainable Chem. Eng. 2021, 9, 12, 4554–4563 (DOI: 10.1021/acssuschemeng.0c09145)

**Abstract:** Atomically precise noble metal nanoclusters protected with proteins have emerged as a new research frontier in nanoscience, due to their unique optical and chemical properties as well as promising applications. In the present work, we have employed an ambient electrospray technique to synthesize protein protected luminescent clusters of gold and silver within the time scale of a few microseconds, which typically takes hours. In the absence of electric field, the spray results in nanoparticles and no cluster formation was noticed. Synthesis of these clusters in microdroplets leads to several fold enhancement in the rate of cluster formation. Spectroscopic investigations such as optical absorption, transmission electron microscopy and matrix-assisted laser desorption ionization mass

spectrometry confirm the molecular nature of the particles formed. Luminescence of electrospray-synthesized clusters show multifold enhancement as compared to the clusters synthesized in the solution phase. Luminescence of the clusters synthesized in microdroplets increases with the distance travelled by the spray. The formation of clusters via electrospray affects the secondary





structure of the protein, and its conformation is different from that of the parent protein. Au@BSA cluster is utilized for in vitro imaging of Retinoblastoma NCC-RbC-51 cells demonstrating a biological application of the resultant material.

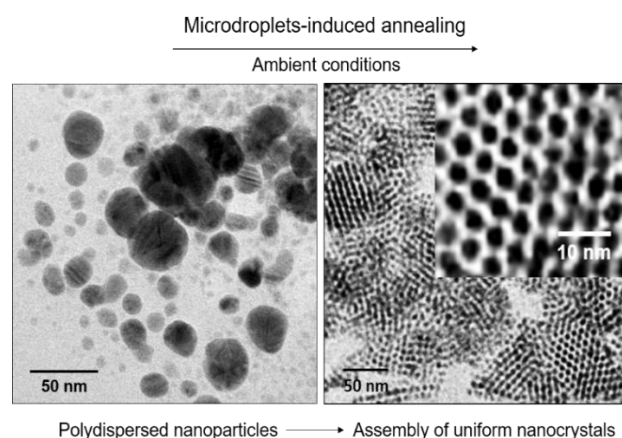
### Ambient microdroplet annealing of nanoparticles

Angshuman Ray Chowdhuri,<sup>‡</sup> B. K. Spoorthi,<sup>‡</sup> Biswajit Mondal, Paulami Bose, Sandeep Bose and Thalappil Pradeep

Chem. Sci., 2021, 12, 6370 (DOI: 10.1039/D1SC00112D)

**Abstract:** Conversion of polydisperse nanoparticles to their monodisperse analogues and formation of organized superstructures using them involve post synthetic modifications, and the process is generally slow. We show that ambient electro spray of preformed polydisperse nanoparticles makes them monodisperse and the product nanoparticles self-assemble spontaneously to form organized films, all within seconds. This phenomenon has been demonstrated with thiol-protected polydisperse silver nanoparticles of  $15 \pm 10$  nm diameter. Uniform silver nanoparticles of  $4.0 \pm 0.5$  nm diameter were formed after microdroplet spray, and this occurred without added chemicals, templates, and temperature, and within the time needed for electro spray, which was of the order of seconds. Well organized nanoparticle assemblies were obtained from such uniform particles. A home-made and simple nanoelectrospray set-up

produced charged microdroplets for the generation of such nanostructures, forming  $\text{cm}^2$  areas of uniform nanoparticles. A free-standing thin film of monodisperse silver nanoparticles was also made on a liquid surface by controlling the electro spray conditions. This unique method may be extended for the creation of advanced materials of many kinds.



### Kinetics of inter-cluster reactions between atomically precise noble metal clusters $[\text{Ag}_{25}(\text{DMBT})_{18}]^-$ and $[\text{Au}_{25}(\text{PET})_{18}]^-$ in room temperature solutions

Marco Neumaier, Ananya Baksi, Patrick Weis, Erik Schneider, Papri Chakraborty, Horst Hahn, Thalappil Pradeep and Manfred Kappes

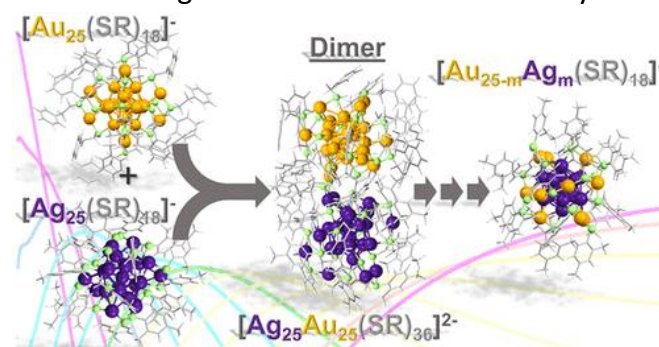
J. Am. Chem. Soc., 143 (2021) 6969–6980 (DOI: 10.1021/jacs.1c01140)

**Abstract:** The kinetics of intercluster metal atom exchange reactions between solvated

$[\text{Ag}_{25}(\text{DMBT})_{18}]^-$  and  $[\text{Au}_{25}(\text{PET})_{18}]^-$  (DMBT and PET are 2,4-dimethylbenzenethiol and 2-

phenylethanethiol, respectively, both  $C_8H_{10}S$ ) were probed by electrospray ionization mass spectrometry and computer-based modeling. Anion mass spectra and collision induced dissociation (CID) measurements show that both cluster monomers and dimers are involved in the reactions. We have modeled the corresponding kinetics assuming a reaction mechanism in which metal atom exchange occurs through transient dimers. Our kinetic model contains three types of generic reactions: dimerization of monomers, metal atom exchange in the transient dimers, and dissociation of the dimers to monomers. There are correspondingly 377 discrete species connected by in total 1302 reactions (i.e., dimerization, dissociation and atom exchange reactions) leading to the entire series of monomeric and dimeric products  $[Ag_m Au_{25-m}]^-$  ( $m = 1-24$ ) and  $[Ag_m Au_{50-m}]^{2-}$  ( $m = 0-50$ ), respectively. The rate constants of

the corresponding reactions were fitted to the experimental data, and good agreement was obtained with exchange rate constants which scale with the probability of finding a silver or gold atom in the respective monomeric subunit of the dimer, i.e., reflecting an entropic driving force for alloying. Allowing the dimerization rate constant to scale with increasing gold composition of the respective reactants improves the agreement further. The rate constants obtained are physically plausible, thus strongly supporting dimer-mediated metal atom exchange in this intercluster reaction system.



### Transformation of Nanodiamonds to Onion-like Carbons by Ambient Electrospray Deposition

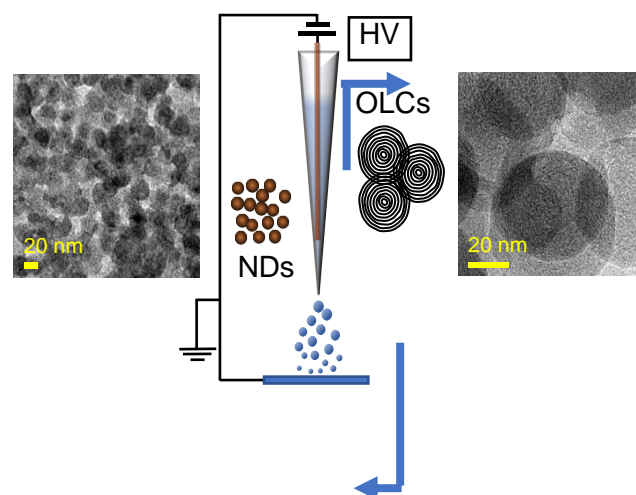
Deeksha Satyabola, Tripti Ahuja, Sandeep Bose, Biswajit Mondal, Pillalamarri Srikrishnarka, M. P. Kannan, B.

K. Spoorthi, and Thalappil Pradeep

J. Phys. Chem. C 2021, 125, 20, 10998–11006 (DOI: 10.1021/acs.jpcc.1c00166)

**Abstract:** Onion-like carbons (OLCs) are a class of fullerene-like circular nanoallotropes of carbon, typically synthesized from nanodiamond (ND) *via* thermal annealing, plasma spraying, and laser ablation. These methods require high temperature, high vacuum, or inert gas. Here, we report an ambient electrospray deposition (AED) process to transform NDs ( $11 \pm 1$  nm in size) into OLCs ( $50 \pm 13$  nm in size) in water. Transmission electron microscopy (TEM), field emission scanning electron microscopy (FESEM), Raman spectroscopy, and X-ray photoelectron spectroscopy (XPS) were used for the characterization of NDs and OLCs. High-resolution TEM images showed an increased interplanar spacing from ND (0.23 nm) to OLC (0.39 nm). Raman spectra showed a shift in the ND peak from

$1336\text{ cm}^{-1}$  to D-band at  $1349\text{ cm}^{-1}$ , and XPS quantitatively estimated an increase in the graphitization ratio ( $sp^2/sp^3$ ) from 0.95 to 3.16



after AED. Comparison of electrospray with sonic spray confirmed that such a transformation

required an external voltage as well. AESD was also performed for NDs dispersed in ethanol and

acetonitrile, which showed a solvent-dependent transformation.

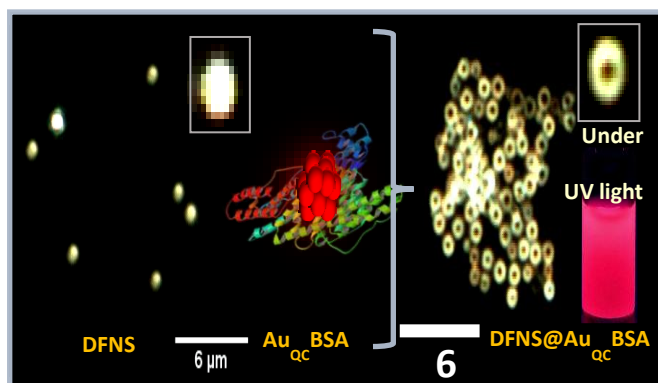
### Gold Clusters-Loaded Dendritic Nanosilica: Single Particle Luminescence and Catalytic Properties in the Bulk

Jyoti Sarita Mohanty, Ayan Maity, Tripti Ahuja, Kamalesh Chaudhari, Pillalamarri Srikrishnarka, Vivek Polshettiwar and Thalappil Pradeep

Nanoscale, 13, 2021, 9788-9797 (DOI: 10.1039/d1nr00619c)

**Abstract:** We report a hybrid material in which surface anchoring-induced enhanced luminescence of Au<sub>qc</sub>@BSA clusters on high surface area dendritic fibrous nanosilica of 800 nm diameter enabled their luminescence imaging at single particle level. The photophysical and structural properties of the hybrid material were characterized by various spectroscopic and microscopic techniques. Concomitant imaging using scattering and luminescence of such mesostructures and their response to analytes have been used to develop a chemical sensor. The hybrid material was found to be catalytically active in silane to silanol conversion, 100% conversion was observed in 4 h when the reaction was carried

out at 30 °C in presence of light. Such materials at submicron dimensions, enhanced surface area, emission in the solid state along with a high quantum yield of 12% in water along with enhanced scattering, and surface functionalities present numerous benefits for the creation of multifunctional materials.



### Triboelectric Generators for Sustainable Reduction Leading to Nanoparticles and Nanoclusters

Vishal Kumar, Pillalamarri Srikrishnarka, Jyoti Sarita Mohanty, Murugesan Paulthangam Kannan, Ramamurthy Nagarajan, and Thalappil Pradeep

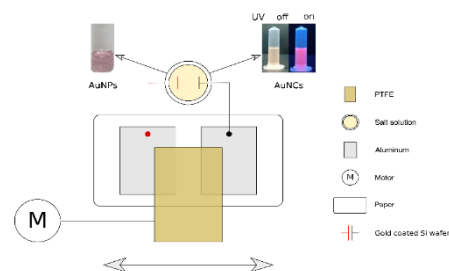
ACS Sustainable Chem. Eng. 2021, 9, 22, 7431–7436 (DOI: 10.1021/acssuschemeng.1c01586)

**Abstract:** In this letter, we demonstrate a sustainable, fast, and facile room temperature synthesis of plasmonic nanoparticles and luminescent nanoclusters of gold. The synthesis was performed using an affordable, easy to build, and robust triboelectric generator (TG). The

electricity generated by the TG was transferred to the solution continuously to synthesize gold nanoclusters (AuNCs). The obtained AuNCs had extremely narrow size distributions with mean particle sizes of ~2 nm and showed bright pink luminescence under UV light. The approach was



also extended to synthesize plasmonic gold nanoparticles (AuNPs). With this method, the synthesis time could be reduced from hours to several minutes without requiring any reducing agents. Tunability in size by simple variation of synthetic conditions and the consequent change in properties make this method usable for diverse applications.



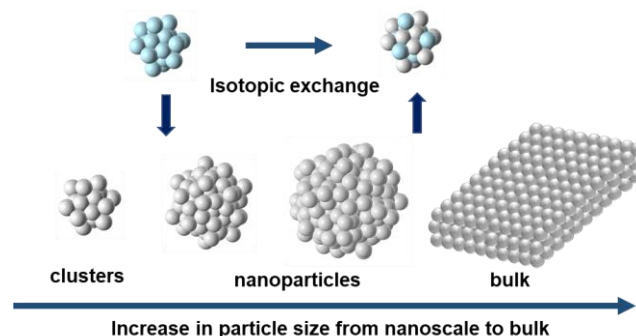
### Isotopic Exchange of Atomically Precise Nanoclusters with Materials of Varying Dimensions: From Nanoscale to Bulk

Papri Chakraborty, Paulami Bose, Jayoti Roy, Abhijit Nag, Biswajit Mondal, Amrita Chakraborty and Thalappil Pradeep

J. Phys. Chem. C 2021, 125, 29, 16110–16117 (DOI: 10.1021/acs.jpcc.1c02264)

**Abstract:** We present isotopic exchange reactions of atomically precise silver nanoclusters (NCs) with materials of different dimensions, namely, NCs, plasmonic nanoparticles (NPs), and bulk metals, all made of silver. Isotopically pure  $^{109}\text{Ag}_{25}(\text{DMBT})_{18}^-$  and  $^{107}\text{Ag}_{25}(\text{DMBT})_{18}^-$  (DMBT is 2,4-dimethyl benzene thiol) were reacted with Ag NPs of different sizes in the range of ~2–11 nm, protected with the same ligand. The exchange of  $^{107}\text{Ag}/^{109}\text{Ag}$  atoms in the NC was monitored using electrospray ionization mass spectrometry. The reaction kinetics was analyzed by fitting the temporal evolution of the reactant concentration to a kinetic model. The reaction timescales of NC–NP reactions were significantly longer compared to those of the NC–NC exchange process under

similar conditions. Differences between NC–NC exchange and NC–NP exchange highlighted the importance of the structure in controlling the reaction. Moreover, isotopic exchanges of the NC were also studied with the bulk metal to obtain a complete understanding of how the kinetics of atom transfer varies upon changing the size of the reacting partner from nanoscale to bulk.



### Cellulosic Ternary Nanocomposite for Affordable and Sustainable Fluoride Removal

Moses Egor, Avula Anil Kumar, Tripti Ahuja, Sritama Mukherjee, Amrita Chakraborty, Chennu

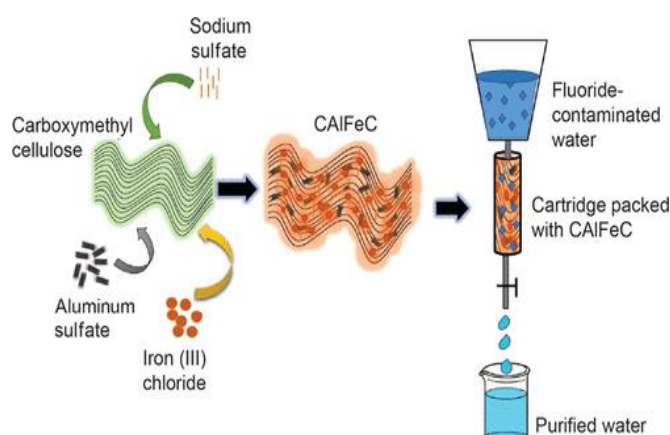
Sudhakar, Pillalamarri Srikrishnarka, Sandeep Bose, Swathy Jakka Ravindran, and Thalappil Pradeep

ACS Sustainable Chem. Eng. 2021, 9, 38, 12788–12799 (DOI: 10.1021/acssuschemeng.1c03272)

**Abstract:** Adsorption is shown to be an extremely affordable and sustainable way of producing clean water, particularly in resource-limited settings.

In this paper, we sought to synthesize an effective cellulose-based composite adsorbent from eco-friendly, earth-abundant, and consequently affordable ingredients at room temperature for fluoride removal from drinking water. We utilized the synergistic effect of various renewable materials and active sites of metal oxyhydroxides in developing an effective adsorbent, which is physically stable under the conditions of use. Nanoscale oxyhydroxides of aluminum and iron were scaffolded into a matrix of carboxymethyl cellulose (CMC) to form a nanocomposite adsorbent, which was prepared in water, eventually making a water-stable porous solid. This was used in batch and cartridge adsorption experiments for fluoride removal. The adsorbent surface before (*in situ*) and after fluoride uptake was characterized using various analytical techniques. The *in-situ* composite exhibited a surface area of  $134.3 \text{ m}^2/\text{g}$  with an amorphous solid structure with Al and Fe uniformly distributed in the cellulose matrix. From the batch adsorption experiments, we observed 80% fluoride removal within the first 3 min of contact, with a maximum uptake capacity of  $75.2 \text{ mg/g}$  as modeled by the Langmuir adsorption isotherm, better than most reported materials. The adsorbent effectively

reduced  $\text{F}^-$  levels in field water from 10 to  $0.3 \text{ mg/L}$ , less than  $1.5 \text{ mg/L}$  the World Health Organization upper limit for drinking water. Optimum  $\text{F}^-$  removal was achieved between the pH of 4–9; however, the effectiveness of the adsorbent was reduced in the presence of competing ions in the order  $\text{PO}_4^{3-} > \text{SiO}_3^{2-} > \text{CO}_3^{2-} > \text{HCO}_3^- > \text{SO}_4^{2-}$ . A cartridge experiment demonstrated the applicability of the adsorbent in a domestic point-of-use water purifier for defluoridation. Sustainability metrics of the material were evaluated. Defluoridation using the material is estimated to cost \$3.3 per 1000 L of treated water at the scale of community implementation projects.



### Aminoclay-Graphene Oxide Composite for Thin-Film Composite Reverse Osmosis Membranes with Unprecedented Water Flux and Fouling Resistance

Md Rabiul Islam, Pratishtha Khurana, Pillalamarri Srikrishnarka, Ankit Nagar, Madhuri Jash, Shantha Kumar Jenifer, Mohd Azhardin Ganayee, Mathava Kumar, and Thalappil Pradeep

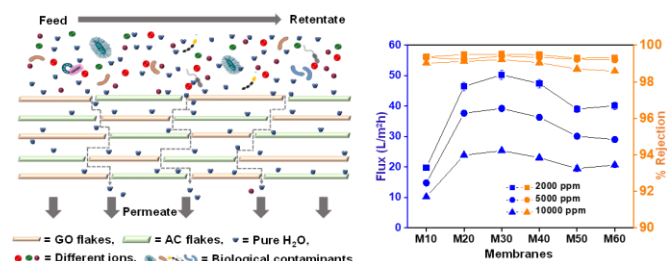
*Adv. Mater. Interfaces*, 2021, 2100533 (DOI:10.1002/admi.202100533)

**Abstract:** Work attempts to incorporate aminoclay-graphene oxide composites into thin-film composite (TFC)-reverse osmosis membranes to improve the desalination efficiency of brackish water. The composite is coated on a polysulfone substrate as a result of interfacial polymerization

of *m*-phenylene diamine and trimesoyl chloride, at different time durations. The prepared membranes are analyzed for their water permeation and salt rejection efficiencies using brackish feed water. The results indicated that the membrane loaded with 0.015 wt% of the

composite delivered maximum flux at 20 bar pressure for 2000 ppm feed. Moreover, the water flow rate increased by  $\approx 3.27$  times (from  $15.62 \pm 0.36$  to  $50.28 \pm 1.69 \text{ L m}^{-2} \text{ h}^{-1}$ ), compared to the unmodified TFC membrane. An enhancement in the salt rejection from  $97.03 \pm 1.07$  to  $99.51 \pm 0.10\%$  is also observed for the same feed water at 20 bar as compared to the unmodified membrane. Furthermore, antifouling tests with model biofoulant humic acid revealed better stability and antifouling performance of the prepared

membranes than the unmodified membranes under identical operating conditions. The membrane, therefore, assures high performance and lifetime owing to its mechanical and chemical stability, and hence suggests energy-efficient desalination.



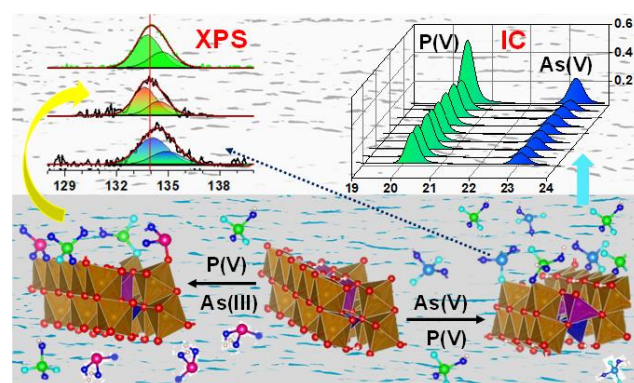
### Interference of Phosphate on the Adsorption of Arsenate and Arsenite Over Confined Metastable 2-Line Ferrihydrite and Magnetite

Chennu Sudhakar, Sritama Mukherjee, Avula Anil Kumar, Ganesan Paramasivam, P. Karthigai Meena, Nonappa, and Thalappil Pradeep

J. Phys. Chem. C 2021, 125, 41, 22502–22512 (DOI: 10.1021/acs.jpcc.1c043)

**Abstract:** Contamination of groundwater by arsenic (As(III/V)) is a serious global issue and phosphate (P(V)) is known to be the biggest interference in adsorption-based remediation methods. The present study is focused on understanding the interaction between phosphate and iron oxides/oxy-hydroxides, with two well-known classes of potential adsorbents in the important pH range of 5-9, and the effect of such interactions on the uptake of arsenite and arsenate. Spectroscopic studies such as XPS and FTIR were used to understand the binding of various oxyanions of phosphorous and arsenic with the iron oxides/oxy-hydroxides, exploring the core levels of P 2p and Fe 2p. Materials used for adsorption experiments were magnetite (MAG) and a nanocomposite, confined metastable 2-line ferrihydrite (CM2LF)); CM2LF is used for arsenic remediation in the affected states of India. Further, we studied the interference of P(V) on As(III/V) adsorption. Kinetics of adsorption was quantified using ion chromatography (IC), where P(V) alone

followed a pseudo-second-order model. In the case of mixed solutions, namely, AP<sub>mix1</sub> (P(V) + As(III)) and AP<sub>mix2</sub> (P(V) + As(V)), kinetics data suggested that P(V) or As(III/V) oxyanions are partially following the pseudo-second-order model. Results also confirmed that CM2LF performed better than magnetite (MAG) for As(III/V) uptake in presence of P(V). As(III) and As(V) species are more competitive than P(V) at neutral pH. A model for the adsorption of P(V) species in water on a ferrihydrite particles was developed using DFT. This accounted for



phosphate complexation at various pH values. The

study is highly useful in developing an affordable solution for sustainable arsenic remediation. Various aspects of sustainability were discussed.

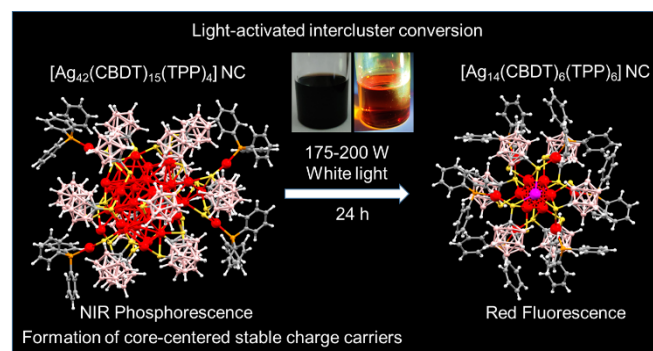
### Light-Activated Intercluster Conversion of an Atomically Precise Silver Nanocluster

Arijit Jana, Madhuri Jash, Ajay Kumar Poonia, Ganesan Paramasivam, Md Rabiul Islam, Papri Chakraborty, Sudhadevi Antharjanam, Jan Machacek, Sundargopal Ghosh, Kumaran Nair Valsala Devi Adarsh, Tomas Base, and Thalappil Pradeep

ACS Nano 2021, 15, 15781–15793 (DOI: 10.1021/acsnano.1c02602)

**Abstract:** Noble metal nanoclusters protected with carboranes, a 12-vertex, nearly icosahedral boron–carbon framework system, have received immense attention due to their different physicochemical properties. We have synthesized *ortho*-carborane-1,2-dithiol (CBDT) and triphenylphosphine (TPP) coprotected  $[\text{Ag}_{42}(\text{CBDT})_{15}(\text{TPP})_4]^{2-}$  (shortly  $\text{Ag}_{42}$ ) using a ligand-exchange induced structural transformation reaction starting from  $[\text{Ag}_{18}\text{H}_{16}(\text{TPP})_{10}]^{2+}$  (shortly  $\text{Ag}_{18}$ ). The formation of  $\text{Ag}_{42}$  was confirmed using UV–vis absorption spectroscopy, mass spectrometry, transmission electron microscopy, X-ray photoelectron spectroscopy, infrared spectroscopy, and multinuclear magnetic resonance spectroscopy. Multiple UV–vis optical absorption features, which exhibit characteristic patterns, confirmed its molecular nature.  $\text{Ag}_{42}$  is the highest nuclearity silver nanocluster protected with carboranes reported so far. Although these clusters are thermally stable up to 200 °C in their solid state, light-irradiation of its solutions in dichloromethane results in its structural conversion to  $[\text{Ag}_{14}(\text{CBDT})_6(\text{TPP})_6]$  (shortly  $\text{Ag}_{14}$ ). Single crystal X-ray diffraction of  $\text{Ag}_{14}$  exhibits  $\text{Ag}_8$ – $\text{Ag}_6$  core–shell structure of this nanocluster. Other spectroscopic and microscopic studies also confirm the formation of  $\text{Ag}_{14}$ . Time-dependent mass spectrometry revealed that this light-activated intercluster conversion went through two sets of

intermediate clusters. The first set of intermediates,  $[\text{Ag}_{37}(\text{CBDT})_{12}(\text{TPP})_4]^{3-}$  and  $[\text{Ag}_{35}(\text{CBDT})_8(\text{TPP})_4]^{2-}$  were formed after 8 h of light irradiation, and the second set comprised of  $[\text{Ag}_{30}(\text{CBDT})_8(\text{TPP})_4]^{2-}$ ,  $[\text{Ag}_{26}(\text{CBDT})_{11}(\text{TPP})_4]^{2-}$ , and  $[\text{Ag}_{26}(\text{CBDT})_7(\text{TPP})_7]^{2-}$  were formed after 16 h of irradiation. After 24 h, the conversion to  $\text{Ag}_{14}$  was complete. Density functional theory calculations reveal that the kernel-centered excited state molecular orbitals of  $\text{Ag}_{42}$  are responsible for light-activated transformation. Interestingly,  $\text{Ag}_{42}$  showed near-infrared emission at 980 nm



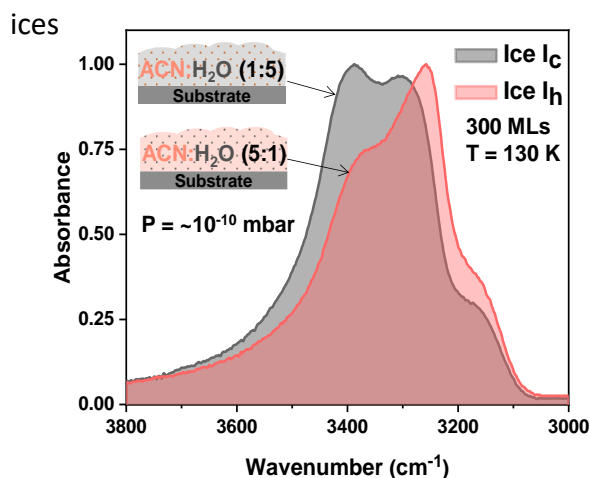
(1.26 eV) with a lifetime of  $>1.5 \mu\text{s}$ , indicating phosphorescence, while  $\text{Ag}_{14}$  shows red luminescence at 626 nm (1.98 eV) with a lifetime of 550 ps, indicating fluorescence. Femtosecond and nanosecond transient absorption showed the transitions between their electronic energy levels and associated carrier dynamics. Formation of the stable excited states of  $\text{Ag}_{42}$  is shown to be responsible for the core transformation.



## Desorption-induced evolution of cubic and hexagonal ices in an ultrahigh vacuum and cryogenic temperatures

Gaurav Vishwakarma, Jyotirmoy Ghosh and Thalappil Pradeep  
*Phys. Chem. Chem. Phys.*, 2021, 23, 24052 (DOI: 10.1039/d1cp03872a)

**Abstract:** Reflection absorption infrared spectroscopic investigations of multilayer films of acetonitrile (ACN) and water in ultrahigh vacuum under isothermal conditions showed the emergence of cubic (Ice  $I_c$ ) and hexagonal (Ice  $I_h$ )

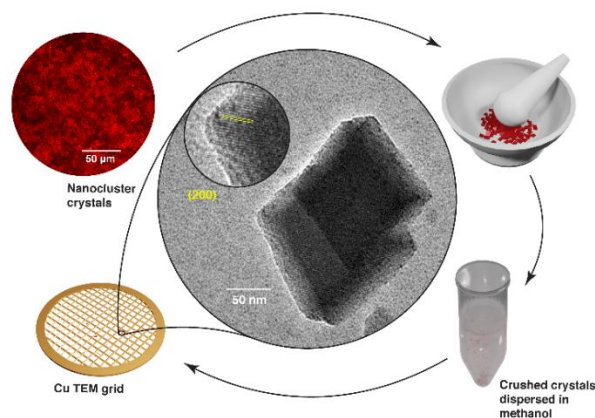


depending on the composition of the film. The experiments were conducted with a mixed film of 300 monolayers thickness and the ACN:H<sub>2</sub>O monolayer ratios were varied from 1:5 to 5:1. Mixed films were deposited at 10 K and warmed to 130-135 K, where ACN desorbed subsequently and IR spectral evolution was monitored continuously. While the emergence of Ice  $I_c$  at 130 K has been reported, the occurrence of Ice  $I_h$  at this temperature was seen for the first time. Detailed investigations showed that Ice  $I_h$  can form at 125 K as well. Crystallization kinetics and activation energy ( $E_a$ ) for the emergence of Ice  $I_h$  were evaluated using the Avrami equation.

## Direct imaging of lattice planes in atomically precise noble metal cluster crystals using a conventional transmission electron microscope

Ananthu Mahendranath, Biswajit Mondal, Korath Sivan Sugi, and Thalappil Pradeep  
*Chem. Commun.*, 2021 (DOI: 10.1039/D1CC05643C)

**Abstract:** Imaging finer structural details of atomically precise noble metal cluster crystals has been difficult with electron microscopy, owing to their extreme beam sensitivity. Here we present a simple method whereby lattice planes in single crystals of nanoclusters can be observed using a conventional transmission electron microscope, enabling further expansion of cluster research.



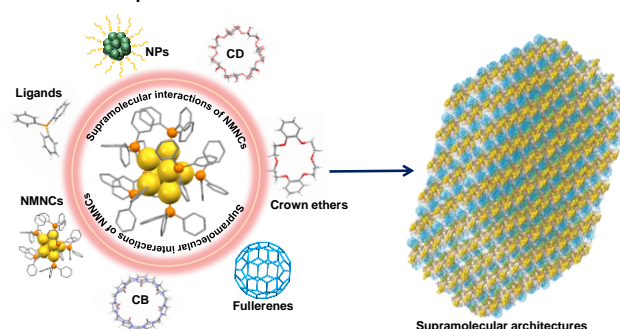
## Assembling Atomically Precise Noble Metal Nanoclusters Using Supramolecular Interactions

Abhijit Nag, and Thalappil Pradeep

ACS Nanoscience Au., 2021 (Just accepted)

**Abstract:** Supramolecular chemistry (SC) of noble metal nanoclusters (NMNCs) is one of the fascinating areas of contemporary materials science. It is principally concerned with the non-covalent interactions between NMNCs, as well as between NMNCs and molecules or nanoparticles. This review focuses on recent advances in the supramolecular assembly of NMNCs and applications of the resulting structures. We have divided the topics into four distinct sub-groups: i) SC of NMNCs in gaseous and solution phases, ii) supramolecular interactions of NMNCs in crystal lattices, iii) supramolecular assemblies of NMNCs with nanoparticles and NMNCs, and iv) SC of NMNCs with other molecules; the last explores their interactions with fullerenes, cyclodextrins, cucurbiturils, crown ethers, and more. After discussing these topics concisely, various

emerging properties of the assembled systems in terms of their mechanical, optical, magnetic, charge transfer, etc., properties and applications are presented. SC is seen to provide a crucial role to induce new physical and chemical properties in such hybrid nanomaterials. Finally, we highlight the scope for expansion and future research in the area. This review would be useful to those working on functional nanostructures in general and NMNCs in particular.



## Gas phase ion chemistry of titanium-oxofullerene with ligated solvents

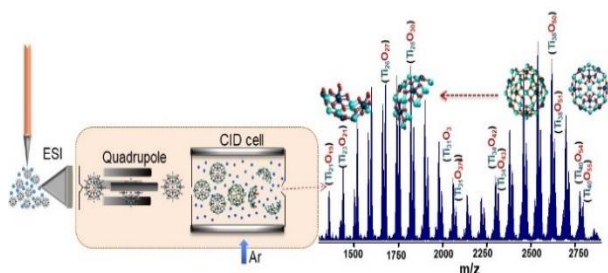
Jayoti Roy, Papri Chakraborty, Ganesan Paramasivam, Ganapati Natarajan, and Thalappil Pradeep

Phys. Chem. Chem. Phys., 2021 (Just accepted)

**Abstract:** We investigated the gas phase fragmentation events of highly symmetric fullerene-like (FN-like) titanium oxo-cluster anions,  $[\text{H}_{12}\text{Ti}_{42}\text{O}_{60}(\text{OCH}_3)_{42}(\text{HOCH}_3)_{10}(\text{H}_2\text{O})_2]^{2-}$  (**1**) and  $[\text{H}_7\text{Ti}_{42}\text{O}_{60}(\text{OCH}_3)_{42}(\text{HOCH}_3)_{10}(\text{H}_2\text{O})_3]^{1-}$  (**2**). These oxo-clusters contain a closed cage  $\text{Ti}_{42}\text{O}_{60}$  core, protected by a specific number of methoxy, methanol, and water molecules acting as ligands. These dianionic and monoanionic species were generated in the gas phase by electrospray ionization of  $\text{H}_6[\text{Ti}_{42}(\mu^3\text{-O})_{60}(\text{O}^i\text{Pr})_{42}(\text{OH})_{12}]$  (TOF) cluster in methanol. Collision induced dissociation

studies of **1** revealed that upon increasing the collision energy, the protecting ligands were stripped off first, and  $[\text{Ti}_{41}\text{O}_{58}]^{2-}$  was formed as the first fragment from the  $\text{Ti}_{42}\text{O}_{60}$  core. Thereafter, systematic  $\text{TiO}_2$  losses were observed giving rise to subsequent fragments like  $[\text{Ti}_{40}\text{O}_{56}]^{2-}$ ,  $[\text{Ti}_{39}\text{O}_{54}]^{2-}$ ,  $[\text{Ti}_{38}\text{O}_{52}]^{2-}$ , etc. Similar fragments were also

observed for monoanionic species, **2** as well.



Systematic 23  $\text{TiO}_2$  losses were observed, which were followed by complete shattering of the cage. We also carried out computational studies using

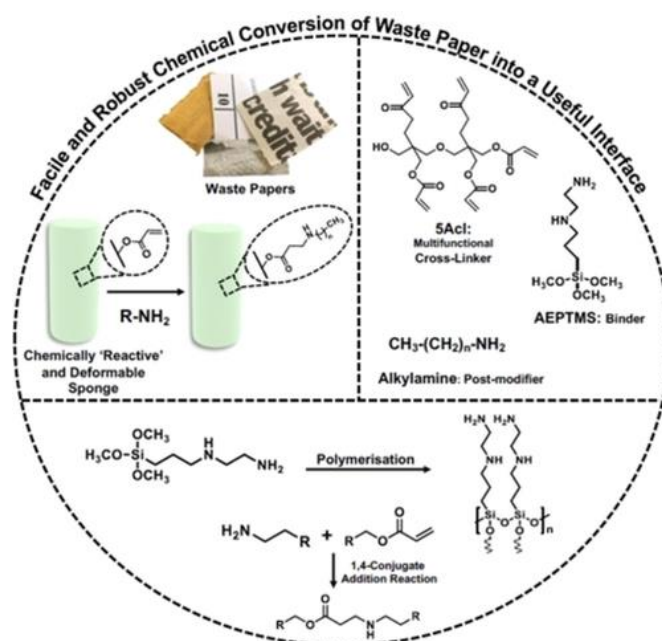
density functional theory (DFT) to investigate the structures and fragmentation mechanism. The fragmentation of TOF was comparable to the fragmentation of  $\text{C}_{60}$  ions, where systematic  $\text{C}_2$  losses were observed. We believe that this is a consequence of topological similarity. The present study provides valuable insights into the structural constitution of TOF clusters and stability of the parent as well as the resulting cage-fragments in the gas phase.

### Design of a Waste Paper-Derived Chemically 'Reactive' and Durable Functional Material with Tailorable Mechanical Property Following an Ambient and Sustainable Chemical Approach

Arpita Shome, Adil Rather, Angana Borbora, Pillalamarri Srikrishnarka, Avijit Baidya, Thalappil Pradeep, and Uttam Manna

Chem. Asian J., 2021 (DOI: 10.1002/asia.202100475)

**Abstract:** Controlled tailoring of mechanical property and wettability is important for designing various functional materials. The integration of these characteristics with waste materials is immensely challenging to achieve, however, it can provide sustainable solutions to combat relevant environmental pollutions and other relevant challenges. Here, the strategic conversion of discarded and valueless waste paper into functional products has been introduced following a catalyst-free chemical approach to tailor both the mechanical property and water wettability at ambient conditions for sustainable waste management and controlling the relevant environmental pollution. In the current design, the controlled and appropriate silanization of waste paper allowed to modulate both the a) porosity and b) compressive modulus of the paper-derived sponges. Further, the association of 1,4-conjugate addition reaction between amine and acrylate groups allowed to obtain an unconventional waste



paper-derived chemically 'reactive' sponge. The appropriate covalent modification of the residual reactive acrylate groups with selected alkylamines at ambient conditions provided a facile basis to tailor the water wettability from moderate

hydrophobicity, adhesive superhydrophobicity to non-adhesive superhydrophobicity. The embedded superhydrophobicity in the waste paper-derived sponge was capable of sustaining large physical deformations, severe physical abrasions, prolonged exposure to harsh aqueous conditions, etc. Further, the waste paper-derived, extremely water-repellent sponges and

membranes were successfully extended for proof-of-concept demonstration of a practically relevant outdoor application, where the repetitive remediation of oil spillages has been demonstrated following both selective absorption (25 times) of oils and gravity-driven filtration-based (50 times) separation of oils from oil/water mixtures at different harsh aqueous scenarios.



## Acknowledgements

We thank our collaborators and students for their hard work.

We are grateful to IIT Madras for its continued support.

Department of Science and Technology,

Government of India is acknowledged for generous funding.

