Annual report | 2016

Pradeep Research Group

Indian Institute of Technology Madras

Our struggle is to be creative…

today and everyday!

This annual report is available here.
Annual reports of 2014 and 2015 are also available (click the respective year).

Our Team

Thalappil Pradeep FNA, FASc., FNASc., FNAE, FRSC
Institute Professor
Institute Chair Professor and Professor of Chemistry
Department of Chemistry
Indian Institute of Technology Madras
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Laboratories: DST Unit of Nanoscience and Thematic Unit of Excellence

Web: www.dstuns.iitm.ac.in/pradeep-research-group.php

Ph.D. Students

Atanu Ghosh
Soujit Sengupta
N. Rahul
Shridevi Bhat
Depanjan Sarkar
Mohd. Azhardin Ganayee
S. Vidhya
C. K. Manju
Avijit Baidya
Jyoti Sarita Mohanty
Sudhakar Chennu
A. Suganya
Madhuri Jash
Sandeep Bose
Debasmita Ghosh
Amrita Chakraborty

Sugi Shivan
J. R. Swathy
Biswajit Mondal
Abhijit Nag
Jyotirmoy Ghosh
Papri Chakraborty
Sritama Mukherjee
Md Bodiuzzaman
Md Rabiul Islam
Esma Khatun
Tripti Ahuja
Pallab Basuri
Srikrishnarka Pillalamarri
Tanvi Gupte
Prosenjit Baidya
Vishal Kumar
Paulami Bose

Postdoctoral/Research Associates

Dr. Gana Natarajan
Dr. P. Mohan Kumar
Dr. Amitava Srimany
Dr. M. Dhivakar
Dr. Anirban Som
Dr. Rabin Rajan J. Methikkalam
Dr. K. R. Krishnadas
Dr. Sourav Kanti Jana
Dr. P. Ganesan

Project Associates

Manoj Kumar Panwar
A. Anil Kumar
Ramesh Kumar
Ananthu Mahendranath
Bibhuti Bhusan Rath

Visiting students

Erick Kiage Mobegi
Sahana Sheshachala

M.Sc. Students

Abhijith Menon
Pratyusha Das
Rohan Chowdhury
Sohini Mukherjee
Arunava Saha

Industrial Consultant

Dr. Kamalesh Chaudhari

Administrative Officer

K. Priya

Project Technicians

E. Sundarraj
R. Sowmya Narayani

Project Consultant

Hemanta R. Naik

Summer Student(s)/Fellow(s)

Neeru Mittal
Astha Chandodwala
S. Saikrithika
Kezia Sasitharan
Jeena N. Baby
K. M. Archana
Dr. Kalpana Gupta
S. Shanjitha

Winter Student

Era Kumari Modi

What's Inside

An Important Milestone

Inauguration of our new laboratory by Prof. C. N. R. Rao on January 11, 2016

THEMATIC UNIT OF EXCELLENCE

Inauguration of our TUE by Professor C. N. R. Rao, with Professors Ashok Jhunjhunwala, P. T. Manoharan and Indrapal Singh Aidhen

A view of our new lab, through the corridor

Publications

JOURNAL PUBLICATIONS

1. Unusual reactivity of dithiol protected clusters in comparison to monothiol protected clusters: Studies using $Ag_{51}(BDT)_{19}(TPP)_3$ and $Ag_{29}(BDT)_{12}(TPP)_4$, Atanu Ghosh, Debasmita Ghosh, Esma Khatun, Papri Chakraborty and T. Pradeep, *Nanoscale,* (2016) (*DOI: 10.1039/C6NR07692K*).
2. Confined metastable 2-line ferrihydrite for affordable point-of-use arsenic free drinking water, Anil Kumar Avula, Anirban Som, Paolo Longo, Chennu Sudhakar, Radha Gobinda Bhuin, Soujit Sen Gupta, Anshup, Mohan Udhaya Sankar, Amrita Chaudhary, Ramesh Kumar and T. Pradeep, *Adv. Mat.,* (2016) (*DOI: 10.1002/adma.201604260).*
3. Diffusion controlled simultaneous sensing and scavenging of heavy metal ions in water using atomically precise cluster – cellulose nanocrystal composites, Nishil Mohammed, Avijit Baidya, Vasanthanarayan Murugesan, Anil Kumar Avula, Mohd Azhardin Ganayee, Jyoti Mohanty, Tam, Kam (Michael) and T. Pradeep, *ACS Sustainable Chem. Eng.*, 4(11) (2016) 6167-6176 *(DOI:10.1021/acssuschemeng.6b01674).*
4. Structure-conserving spontaneous transformations between nanoparticles, K. R. Krishnadas, Ananya Baksi, Atanu Ghosh, Ganapati Natarajan and T. Pradeep, *Nat. Commun.,* 7 (2016) 13447 *(DOI: 10.1038/ncomms13447).*
5. Cooking induced corrosion of metals, Soujit Sen Gupta, Ananya Baksi, Vidhya Subramanian and T. Pradeep, *ACS Sustain. Chem. Eng.,* 4 (2016) 4781-4787 *(DOI: 10.1021/acssuschemeng.6b00980).*
6. Nucleolin-aptamer therapy in retinoblastoma: molecular changes and mass spectrometry–based imaging, Nithya Subramanian, Amitava Srimany, Jagat R Kanwar, Rupinder K Kanwar, Balachandran Akilandeswari, Pukhraj Rishi, Vikas Khetan, Madavan Vasudevan, T. Pradeep and Subramanian Krishnakumar, *Mol. Ther. Nucleic Acids,* 5 (2016) e358 *(DOI: 10.1038/mtna.2016.70).*
7. Towards a Janus cluster: Regiospecific decarboxylation of Ag_{44}(4-MBA)$_{30}$@Ag nanoparticles, Indranath Chakraborty, Anirban Som, Tuhina Adit Maark, Biswajit Mondal, Depanjan Sarkar and T. Pradeep, *J. Phys. Chem. C,* 120 (28) (2016) 15471-15479 *(DOI: 10.1021/acs.jpcc.6b04769).*
8. Desorption electrospray ionization (DESI) mass spectrometric imaging of the distribution of rohitukine in the seedling of *Dysoxylum binectariferum Hook. f.*, Mohana Kumara P, Amitava

Srimany, Suganya Arunan, Ravikanth G, Uma Shaanker R and T. Pradeep, *PLoS. ONE,* 11(6) (2016) 1-14 *(DOI:10.1371/journal.pone.0158099)*.

9. $[Au_{25}(SR)_{18}]_2^{2-}$: A noble metal cluster dimer in the gas phase, Ananya Baksi, Papri Chakraborty, Shridevi Bhat, Ganapati Natarajan and T. Pradeep, *Chem. Commun.,* 52 (2016) 8397-8400 *(DOI: 10.1039/c6cc03202h)*.
10. Sparingly soluble constant carbonate releasing inert monolith for enhancement of antimicrobial silver action and sustainable utilization, Swathy Jakka Ravindran, Nalenthiran Pugazhenthiran, Sudhakar Chennu, Anil Kumar Avula and T. Pradeep, *ACS Sustain. Chem. Eng.,* 4 (2016) 4043-4049 *(DOI: 10.1021/acssuschemeng.6b00979)*.
11. Diffusion and crystallization of dichloromethane within the pores of amorphous solid water, Radha Gobinda Bhuin, Rabin Rajan J. Methikkalam, Soumabha Bag and T. Pradeep, *J. Phys. Chem. C*, 120 (2016) 13474-13484 *(DOI: 10.1021/acs.jpcc.6b00436)*.
12. Monitoring of changes in lipid profiles during PLK1 knockdown in cancer cells using DESI MS, Balasubramanyam Jayashree, Amitava Srimany, Srinidhi Jayaraman, Anjali Bhutra, Narayanan Janakiraman, Srujana Chitipothu, Subramanian Krishnakumar, Lakshmi Subhadra Baddireddi, Sailaja Elchuri and T. Pradeep, *Anal. Bioanal. Chem.*, 408 (2016) 5623-5632 *(DOI: 10.1007/s00216-016-9665-y)*.
13. Electrospun nanofiber mats as "smart surfaces" for desorption electrospray ionization mass spectrometry (DESI MS)-based analysis and imprint imaging, R. G. Hemalatha, Mohd Azhardin Ganayee and T. Pradeep, *Anal. Chem.,* 88 (2016) 5710-5717 *(DOI: 10.1021/acs.analchem.5b04520)*.
14. Highly luminescent monolayer protected $Ag_{56}Se_{13}S_{15}$ clusters, C. K. Manju, Indranath Chakraborty and T. Pradeep, *J. Mater. Chem. C,* 4 (2016) 5572-5577 *(DOI: 10.1039/c6tc01388k)*.
15. Thio residue from thermal processing of cometary ices containing carbon disulfide and ammonia, Rabin Rajan J. Methikkalam, S. Pavithraa, S. P. Murali Babu, H. Hill, Raja Sekhar, T Pradeep and B. Sivaraman, *Adv. Space. Res.,* 58 (2016) 438-443 *(DOI:10.1016/j.asr.2016.04.028)*.
16. Unusual reactivity of MoS_2 nanosheets, Biswajit Mondal, Anirban Som, Indranath Chakraborty, Ananya Baksi, Depanjan Sarkar and T. Pradeep, *Nanoscale,* 8 (2016) 10282-10290 *(DOI: 10.1039/c6nr00878j)*.
17. Extraction of silver by glucose, Ananya Baksi, Mounika Gandi, Swathi Chaudhari, Soumabha Bag, Soujit Sen Gupta and T. Pradeep, *Angew. Chem. Int. Ed.*, 55 (2016) 7777-7781 *(DOI: 10.1002/anie.201510122)*.

18. Atomically precise and monolayer protected iridium clusters in solution, Shridevi Bhat, Indranath Chakraborty, Tuhina Adit Maark, Anuradha Mitra, Goutham De and T. Pradeep, *RSC Adv.,* 6 (2016) 26679-26688 *(DOI: 10.1039/c5ra27972k).*
19. Developmental patterning and segregation of alkaloids in areca nut (seed of Areca catechu) revealed by magnetic resonance and mass spectrometry imaging, Amitava Srimany, Christy George, Hemanta R. Naik, Danica Glenda Pinto, N. Chandrakumar and T. Pradeep, *Phytochemistry,* 125 (2016) 35-42 *(DOI: 10.1016/j.phytochem.2016.02.002).*
20. Possible isomers in ligand protected Ag_{11} cluster ions identified by ion mobility mass spectrometry and fragmented by surface induced dissociation, Ananya Baksi, Sophie H. Harvey, Ganapati Natarajan, Vicki H. Wysocki and T. Pradeep, *Chem. Commun.*, 52 (2016) 3805-3808 *(DOI: 10.1039/C5CC09119E).*
21. Cluster mediated crossed bilayer precision assemblies of 1D nanowires, Anirban Som, Indranath Chakraborty, Tuhina Adit Maark, Shridevi Bhat and T. Pradeep, *Adv. Mater.*, 28 (2016) 2827-2833 *(DOI: 10.1002/adma.201505775).*
22. Rapid dehalogenation of pesticides and organics at the interface of reduced graphene oxide-silver nanocomposite, Dibyashree Koushik, Soujit Sen Gupta, Shihabudheen M. Maliyekkal and T. Pradeep*, J. Haz. Mater.,* 308 (2016) 192-198 *(DOI:10.1016/j.jhazmat.2016.01.004).*

OTHER PUBLICATIONS

23. **Editorial:** Joyful Years with the Journal: Balancing the Editor–Professor Life, Thalappil Pradeep, *ACS Sustainable Chem. Eng.*, 4 (12) (2016) 6252 *(DOI: 10.1021/acssuschemeng.6b02786).*
24. Direct observation of the formation pathway of [Mo132] keplerates, Subharanjan Biswas, Dolores Melgar, Amitava Srimany, Antonio Rodríguez-Fortea, T. Pradeep, Carles Bo, Josep M. Poblet and Soumyajit Roy, *Inorg. Chem.,* 55 (2016) 8285-8291 *(DOI: 10.1021/acs.inorgchem.5b02570).*
25. **Meeting report:** Bridging innovations in academic institutions to society, T. Pradeep, Baldev Raj, V. Ramgopal Rao, Anil Kumar, Bodh Raj Mehta, G. U. Kulkarni, Tata Narasinga Rao, A. K. Ghosh, Satish Vasu Kailas, Kishore M. Paknikar, Mohan Kumar, S. G. Sreekanteswara Swamy, Anshup, Nitin Kale, Praveen Poddar, Radhica Sastry, Saket Kumar, Abhijeet Gaan, Krishnan Swaminathan, Prashanth Vaijayanth, Vijaya Lakshmi, Rajeev Kumar, D. R. Prasada Raju, Debapriya Dutta, Sanjay Bajpai, Soujit Sen Gupta, Devaraju, *Curr. Sci.*, 110 (2016) 482-486.

BOOK CHAPTER

26. Evolution of atomically precise clusters through the eye of mass spectrometry, Shridevi Bhat, Indranath Chakraborty, Ananya Baksi, Raghu Pradeep Narayanan and T. Pradeep, Nanoscience : Volume 3 Paul O'Brien (Ed.) and P John Thomas (Ed.), Royal Society of Chemistry, London, 3 (2016) 343-385 *(DOI:10.1039/9781782623717-00343)*.

Lectures Delivered

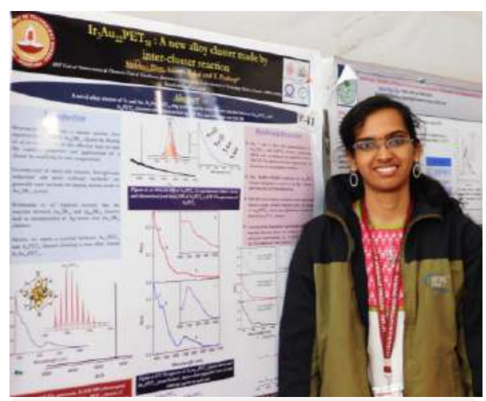
1. Inter-cluster reactions between $Au_{25}(SR)_{18}$ and $Ag_{44}(SR)_{30}$, Nano-Scaled Systems for Energy Harvesting, VIT University, February 1, 2016.
2. Affordable point-of-use water purification using nanomaterials, PSG Institute of Advanced Studies, February 11, 2016.
3. Nanomaterials to clean water: Lab to industry, Institute lecture at IISER Thiruvananthapuram, February 12, 2016.
4. Affordable point-of-use water purification using nanomaterials, Sixth International Conference on Metals in Genetics, Chemical Biology and Therapeutics (ICMG-2016), February 12, 2016.
5. Nanomaterials to clean water: Lab to industry, National Science Day Lecture at IIT Madras, February 28, 2016.
6. Inter-cluster reactions between $Au_{25}(SR)_{18}$ and $Ag_{44}(SR)_{30}$, ICONSAT 2016, February 29, IISER Pune.
7. Clean water using nanomaterials, Bangalore Nano, March 3, 2016.
8. Inter-cluster reactions between $Au_{25}(SR)_{18}$ and $Ag_{44}(SR)_{30}$, Plenary talk at ISCAN 2016, IISER Thiruvananthapuram, March 9, 2016.
9. Affordable clean water using advanced materials, Frontier Lecture Series, University of Calicut, March 22, 2016.
10. Affordable clean water using advanced materials, Inaugural lecture at the international symposium, VIT University, Vellore, May 2, 2016.
11. Innovations to address groundwater contamination, South Asia Groundwater Forum, Jaipur, June 1-3, 2016.
12. Atomically precise clusters of noble metals: From basic science to applications, School of Materials

Science and Engineering, Nanyang Technological University, June 17, 2016.

13. Nanotechnology: Prospects for tomorrow, Hindu Senior Secondary School, Triplicane, Chennai, July 5, 2016.
14. Inter-cluster reactions between atomically precise noble metal clusters, ISCAN 2016, IIST Thiruvananthapuram, July 14, 2016.
15. Affordable point-of-use water purification using nanomaterials, Indo-UK Workshop on Clean Water through Advanced and Affordable Materials, Chennai, August 8-10, 2016.
16. Clean water using advanced materials: Science, incubation and industry, Ahmedabad University, August 24, 2016.
17. Clean water using advanced materials: Science, incubation and industry Journey, from foundational research in nanotechnology to innovation led entrepreneurship, NANOBIOTECK - 2016, All India Institute of Medical Science, November 24-26, 2016.
18. Affordable Clean water using advanced materials: Science, incubation and industry, Pan Africa Chemistry Network, Nairobi, November 30 - December 2, 2016.
19. Intercluster reactions between atomically precise noble metal clusters, Asian Academic Seminar 2016, The University of Tokyo, December 14-20, 2016.

Student Activities

1. Highly luminescent silver selenide by C. K. Manju (18th Chemical Research Society of India Symposium, CRSI 2016, Punjab University), February 5-7, 2016.
2. $Ir_3Au_{22}PET_{18}$: A new alloy cluster made by inter-cluster reaction by Shridevi Bhat (18th Chemical Research Society of India Symposium, CRSI 2016, Punjab University), February 5-7, 2016.



Shridevi Bhat @ CRSI

3. Molecular ionization at low voltage from one-dimensional nanostructures by Rahul Narayanan, 64th ASMS conference on Mass Spectrometry, Texas, USA, June 5-9, 2016.
4. Avijit Baidya, Madhuri Jash, K. S. Sugi and Srikrishnarka Pillalamarri attended “The 27th Jyväskylä Summer School” at University of Jyväskylä, Finland, August 7-18, 2016

5. Avijit Baidya, Madhuri Jash, K. S. Sugi and Srikrishnarka Pillalamarri attended XVIII - International Symposium on Small Particles and Inorganic Clusters (ISSPIC), 2016, by University of Jyväskylä, Finland, August 14-19, 2016

6. Avijit Baidya, Madhuri Jash, K. S. Sugi and Srikrishnarka Pillalamarri visited Aalto University Finland – Lab visit, August 20-23, 2016.

From Left: Atanu Gosh, Papri Chakraborty, C.K. Manju, Madhuri Jash @ JSPS-DST Asian Academic Seminar

7. Unusual reactivity of dithiol protected clusters in comparison to monothiol protected clusters by Atanu Ghosh, JSPS-DST Asian Academic Seminar; Advanced Materials, Processes and Systems for Sustainable Development, 2016, The University of Tokyo, Japan, December 14-20, 2016.

8. Highly luminescent monolayer protected $Ag_{56}Se_{13}S_{15}$ clusters by C. K. Manju, JSPS-DST Asian Academic Seminar; Advanced Materials, Processes and Systems for Sustainable Development, The University of Tokyo, Japan, December 14-20, 2016.

9. Dissociation of gas phase ions of atomically precise silver clusters establishes their electronic stability by Papri Chakraborty, JSPS-DST Asian Academic Seminar; Advanced Materials, Processes and Systems for Sustainable Development, The University of Tokyo, Japan, December 14-20, 2016.

10. Naked clusters of noble metals in air formed from ligand protected clusters in solution by Madhuri Jash, JSPS-DST Asian Academic Seminar; Advanced Materials, Processes and Systems for Sustainable Development, The University of Tokyo, Japan, December 14-20, 2016.

Patents/Technology/Grants

Patent Applications

1. Cellulose nanocrystal templated iron oxyhydroxide based adsorbent for arsenic removal from water and a device thereof, T. Pradeep, Avijit Baidya, Bibhuti Bhusan Rath and A. Anil Kumar, 201641027660, filed on August 12, 2016.

2. Method of synthesis of atomically precise metal cluster-cellulose nanocrystal composite for diffusion controlled simultaneous sensing and scavenging of heavy metal ions in water, T. Pradeep, Nishil Muhammed, Avijit Baidya, A. Anil Kumar and Michael K. C. Tam, 201641031815, September 19, 2016.
3. Structure and topology conserving transformations between two archetypal nanoparticles, T. Pradeep, K. R. Krishnadas, Atanu Ghosh, Ananya Baksi and Gana Natarajan, 201641034921, October 13, 2016.
4. Method to produce unprotected naked clusters of metals of precise composition in air without mass selection, 201641035574, October 18, 2016.
5. Inbuilt water purification device for storage containers. Design patent. 287785, October 18, 2016.
6. Domestic water purification unit. Design patent. 288810, November 24, 2016.
7. Chitosan reinforced mixed oxide nanocomposite for fluoride removal from water and a device thereof, T. Pradeep, A. Anil Kumar, Bibhuti Bhusan Rath, filed on December 29, 2016.
8. Patterned metallic nanobrushes for capture of atmospheric humidity, T. Pradeep, Depanjan Sarkar, Anindita Mahapatra, Anirban Som, Avijit Baidya, filed on December 29, 2016.
9. Cellulose microstructures templated nanocomposites with enhanced arsenic removal capacity and a purifier thereof, T. Pradeep, Sritama Mukherjee, A. Anil Kumar, filed on December 30, 2016.

Patents Granted

1. On-line water purifier for hand pumps, Design application, Patent No. 271059, filed on April 6, 2015, granted on July 12, 2016.
2. A method to produce supported noble metal nanoparticles in commercial quantities for drinking water purification, T. Pradeep filed along with Aquamall Water Solutions Ltd., Patent No. 277112, filed on August 22, 2007, granted on November 10, 2016.
3. Coated mesoflowers for molecular detection and smart barcode materials, Sajanlal, P. R. and T. Pradeep, Patent No. US20160077010 A1, filed on April 30, 2014, granted on March 17, 2016.
4. Multielement and multiproperty tagging, Sajanlal, P. R. and T. Pradeep, Patent No. JP5931725 (B2), filed on August 2010, granted on June 8, 2016.

Technology Development

1. Generated over Rs. 65 lakhs of additional revenue for the Institute through royalties of one patent.

Incubation

1. InnoNano Research Private Limited (a start-up company at IIT Madras) has received orders worth over Rs. 3 crores this year.
2. Safewater Nano Pte. Ltd. The company is incorporated in Singapore, to take our water technologies to international markets. It has received funding to the tune of US$18 million.

Both are co-owned by IIT Madras.

Ongoing Research Grants

1. Thematic Unit of Excellence (TUE) on water purification using nanotechnology at IIT Madras, DST, Rs. 1081 lakhs (principal investigator)
2. Soft ionization ion mobility mass spectrometry of atomically precise clusters of noble metals, Rs. 608 lakhs (principal investigator)
3. Improve rubber to steel bonding in steel radial tyres through scientific understanding, MRF Ltd. Rs. 130 lakhs (principal investigator)
4. Dust free glass, Saint-Gobain Research India Ltd. Rs. 36 lakhs (principal investigator with Prof. R. Nagarajan)

Grants Sanctioned in 2016

1. Development of a novel combined arsenic filtration/monitoring system for community-scale water supplies, India-UK project supported by GITA, total funds Rs. 130 lakhs (principal investigator along with InnoNano Research Pvt. Ltd.)
2. Arsenic free South 24 Parganas district, DST, Rs. 374.88 lakhs (principal investigator)
3. Cluster composite nanofibre membranes for rapid, ultra-trace detection of waterborne contaminants, India-German Science and Technology Forum, Total funds Rs. 191.324 lakhs (principal investigator along with InnoNano Research Pvt. Ltd.)

Others such as JC Bose Fellowship, R&D Awards, technology development and instrument maintenance activities are managed as projects.

Media Reports (selected)

08/06/2016 IIT Madras researchers dissolve silver using glucose water - Thrissur - The Hindu

THE HINDU

» TODAY'S PAPER » EDUCATION PLUS

June 6, 2016

IIT Madras researchers dissolve silver using glucose water

- R. Prasad

Dissolution of silver by glucose is enhanced by the presence of carbonates and phosphates.Photo: Special Arrangement.

In a finding that may have many implications, IIT Madras researchers have found that silver can slowly dissolve in water if heated to about 70 degree C in the presence of glucose. As much as 0.5 weight per cent of a silver plate can get dissolved in glucose water within a week. The results of a study were published recently in the journal *Angewandte Chemie* .

Like gold, silver is a noble metal and is therefore supposed to be inert (resistant to chemical corrosion, especially to chemical reagents used in daily life). However, Prof. T. Pradeep from the Department of Chemistry, IIT Madras and his team found that silver atoms gets released from a plate in a simple, two-step mechanism — silver ions are first formed at the metal surface, which later form specific metal complexes with sugar.

"Atoms are highly reactive on the surface of the metal as they less connected and less bound and this allows the atoms to be released," said Prof. Pradeep.

Metal dissolution leads to corrosion of the plate and nanoscale pits get formed on the plate. Further dissolution occurs at the pits and as a result the pits get bigger, making a polished silvery metal appear black. Under favourable conditions, up to 10 per cent of the metal can get dissolved in 90 days.

1/6/2016 IIT-M: designer alloys by chemical reactions - The Hindu

THE HINDU

SCI-TECH » SCIENCE

Published: January 3, 2016 17:00 IST | Updated: January 4, 2016 09:41 IST January 3, 2016

IIT-M: designer alloys by chemical reactions

- R. Prasad

Photo: Special Arrangement

Clusters of gold and silver react spontaneously to make alloy clusters

Nothing whatsoever will happen if large chunks of silver and gold kept in proximity even for infinite period. But the same cannot be said when the two metals are at nanoscale.

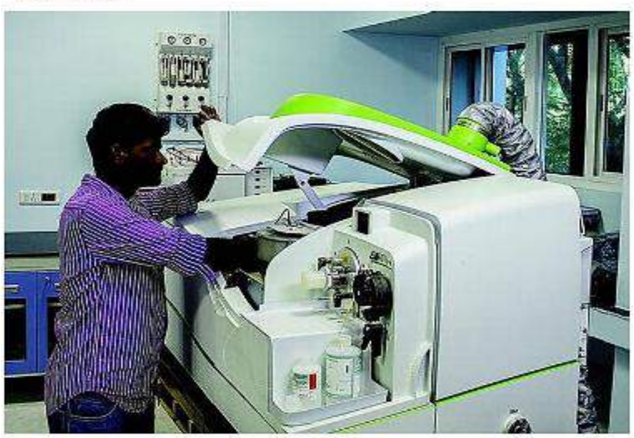
A path-breaking work by a team led by Prof. T. Pradeep, Department of Chemistry, IIT Madras has shown that two nanoscale pieces of metals react spontaneously at room temperature even in solution to make new alloys of well-defined composition. The study was published recently

23/12/2016 IIT Madras researchers prove the superiority of arsenic water filter - The Hindu

THE HINDU

SCIENCE

IIT Madras researchers prove the superiority of arsenic water filter



R. Prasad

DECEMBER 16, 2016 18:54 IST
UPDATED: DECEMBER 17, 2016 18:55 IST

Exhaustive research carried out by a team of researchers led by Prof. T. Pradeep from the Department of Chemistry at the Indian Institute of Technology (IIT) Madras, spread over four years, has put to rest the scepticism about the merits of the arsenic water filter developed by

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THE NEW INDIAN EXPRESS

Monday, March 07, 2016

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Karnataka Invites Nanotech Ventures

By Express News Service | Published: 04th March 2016 04:02 AM Last Updated: 04th March 2016 04:02 AM

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Students and delegates participating in the 8th Bangalore India Nano event in Bengaluru on Thursday | S Manjunath

BENGALURU: Karnataka on Thursday rolled out the red carpet to scientists,

MORE FROM THIS SECTION

- Karnataka Artists Hug Venkatappa Art Gallery, Fight Bid to Privatise It
- Chennabhairadevi, The Pepper Queen of India Who Ruled for 54 Years
- Man Stabbed to Death for not Recharging Mobile Phone
- Actors Sign Petition for Cheaper Movies at Karnataka Multiplexes
- Heartwarming Story of Organ Transplants
- Hold on to Your Bladder at MG Road Metro Station

THE HINDU

Tue, 10 May-16; Hindu - Chennai; Size : 198 sq.cm.; Page : 5

IIT-M incubated firm gets $ 18 million funding

SANGEETHA KANDAVEL

CHENNAI: InnoNano Research (INR), a clean water technology company incubated at IIT Madras, has received funding of $ 18 million from Nano Holdings, a US-based energy and water investment specialist firm. With this funding, INR will expand its global presence.

The clean water tech firm plans labs and offices in North America, Asia and Africa

The eight-year-old firm plans to set up a manufacturing unit, a laboratory and technology delivery offices across North America, Asia and Africa.

Thalappil Pradeep of the Department of Chemistry, IIT-M, who is one of the key members of this start up, said the funding would come over a five-year window. Of this, $ 6 million would be spent over the next three years.

"A substantial amount would be spent on research and new technologies like new membranes and new sensors. A part of this fund would be used for patent protection," he said.

INR, with the help of technology, provides drinking water, free of arsenic, fluoride and micro organisms to rural India.

This technology has been implemented across 700 villages in India including Punjab, West Bengal and Karnataka. By 2017, more than 1,500 villages will be covered, he claimed.

"The presence of arsenic and iron in drinking water affects the quality and human health. With the help of nanotechnology, it is possible to address contaminants, such as arsenic, at affordable cost," explained H. Anshup, who did his project with Prof. Pradeep. He is now the co-founder and managing director of INR.

INR's co-founders are Udhaya Shankar and Amrita Chaudhary.

The team, along with other research scholars and post-doctoral fellows, have developed a range of technologies to tackle diverse contaminants in drinking water, maintaining international quality standards.

Currently, the firm has a turnover of Rs. 2.5 crore.

23/12/2016 Produ

Indiatimes | The Times of India | The Economic

THE ECONOMIC TIMES

Science

Producing 2,000 litres of water at 140 paise per litre through renewable energy?

By HARI PULAKKAT, ET Bureau | Updated: Dec 15, 2016, 01.46 PM IST Post a Comment

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Making water at 14 paise a litre is a challenge that requires deep science and engineering. Engineers will have to apply knowledge from many fields and try to make the materials cheaply.

When T Pradeep, professor at IIT Madras, began to work on solving the world's water scarcity problem, one of his first inspirations was the darkling beetles living in deserts. These tiny creatures have learned to live in the driest of environments, by developing a mechanism to draw water out of thin air. Humanity will have enough water if it learns to mimic the insects, and yet do it in a large scale with minimum energy consumption. It is a tall order, but Pradeep and his team set to work on the problem two years ago.

Pradeep is a chemist who develops and probes nanostructures, surfaces that show their properties at scales of a few billionths of a meter. He had made a surface on which water droplets would collect, and was working on developing a device when he heard about an XPrize challenge to draw water from the atmosphere. IIT Madras quickly assembled a 30-member team with Pradeep as the lead. They would have two years to develop a product that can draw 2,000 litres of water from the atmosphere in one day. The XPrize challenge was announced late last month, and its parameters went well beyond what anybody could do at the moment.

The winning team has to use only renewable energy, and has to produce 2,000 litres of water costing two cents (roughly 140 paise) per litre. There are a large number of water capture devices selling around the world, but none that could work at this efficiency and cost. "To make water at two cents a litre is audacious," says Zenia Tata, executive director

Tiny particles with mega impacts | The Source http://www.thesourcemagazine.org/tiny-particles

Tiny particles with mega impacts

By quad011 - February 29, 2016

A water purification unit using nanomaterials connected to a handpump © Indian Institute of Technology, Madras

In India, a research scientist and his team are manipulating invisible n
in ways that could quietly disrupt the global water purification industr

Service 2016

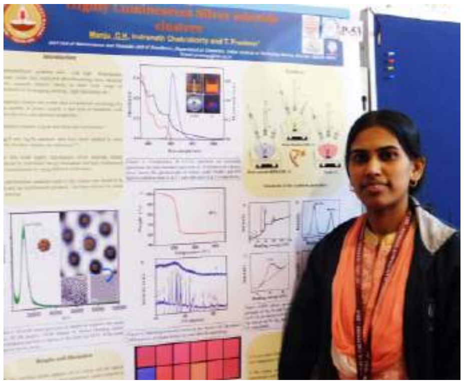
1. Associate Editor of the Journal, *ACS Sustainable Chemistry & Engineering.*
2. Member, Editorial Board of the Journal, *Chemistry – An Asian Journal.*
3. Member, Advisory Board of the Journal, *Nanoscale.*
4. Member, Editorial Board of the Journal, *Scientific Reports (Nature Group).*
5. International Editorial Advisory Board Member of the Journal, *Particle.*
6. International Editorial Advisory Board Member of the Journal, *Surface Innovations.*
7. Member, Editorial board of *International Journal of Water and Wastewater Treatment.*
8. Member, India-Japan Council of the Department of Science and Technology.
9. Member, Nanoscience Advisory Committee, Nano Mission, Department of Science and Technology.
10. Member, Proof of Concept Expert Committee, Nano Mission, Department of Science and Technology.
11. Member, Executive Committee, Neutron Scattering Society of India.
12. Vice President of the Indian Society for Mass Spectrometry.
13. Member of the Council of Materials Research Society of India.
14. Member, Bureau of Indian Standards – on drinking water products.
15. Member, Board of studies of the Department of Atomic and Molecular Physics, Manipal University.
16. Member, Board of School of Life Sciences, Ahmedabad University.

Recognition

Students

1. C. K. Manju, CRSI- RSC Best Poster Award for the poster titled "Highly Luminescent Silver Selenide Clusters", February 7, 2016.
2. K. R. Krishnadas received one of the best posters award at the 8th Bangalore India Nano conference, The Lalit Ashok, Bengaluru, March 4, 2016.
3. Depanjan Sarkar, 'Malhotra Weikfield Foundation-Bangalore Nano Young Scientist Award 2016' for the young researchers in the field of nanotechnology by the Govt. of Karnataka, March 4, 2016.

4. The group won "Best exhibitor award" in the category of innovative display at the 8th Bangalore India Nano conference, The Lalit Ashok, Bengaluru, 2016.
5. Depanjan Sarkar, Institute research scholar award, 57th Institute day, IIT Madras, April 25, 2016.
6. C. K. Manju, I. Chakraborty and T. Pradeep. (2016). ***DOI: 10.1039/c6tc01388k*** is considered as part of themed collection: 2016 Journal of Materials Chemistry C ***Hot Papers,*** June 15, 2016.
7. Avijit Baidya, Best Presentation award at Research Scholars Day ID, August 23, 2016.
8. Papri Chakraborty, One of the best Poster Awards at DST-JSPS Asian Academic Seminar, Tokyo, December 19, 2016.
9. Atanu Ghosh, One of the best Poster Awards at DST-JSPS Asian Academic Seminar, Tokyo, December 19, 2016.



C. K. Manju @ CRSI

Alumni News

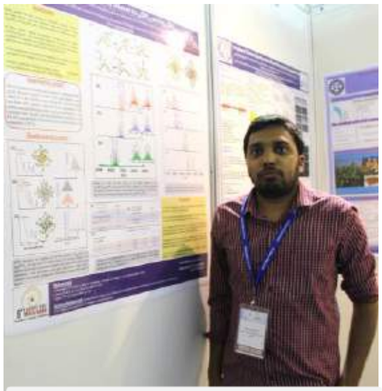
1. Radha Gobinda Bhuin, received SERB overseas Postdoctoral fellow fellowship 2016.
2. Radha Gobinda Bhuin, joined Friedrich Alexander Universität Erlangen Nürnberg (Hans- Peter Steinrück's research group) as a Postdoctoral fellow.
3. G. Velmurugan, Postdoctoral fellow, Cancer and Genetics Research Centre, College of Medicine, University of Florida, Gainesville, Florida, USA.
4. Udayabhaskararao Thumu, Postdoctoral fellow Nanophotonics Group, Prof. Dan Oron, Dept of Physics of Complex Systems, Weizmann Institute of Science Rehovot, Israel.
5. Balanagulu Busupalli (Bala), Postdoctoral fellow in the 'Origins of Life Initiative' at Harvard University from June 1st, 2016.
6. M. S. Bootharaju, Postdoctoral fellow, C/O Prof. Jean-Marie Basset KAUST Catalysis Center (KCC) King Abdullah University of Science and Technology, Saudi Arabia.

Depanjan Sarkar receiving 'Malhotra Weikfield Foundation - Young Scientist Award' from Prof. C. N. R. Rao @ 8th Bangalore India Nano conference

7. Soumabha Bag, Postdoctoral fellow at Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany.
8. Ananya Bakshi, Postdoctoral fellow at Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany.
9. Kamalesh Chaudhari, Principal scientist in Safe Water Innovation India Pvt. Ltd. under the project title, "Development of in-line arsenic sensor for Amrit water filter".
10. Akshaya Kumar Samal, Postdoctoral Researcher KAUST Catalysis Center, King Abdullah University of Science & Technology, Thuwal 23955-6900, Kingdom of Saudi Arabia.
11. David Jeba Singh, Mass spectrometry specialist, Agilent Partner Laboratory, Gulf Bio Analytical Dubai, UAE.
12. Aniruddha Molla, Postdoctoral Researcher, BK21 Plus (Korea Research Foundation) C/O Prof. Jin Suk Chung School of Chemical Eng. & Bioeng, University of Ulsan.
13. T. S. Sreeprasad, NASA space grant: to develop 2D polymer-based solar cells.
14. T. S. Sreeprasad, A seed funding to work on next-gen, nanomaterial-based energy generators.
15. T. S. Sreeprasad, Industrial funding to develop novel wash down coating for gear

Graduation

PhD (viva completed, convocation 2017)



K. R. Krishnadas @ 8th Bangalore India Nano conference

1. **Anirban Som**, Department of Chemistry, IIT Madras, 2016.
   Investigations into the reactivity of tellurium nanowires with ionic, molecular and metallic silver, 2016.

2. **Rabin Rajan Methikkalam**, Department of Chemistry, IIT Madras, 2016.
   Physico-chemical changes at icy surfaces of relevance to astrochemical processes, 2016.

3. **K. R. Krishnadas**, Department of Chemistry, IIT Madras, 2016.
   Chemical reactions of atomically precise noble metal clusters, 2016.

4. **Soujit Sengupta**, Department of Chemistry, IIT Madras, 2016.
   Graphenic materials for affordable clean water, 2016.

M.Sc.

1. **Anindita Mahapatra**, Department of Chemistry, IIT Madras, 2016
2. **Bibhuti Bhusan Rath**, Department of Chemistry, IIT Madras, 2016
3. **Esma Khatun**, Department of Chemistry, IIT Madras, 2016
4. **Pallab Basuri**, Department of Chemistry, IIT Madras, 2016
5. **Tripti Ahuja**, Department of Chemistry, IIT Madras, 2016

Summer Student(s) / Fellow(s) - 2016

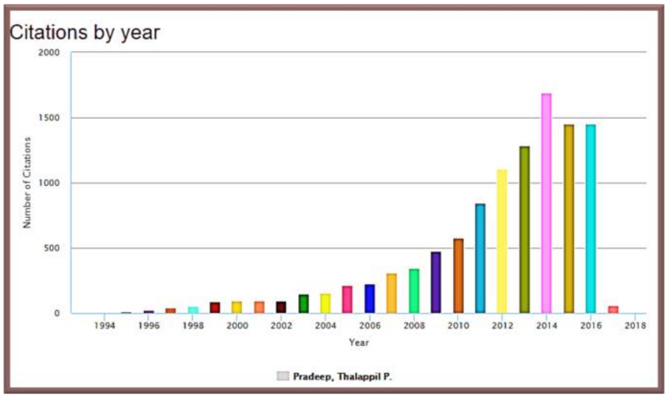
Visiting Student(s) - 2016

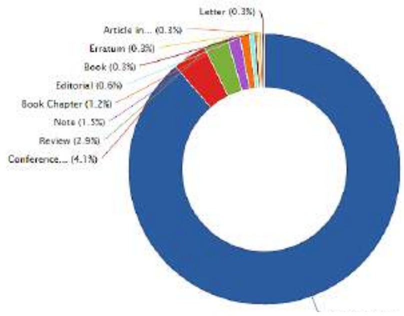
Erick Kiage Mobegi from Kenyatta University, Kenya, NAM S&T Centre Research Training Fellowship for Developing Country Scientists (RTF-DCS)

Sahana Sheshachala from Karlsruhe Institute for Technology, Indo-German Project

Publication Analysis

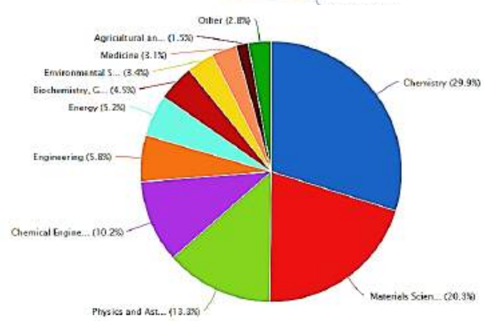
Source: Scopus, December 22, 2016





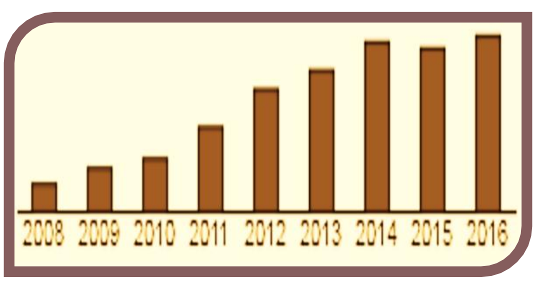
Documents by type

Citations	10850
Average Citation per Items	31.53
h-index	51



Documents by subject area

Source: Google Scholar, December 21, 2016



Citation indices	
Citations	15223
H-index	60
i10 index	239

Glimpses of 2016

Our team during the inauguratation of TUE

Chief guest at the convocation ceremony of Sankara Nethralaya, with Dr. S. S. Badrinath

ISCAN 2016, organised by IISER Thiruvananthapuram

InnoNano team with representatives of the institute, alumini & DST (product AMRIT on display)

Stall at Banglore India Nano

DST-JSPS Asian Academic Seminar, Tokyo

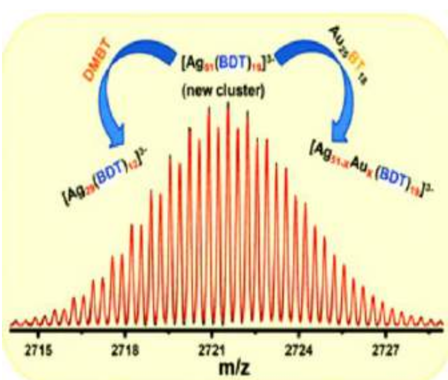
ABSTRACTS OF JOURNAL PAPERS

UNUSUAL REACTIVITY OF DITHIOL PROTECTED CLUSTERS IN COMPARISON TO MONOTHIOL PROTECTED CLUSTERS: STUDIES USING $Ag_{51}(BDT)_{19}(TPP)_3$ AND $Ag_{29}(BDT)_{12}(TPP)_4$

Atanu Ghosh, Debasmita Ghosh, Esma Khatun, Papri Chakraborty and T. Pradeep

Nanoscale, DOI: 10.1039/C6NR07692K

ABSTRACT: We report the synthesis and unique reactivity of a new green dithiol protected cluster (DTPC), $Ag_{51}(BDT)_{19}(TPP)_3$ (BDT and TPP are 1,3-benzenedithiol and triphenylphosphine, respectively). The cluster composition was confirmed by electrospray ionization (ESI) and matrix-assisted laser desorption ionization (MALDI) mass spectrometric studies as well as by other supporting data. Surprisingly, the chemical reactivity between this DTPC and $Au_{25}(SR)_{18}$ involves only metal ion exchange in $Au_{25}(SR)_{18}$ without any ligand exchange, while reactions between monothiol protected clusters (MTPCs) show both metal and ligand exchange, an example being the reaction between $Ag_{25}DMBT_{18}$ and $Au_{25}PET_{18}$ (where DMBT and PET are 2,4-dimethylbenzenethiol and phenylethanethiol, respectively). The conclusions have been confirmed by the reaction of another DTPC, $Ag_{29}(BDT)_{12}(TPP)_4$ with $Au_{25}BT_{18}$ (where BT corresponds to butanethiol) in which only metal exchange happens in $Au_{25}BT_{18}$. We also show the conversion of $Ag_{51}(BDT)_{19}(TPP)_3$ to $Ag_{29}(BDT)_{12}(TPP)_4$ in the presence of a second monothiol, DMBT which does not get integrated into the product cluster. This is completely different from the previous understanding wherein the reaction between MTPCs and a second thiol leads to either mixed thiol protected clusters with the same core composition or a completely new cluster core protected with the second thiol. The present study exposes a new avenue of research for monolayer protected clusters, which in turn will give additional impetus to explore the chemistry of DTPCs.

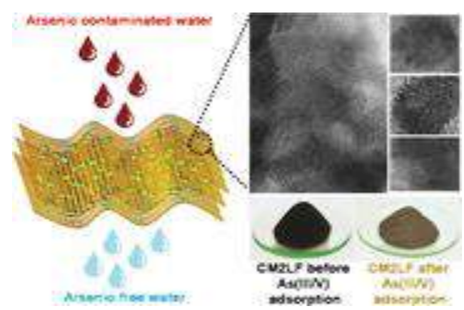


CONFINED METASTABLE 2-LINE FERRIHYDRITE FOR AFFORDABLE POINT-OF-USE ARSENIC FREE DRINKING WATER

Anil Kumar Avula, Anirban Som, Paolo Longo, Chennu Sudhakar, Radha Gobinda Bhuin, Soujit Sen Gupta, Anshup, Mohan Udhaya Sankar, Amrita Chaudhary, Ramesh Kumar and T. Pradeep

Adv. Mat., **DOI:** 10.1002/adma.201604260

ABSTRACT: Arsenic-free drinking water, independent of electrical power and piped water supply, is possible only through advanced and affordable materials with large uptake capacities. Confined metastable 2-line ferrihydrite, stable at ambient temperature, shows continuous arsenic uptake in the presence of other complex species in natural drinking water and an affordable water purification device has been made using the same.

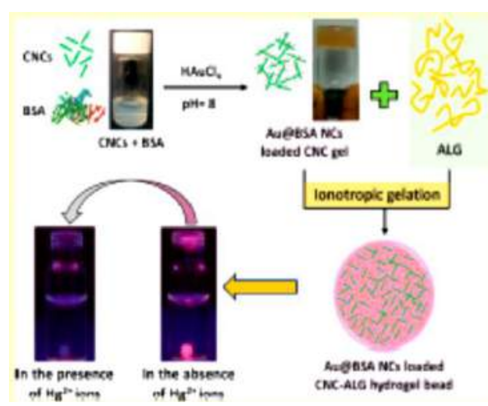


DIFFUSION CONTROLLED SIMULTANEOUS SENSING AND SCAVENGING OF HEAVY METAL IONS IN WATER USING ATOMICALLY PRECISE CLUSTER – CELLULOSE NANOCRYSTAL COMPOSITES

Nishil Mohammed, Avijit Baidya, Vasanthanarayan Murugesan, Anil Kumar Avula, Mohd Azhardin Ganayee, Jyoti Mohanty, Tam, Kam (Michael) and T. Pradeep

ACS Sustainable Chem. Eng., **DOI:** 10.1021/acssuschemeng.6b01674

ABSTRACT: Development of a system that can simultaneously sense and scavenge toxic heavy metal ions at low concentrations is an ideal solution for in-situ monitoring and purification of contaminated water. In this paper, we report on the synthesis and application of a novel system, luminescent atomically precise cluster – cellulose nanocrystal composite namely bovine serum albumin protected gold nanoclusters (Au@BSA NCs) loaded cellulose nanocrystal – alginate hydrogel beads that can simultaneously sense and scavenge heavy metal ions, specifically mercury ions in water. Characterization of the system performed using scanning electron microscopy coupled with



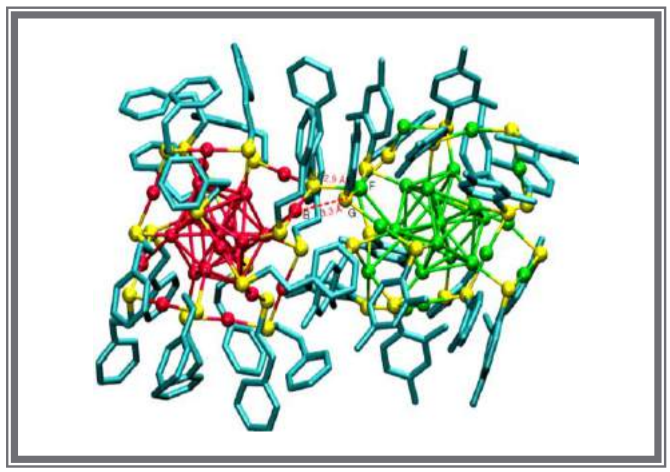
energy dispersive spectroscopy and X-ray photoelectron spectroscopy elucidated the physical and chemical characteristics of the system. Additionally, we proposed a new method to visualize the diffusion phenomenon and calculated the effective diffusion coefficient of heavy metal ions in hydrogel beads by monitoring the fluorescence quenching dynamics of Au@BSA NCs upon binding with mercury ions. Finally, practical applications of this nanocomposite were demonstrated using batch adsorption experiments as well as using a dip pen device loaded with the hydrogel beads for in-situ monitoring of heavy metal ions in water.

STRUCTURE-CONSERVING SPONTANEOUS TRANSFORMATIONS BETWEEN NANOPARTICLES

K. R. Krishnadas, Ananya Baksi, Atanu Ghosh, Ganapati Natarajan and T. Pradeep

Nat. Commun., **DOI**: 10.1038/ncomms13447

ABSTRACT: Ambient, structure- and topology-preserving chemical reactions between two archetypal nanoparticles, $Ag_{25}(SR)_{18}$ and $Au_{25}(SR)_{18}$ are presented. Despite their geometric robustness and electronic stability, reactions between them in solution produce alloys, $Ag_mAu_n(SR)_{18}$ (m+n=25) keeping their M25(SR)18 composition, structure and topology intact. We demonstrate that a mixture of $Ag_{25}(SR)_{18}$ and $Au_{25}(SR)_{18}$ can be transformed to any arbitrary alloy composition, AgmAun(SR)18 (n=1-24) merely by controlling the reactant compositions. We capture one of the earliest events of the process, namely the formation of the dianionic adduct, $[Ag_{25}Au_{25}(SR)_{36}]^{2-}$, by electrospray ionization mass spectrometry. Molecular docking simulations and density functional theory (DFT) calculations also suggest that metal atom exchanges occur through the formation of an adduct between the two clusters. DFT calculations further confirm that metal atom exchanges are thermodynamically feasible. Such isomorphous transformations between nanoparticles imply that microscopic pieces of matter can be transformed completely to chemically different entities, preserving their structures, at least in the nanometric regime



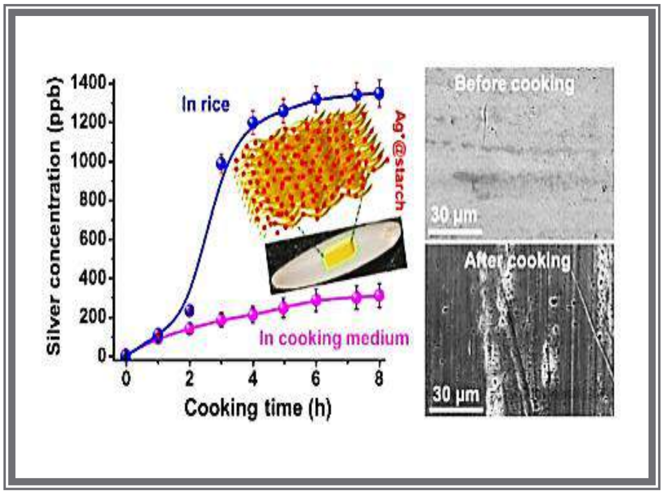
COOKING INDUCED CORROSION OF METALS

Soujit Sen Gupta, Ananya Baksi, Vidhya Subramanian and T. Pradeep

ACS Sustain. Chem. Eng., **DOI**: 10.1021/acssuschemeng.6b00980

ABSTRACT: Uptake of metal ions into rice occurs while it is being cooked in metal vessels, leading to corrosion of the utensils. This study deals with silver, copper, and aluminium uptake during cooking in respective vessels, with a special emphasis on silver. The metal uptake is routed

through solution, enhanced in the presence of specific anions like carbonate, and attenuated when the rice is polished. The concentration of silver in rice increases with the time of cooking with a concomitant decrease in the concentrations of Fe and Zn, suggesting a substitution mechanism for metal ion uptake. The results for some common rice varieties of use across the Indian subcontinent are presented. Similar behavior was observed for cooking in copper and aluminum vessels. Among the three metals studied, aluminum showed reduced uptake. Studies have been done to probe the interaction of metal ions with glucose and sucrose, and efficient complex formation was detected with all these ions, implying that starch



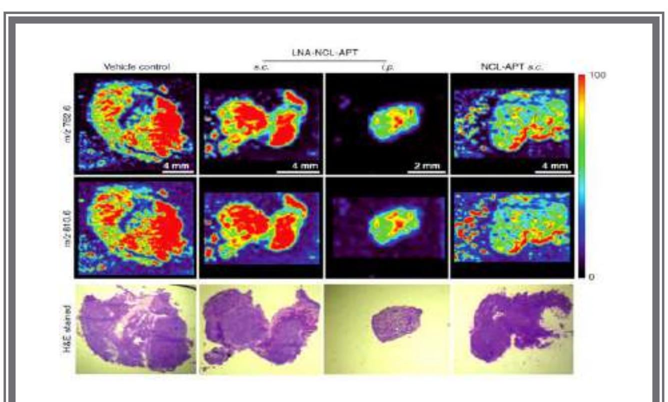
can also form complexes with them. The cooking practices used in this study are reminiscent of local customs and practices that were chosen deliberately to relate to the true implications of these results.

NUCLEOLIN-APTAMER THERAPY IN RETINOBLASTOMA: MOLECULAR CHANGES AND MASS SPECTROMETRY–BASED IMAGING

Nithya Subramanian, Amitava Srimany, Jagat R Kanwar, Rupinder K Kanwar, Balachandran Akilandeswari, Pukhraj Rishi, Vikas Khetan, Madavan Vasudevan, T. Pradeep and Subramanian Krishnakumar

Mol. Ther. Nucleic Acids, **DOI:** 10.1021/acssuschemeng.6b00980

ABSTRACT: Retinoblastoma (RB) is an intraocular childhood tumor which, if left untreated, leads to blindness and mortality. Nucleolin (NCL) protein which is differentially expressed on the tumor cell surface, binds ligands and regulates carcinogenesis and angiogenesis. We found that NCL is over expressed in RB tumor tissues and cell lines compared to normal retina. We studied the effect of nucleolin-aptamer (NCL-APT) to reduce proliferation in RB tumor cells. Aptamer treatment on the RB cell lines (Y79 and WERI-Rb1) led to significant inhibition of cell proliferation. Locked nucleic acid (LNA) modified NCL-APT administered subcutaneously (s.c.) near tumor or intraperitoneally (i.p.) in Y79 xenografted nude mice resulted in 26 and 65% of tumor growth inhibition, respectively. Downregulation of inhibitor of apoptosis proteins, tumor miRNA-18a, altered serum cytokines, and serum miRNA-18a levels were observed upon NCL-APT treatment. Desorption electrospray ionization mass



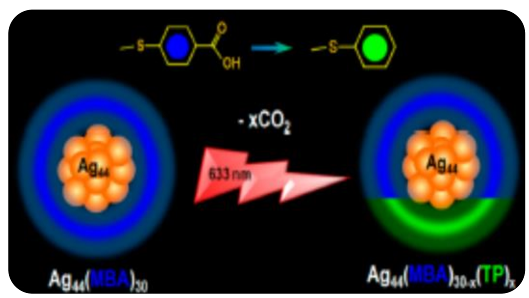
spectrometry (DESI MS)-based imaging of cell lines and tumor tissues revealed changes in phosphatidylcholines levels upon treatment. Thus, our study provides proof of concept illustrating NCL-APT-based targeted therapeutic strategy and use of DESI MS-based lipid imaging in monitoring therapeutic responses in RB.

TOWARDS A JANUS CLUSTER: REGIOSPECIFIC DECARBOXYLATION OF Ag_{44}(4-MBA)$_{30}$@Ag NANOPARTICLES

Indranath Chakraborty, Anirban Som, Tuhina Adit Maark, Biswajit Mondal, Depanjan Sarkar, and Thalappil Pradeep

J. Phys. Chem. C, **DOI:** 10.1021/acs.jpcc.6b04769

ABSTRACT: The ligand shell structure of the aspicule Ag_{44}(4-MBA)$_{30}$ (MBA: mercaptobenzoic acid, in the thiolate form) was modified in a precise, site-specific manner. Laser irradiation at 633 nm of a monolayer assembly of plasmonic Ag nanoparticles (NPs) covered with Ag_{44}(4-MBA)$_{30}$ clusters leads to decarboxylation of 4-MBA ligands forming thiophenolate (TP) ligands. While the molecular identity and integrity of aspicules post laser irradiation were confirmed by ESI MS, time-dependent SERS spectra and computational studies suggest that the phenomenon of decarboxylation is limited to the 4-MBA ligands facing the NP surface. This creates modified Ag_{44} clusters, with 4-MBA ligands on one side and TP ligands on the other, giving them a two-faced (Janus) ligand structure. The ligand distribution of such clusters gets equilibrated in solution. We show that such selective transformation can be used to create molecular patterns. Janus clusters may be important in chemistry at biphasic interfaces.

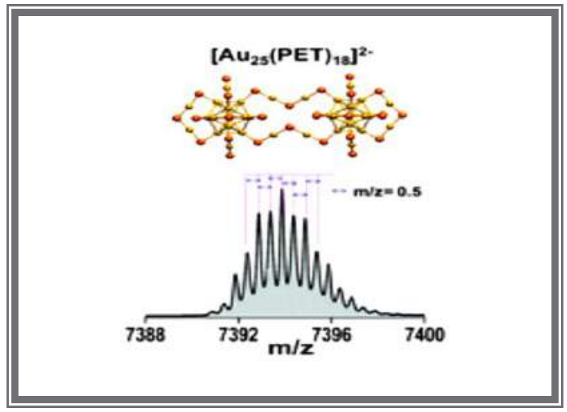


$[AU_{25}(SR)_{18}]_2^{2-}$: A NOBLE METAL CLUSTER DIMER IN THE GAS PHASE

Ananya Baksi, Papri Chakraborty, Shridevi Bhat, Ganapati Natarajan and T. Pradeep

Chem. Commun., **DOI:** 10.1039/c6cc03202h

ABSTARCT: We present the first example of dimer formation in the monolayer protected atomically precise cluster system, $Au_{25}(SR)_{18}$, using ion mobility mass spectrometry. These transient species are shown to be important in explaining chemical reactivity between clusters.

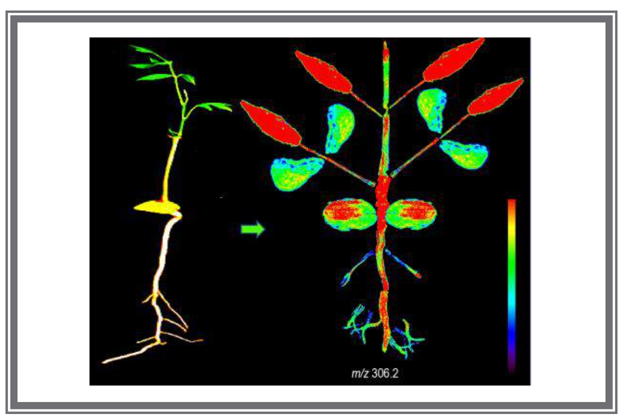


DESORPTION ELECTROSPRAY IONIZATION (DESI) MASS SPECTROMETRIC IMAGING OF THE DISTRIBUTION OF ROHITUKINE IN THE SEEDLING OF *DYSOXYLUM BINECTARIFERUM* HOOK. F

Mohana Kumara P, Amitava Srimany, Suganya Arunan, Ravikanth G, Uma Shaanker R and T. Pradeep

PLoS. ONE., **DOI:** 10.1371/journal.pone.0158099

ABSTRACT: Ambient ionization mass spectrometric imaging of all parts of the seedling of *Dysoxylum binectariferum* Hook. f (Meliaceae) was performed to reconstruct the molecular distribution of rohitukine (Rh) and related compounds. The species accumulates Rh, a prominent chromone alkaloid, in its seeds, fruits, and stem bark. Rh possesses anti-inflammatory, anticancer, and immuno-modulatory properties. Desorption electrospray ionization mass spectrometry imaging (DESI MSI) and electrospray ionization (ESI) tandem mass spectrometry (MS/MS) analysis detected Rh as well as its glycosylated, acetylated, oxidized, and methoxylated analogues. Rh was predominantly distributed in the main roots, collar region of the stem, and young leaves. In the stem and roots, Rh was primarily restricted to the cortex region. The identities of the metabolites were assigned based on both the fragmentation patterns and exact mass analyses. We discuss these results, with specific reference to the possible pathways of Rh biosynthesis and translocation during seedling development in *D. binectariferum.*

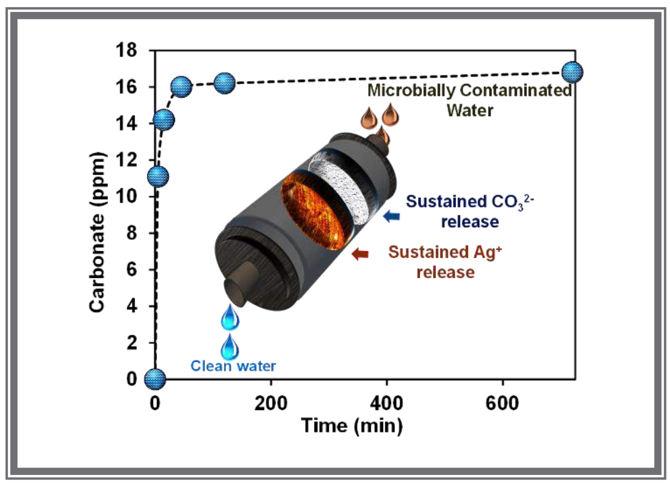


SPARINGLY SOLUBLE CONSTANT CARBONATE RELEASING INERT MONOLITH FOR ENHANCEMENT OF ANTIMICROBIAL SILVER ACTION AND SUSTAINABLE UTILIZATION

Swathy Jakka Ravindran, Nalenthiran Pugazhenthiran, Sudhakar Chennu, Anil Kumar Avula and T. Pradeep

ACS Sustain. Chem. Eng., **DOI:** 10.1021/acssuschemeng.6b00979

ABSTRACT: Silver, a metal with phenomenal commercial importance has been exploited in its ionic form in the field of water purification, with the objective of delivering microbially safe drinking water. Silver released at such concentrations is unrecoverable and has to be reduced to ensure sustainable utilization of the metal. We have shown that small concentrations of carbonate can effectively brin g down the amount of silver ion used for microbial disinfection by half. Implementation of this finding requires constant carbonate releasing materials in natural water for an extended period. In this work, we describe a hybrid material with intrinsically high stability in water that is prepared using naturally abundant ingredients which releases carbonate constantly and in a controlled fashion. This composition in conjunction with reduced silver ion concentration delivers mircobially safe water, tested with *E. coli* and MS2 phage. Use of constant carbonate releasing material for antimicrobial applications can reduce the unrecoverable silver released into the environment by ~1300 tons/year. We also show that the composition can be modified to release cations of choice without disturbing the CO_3^{2-} release from the same. A sustained release of selective cations along with carbonate can supplement drinking water with the minerals of interest.



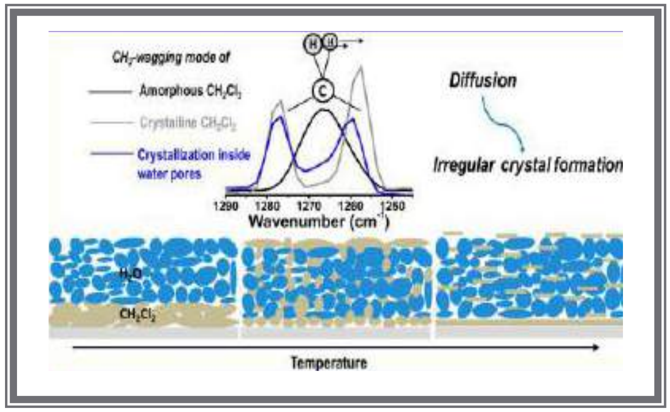
DIFFUSION AND CRYSTALLIZATION OF DICHLOROMETHANE WITHIN THE PORES OF AMORPHOUS SOLID WATER

Radha Gobinda Bhuin, Rabin Rajan J. Methikkalam, Soumabha Bag and T. Pradeep

J. Phys. Chem. C, **DOI:** 10.1021/acs.jpcc.6b00436

ABSTRACT: Dichloromethane (CH_2Cl_2) thin films deposited on Ru(0001) at low temperatures (~80 K or lower) undergo a phase transition at ~95 K, manifested by the splitting of its wagging mode

at 1265 cm−1, due to factor group splitting. This splitting occurs at relatively higher temperatures (~100 K) when amorphous solid water (ASW) is deposited over it, with a significant reduction in intensity of the high-wavenumber component (of the split peaks). Control experiments showed that the intensity of the higher wavenumber peak is dependent on the thickness of the water overlayer. It is proposed that diffusion of CH_2Cl_2 into ASW occurs and it crystallizes within the pores of ASW, which increases the transition temperature. However, the dimensions of the CH_2Cl_2 crystallites get smaller with increasing thickness of ASW with concomitant change in the intensity of the factor group split peak. Control experiments support this suggestion. We propose that the peak intensities can be correlated with the porosity of the ice film. Diffusion of CH_2Cl_2 has been supported by low-energy Cs^+ scattering and temperature-programmed desorption spectroscopies

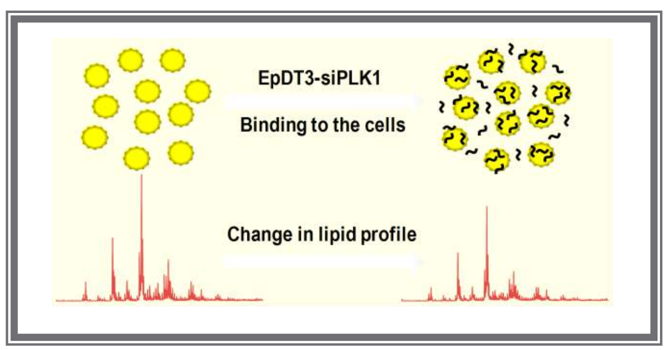


MONITORING OF CHANGES IN LIPID PROFILES DURING PLK1 KNOCKDOWN IN CANCER CELLS USING DESI MS

Balasubramanyam Jayashree, Amitava Srimany, Srinidhi Jayaraman, Anjali Bhutra, Narayanan Janakiraman, Srujana Chitipothu, Subramanian Krishnakumar, Lakshmi Subhadra Baddireddi, Sailaja Elchuri and T. Pradeep

Anal. Bioanal. Chem., **DOI:** 10.1007/s00216-016-9665-y

ABSTRACT: The importance of the polo-like kinase 1 (PLK1) gene is increasing substantially both as a biomarker and as a target for highly specific cancer therapy. This is due to its involvement in multiple points of cell progression and carcinogenesis. PLK1 inhibitors' efficacy in treating human cancers has been limited due to the lack of a specific targeting strategy. Here, we describe a method of targeted downregulation of PLK1 in cancer cells and the concomitant rapid detection of surface lipidomic perturbations using desorption electrospray ionization mass spectrometry (DESI MS). The efficient delivery of siRNA targeting PLK1 gene selectively to the cancer cells is achieved by targeting overexpressed cell surface epithelial cell adhesion molecule (EpCAM) by the EpDT3 aptamer. The chimeric aptamer (EpDT3-siPLK1) showed the knockdown of PLK1 gene expression and PLK1 protein levels by quantitative PCR and western blotting, respectively. The abundant sur face lipids, phosphatidylcholines (PCs), such as PC(32:1) (m/z



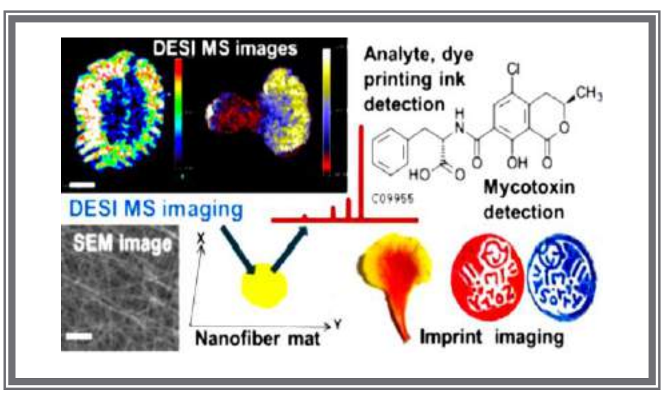
754.6), PC(34:1) (*m/z* 782.6), and PC(36:2) (*m/z* 808.6), were highly expressed in MCF-7 and WERI-RB1 cancer cells compared to normal MIO-M1 cells and they were observed using DESI MS. These overexpressed cell surface lipids in the cancer cells were downregulated upon the treatment of EpDT3-siPLK1 chimera indicating a novel role of PLK1 to regulate surface lipid expression in addition to the efficient selective cancer targeting ability. Our results indicate that DESI MS has a potential ability to rapidly monitor aptamer-mediated cancer therapy and accelerate the drug discovery process.

ELECTROSPUN NANOFIBER MATS AS "SMART SURFACES" FOR DESORPTION ELECTROSPRAY IONIZATION MASS SPECTROMETRY (DESI MS)-BASED ANALYSIS AND IMPRINT IMAGING

R. G. Hemalatha, Mohd Azhardin Ganayee and T. Pradeep

Anal. Chem., **DOI:** 10.1021/acs.analchem.5b04520

ABSTRACT: In this paper, desorption electrospray ionization mass spectrometry (DESI MS)-based molecular analysis and imprint imaging using electrospun nylon-6 nanofiber mats are



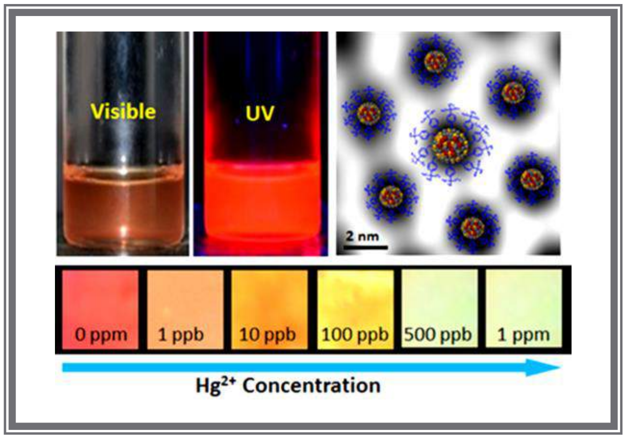
demonstrated for various analytical contexts. Uniform mats of varying thicknesses composed of ~200 nm diameter fibers were prepared using needleless electrospinning. Analytical applications requiring rapid understanding of the analytes in single drops, dyes, inks, and/or plant extracts incorporated directly into the nanofibers are discussed with illustrations. The possibility to imprint patterns made of printing inks, plant parts (such as petals, leaves, and slices of rhizomes), and fungal growth on fruits with their faithful reproductions on the nanofiber mats is illustrated with suitable examples. Metabolites were identified by tandem mass spectrometry data available in the literature and in databases. The results highlight the significance of electrospun nanofiber mats as smart surfaces to capture diverse classes of compounds for rapid detection or to imprint imaging under ambient conditions. Large surface area, appropriate chemical functionalities exposed, and easiness of desorption due to weaker interactions of the analyte species are the specific advantages of nanofibers for this application.

HIGHLY LUMINESCENT MONOLAYER PROTECTED $Ag_{56}Se_{13}S_{15}$ CLUSTERS

C. K. Manju, Indranath Chakraborty and T. Pradeep

J. Mater. Chem. C, **DOI:** 10.1039/c6tc01388k

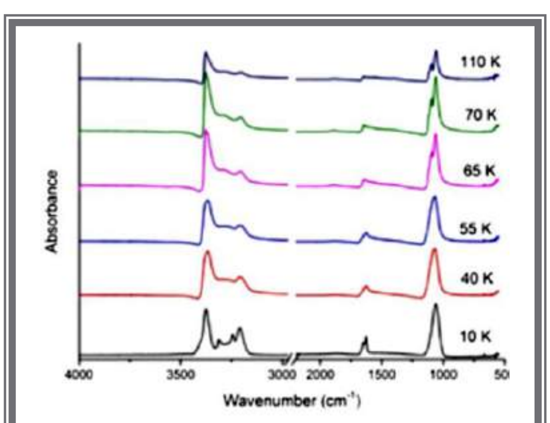
ABSTRACT: A highly luminescent (quantum yield 21%) mixed chalcogenide silver cluster, $Ag_{56}Se_{13}S_{15}$ cluster of Ag_2X stoichiometry, protected with 4-tert-butylbenzyl mercaptan ligand has been synthesized and characterized. Collective investigation from diverse tools of analyses such as mass spectrometry, elemental analysis, thermogravimetry and X-ray diffraction point to this composition. The cluster emits in the solution and in the solid state and has been deposited on oxide supports to get red emitting films. The specificity of cluster emission to mercuric ion, among a rage of heavy metal ions has been used to develop a sensor, which shows sensitivity down to 1 ppb. A pH paper-like visual detector has been developed by combining the Hg(II)-sensitive emission of the cluster and insensitive emission of fluorescein isothiocyanate. The test strip shows visual detection down to 1 ppb in real water samples.



THIO RESIDUE FROM THERMAL PROCESSING OF COMETARY ICES CONTAINING CARBON DISULFIDE AND AMMONIA

Rabin Rajan J. Methikkalam, S. Pavithraa, S. P. Murali Babu, H. Hill, Raja Sekhar, T Pradeep and B. Sivaraman

Adv. Space. Res., **DOI:**10.1016/j.asr.2016.04.028



ABSTRACT: We have carried out experimental investigation on binary ice mixture containing carbon disulfide (CS_2) and ammonia (NH_3) ices formed at 10 K. Icy films were formed in various combinations to investigate the reactivity of CS_2 and NH_3 molecules on cometary nucleus. In the case of NH_3 ices, deposition carried out at 10 K was found to contain NH3 homo-dimers that was found to reorient upon annealing to 40 K. Phase transition was found to take place as the 10 K ice

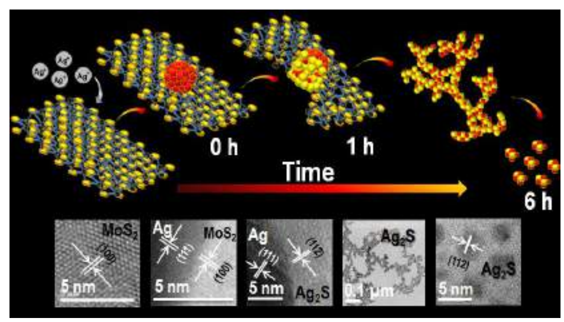
was warmed to higher temperatures and the phase transition temperature was found to be 5 K higher for the mixed ice in comparison to the layered deposits. Thermal processing of the mixed deposition of CS_2-NH_3 ice was found to leave thio residue, which could be ammonium dithiocarbamate that was even found to be present at 340 K.

UNUSUAL REACTIVITY OF MoS_2 NANOSHEETS

Biswajit Mondal, Anirban Som, Indranath Chakraborty, Ananya Baksi, Depanjan Sarkar and T. Pradeep

Nanoscale, **DOI:** 10.1039/c6nr00878j

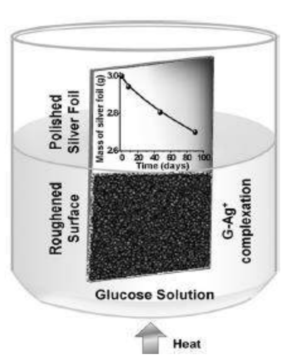
ABSTRACT: The reactivity of the 2D nanosheets of MoS_2 with silver ions in solution, leading to their spontaneous morphological and chemical transformations, is reported. This unique reactivity of the nanoscale form of MoS_2 was in stark contrast to its bulk counterpart. While the gradual morphological transformation involving several steps has been captured with an electron microscope, precise chemical identification of the species involved was achieved by electron spectroscopy and mass spectrometry. The energetics of the system investigated supports the observed chemical transformation. The reaction with mercury and gold ions shows similar and dissimilar reaction products, respectively and points to the stability of the metal–sulphur bond in determining the chemical compositions of the final products.



EXTRACTION OF SILVER BY GLUCOSE

Ananya Baksi, Mounika Gandi, Swathi Chaudhari, Soumabha Bag, Soujit Sen Gupta and T. Pradeep

Angew. Chem. Int. Ed, **DOI:** 10.1002/anie.201510122



ABSTRACT: Unprecedented silver ion leaching, in the range of 0.7 ppm was seen when metallic silver was heated in water at 70°C in presence of simple carbohydrates, such as glucose, making it a green method of silver extraction. Extraction was facilitated by the presence of anions, such as carbonate and phosphate. Studies confirm a two-step mechanism of silver release, first forming silver ions at the metal surface and later

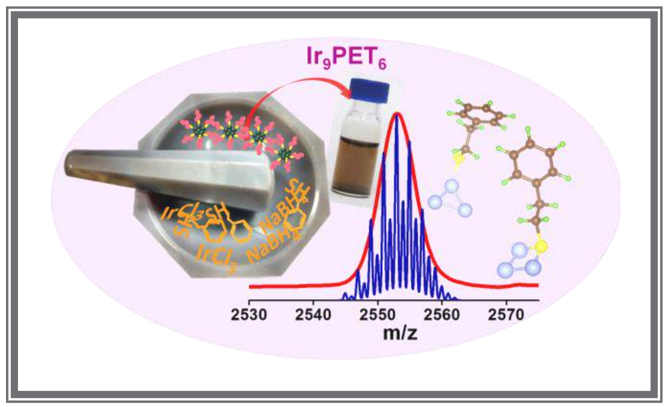
complexation of ionic silver with glucose; such complexes have been detected by mass spectrometry. Extraction leads to microscopic roughening of the surface making it Raman active with an enhancement factor of 5×10^8.

ATOMICALLY PRECISE AND MONOLAYER PROTECTED IRIDIUM CLUSTERS IN SOLUTION

Shridevi Bhat, Indranath Chakraborty, Tuhina Adit Maark, Anuradha Mitra, Goutham De and T. Pradeep

RSC Adv., **DOI:** 10.1039/c5ra27972k

ABSTRACT: The first atomically precise and monolayer protected iridium cluster in solution, $Ir_9(PET)_6$ (PET–2-phenyethanethiol) was synthesized via a solid state method. The absence of a plasmonic band at ~350 nm, expected in the UV/Vis spectra for spherical Ir particles of 10 nm size indicated that the synthesized cluster is smaller than this dimension. Small angle X-ray scattering (SAXS) showed that the cluster has a particle size of ~2 nm in solution which was confirmed by transmission electron microscopy (TEM). The blue emission of the cluster is much weaker than many noble metal clusters investigated so far. X-ray photoelectron spectroscopy (XPS) measurements showed that all Ir atoms of the cluster are close to the zero oxidation state. The characteristic S–H vibrational peak of PET at 2560 cm^{-1} was absent in the FT-IR spectrum of the cluster indicating RS–Ir bond formation. The molecular formula of the cluster, $Ir_9(PET)_6$ was assigned based on the most significant peak at *m/z* 2553 in the matrix assisted laser desorption ionization mass spectrum (MALDI MS), measured at the threshold laser intensity. Density functional theory calculations on small $Ir@SCH_3$ and Ir@PET clusters and comparison of the



predictions with the IR and 1 H- NMR spectra of $Ir_9(PET)_6$ suggested that the PET ligands have two distinct structural arrangements and are likely to be present as bridging thiolates –(Ir–SR–Ir)– and singly attached thiolates –(Ir–SR).

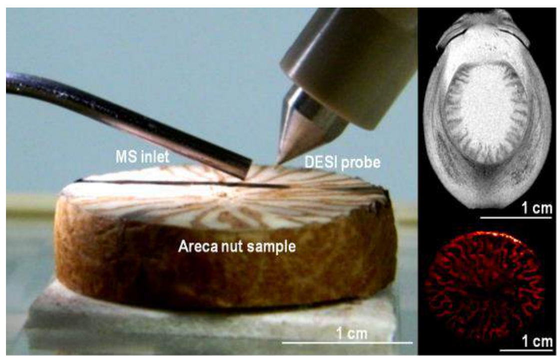
DEVELOPMENTAL PATTERNING AND SEGREGATION OF ALKALOIDS IN ARECA NUT (SEED OF *ARECA CATECHU*) REVEALED BY MAGNETIC RESONANCE AND MASS SPECTROMETRY IMAGING

Amitava Srimany, Christy George, Hemanta R. Naik, Danica Glenda Pinto, N. Chandrakumar and T. Pradeep

Phytochemistry, **DOI:** http://dx.doi.org/10.1016/j.phytochem.2016.02.002

ABSTRACT: Areca nut (seed of *Areca catechu*) is consumed by people from different parts of Asia, including India. The four major alkaloids present in areca nut are arecoline, arecaidine, guvacoline and

guvacine. Upon cutting, the nut reveals two kinds



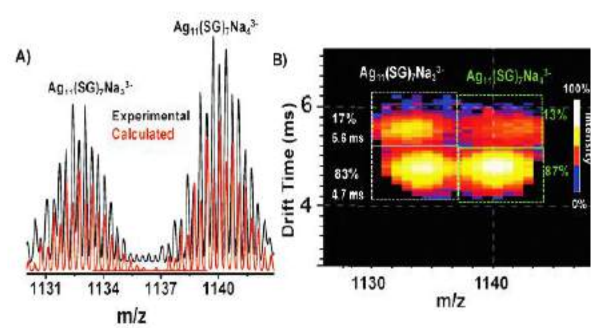
of regions; white and brown. In our present study, we have monitored the formation of these two regions within the nut during maturation, using the non-invasive techniques of magnetic resonance imaging (MRI) and volume localized magnetic resonance spectroscopy (MRS). Electrospray ionization mass spectrometry (ESI MS) and desorption electrospray ionization mass spectrometry (DESI MS) imaging have been used to study the associated change in the alkaloid contents of these two regions during the growth of the nut. Our study reveals that white and brown regions start forming within the nut when the liquid within starts solidifying. At the final stage of maturity, arecoline, arecaidine and guvacoline get segregated in the brown region whereas guvacine gets to the white region of the nut. The transport of molecules with maturity and corresponding pattern formation are expected to be associated with a multitude of physiochemical changes.

POSSIBLE ISOMERS IN LIGAND PROTECTED Ag_{11} CLUSTER IONS IDENTIFIED BY ION MOBILITY MASS SPECTROMETRY AND FRAGMENTED BY SURFACE INDUCED DISSOCIATION

Ananya Baksi, Sophie H. Harvey, Ganapati Natarajan, Vicki H. Wysocki and T. Pradeep

Chem. Commun., **DOI:** 10.1039/C5CC09119E

ABSTRACT: This communication reports the identification of gas phase isomers in monolayer-protected silver clusters. Two different isomers of $Ag_{11}(SG)_7$ (SG-gulathione thiolate) with different drift times have been detected using combined electrospray ionization (ESI) and ion mobility (IM) mass spectrometry (MS). Surface induced dissociation (SID) of the 3^- charge state of such clusters shows charge stripping to give the 1^- charged ion with some sodium attachment, in addition to fragmentation. SID and collision induced dissociation (CID) for $Ag_{11}(SG)_7$ suggest different pathways being accessed with each



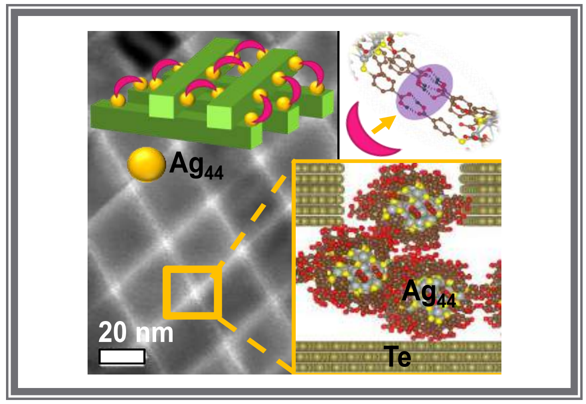
method. SID was introduced for the first time for the study of monolayer-protected clusters

CLUSTER MEDIATED CROSSED BILAYER PRECISION ASSEMBLIES OF 1D NANOWIRES

Anirban Som, Indranath Chakraborty, Tuhina Adit Maark, Shridevi Bhat and T. Pradeep

Adv. Mater., DOI: 10.1002/adma.201505775

ABSTRACT: Highly organized crossed bilayer assemblies of nanowires (NWs) are made using directed hydrogen bonding between the protecting ligand shells of atomically precise cluster molecules anchored on NWs. Layers of quantum clusters remain sandwiched between two neighboring NWs at a defined distance, dictated by the core-size of the cluster, while the orientation of the ligands in space dictates the interlayer geometry.

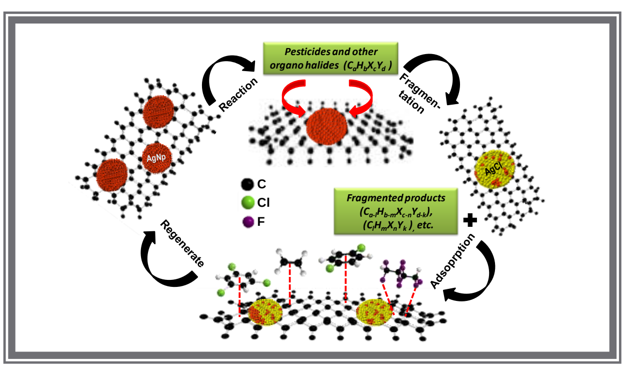


RAPID DEHALOGENATION OF PESTICIDES AND ORGANICS AT THE INTERFACE OF REDUCED GRAPHENE OXIDE-SILVER NANOCOMPOSITE

Dibyashree Koushik, Soujit Sen Gupta, Shihabudheen M. Maliyekkal and T. Pradeep

J. Haz. Mater., DOI:10.1016/j.jhazmat.2016.01.004

ABSTRACT: This paper reports dehalogenation of



various organohalides, especially aliphatic halocarbons and pesticides at reduced graphene oxide–silver nanocomposite (RGO@Ag). Several pesticides as well as chlorinated and fluorinated alkyl halides were chosen for this purpose. The composite and the products of degradation were characterized thoroughly by means of various microscopic and spectroscopic techniques. A sequential two-step mechanism involving dehalogenation of the target pollutants by silver nanoparticles followed by adsorption of the degraded compounds onto RGO was revealed. The composite showed unusual adsorption capacity, as high as 1534 mg/g, which facilitated the complete removal of the pollutants. Irrespective of the pollutants tested, a pseudo-second-order rate equation best described the adsorption kinetics. The affinity of the composite manifested chemical differences. The high adsorption capacity and re-usability makes the composite an excellent substrate for purification of water.

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