ANNUAL REPORT 2015

Pradeep Research Group

Indian Institute of Technology Madras

Our Team

Publications

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Patents/Technology/New Grants

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Service

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Publication Analysis

Abstracts of Journal Papers

T. Pradeep
Institute Professor and Professor of Chemistry
Department of Chemistry
DST Unit of Nanoscience (DSTUNS) and Thematic Unit of Excellence (TUE)
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http://www.dstuns.iitm.ac.in/pradeep-research-group.php

Our Team

Ph.D. Students

Anirban Som
K. R. Krishnadas
Atanu Ghosh
Rabin Rajan J. Methikkalam
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
M. K. Mahitha
Amrita Chakraborty
Sugi Shivan
J. R. Swathy
Biswajit Mondal
Abhijit Nag
Jyotirmoy Ghosh
Papri Chakraborty
Sritama Mukherjee
M. D. Bodiuzzaman
M. D. Rabiul Islam

Project Technicians

P. Gautham
E. Sundarraj

Administrative Officer

K. Priya

Postdoctoral/Research Associates

Dr. Gana Natarajan
Dr. N. Pugazhenthiran
Dr. P. Mohan Kumar
Dr. P. Saravanan
Dr. G. Velmurugan
Dr. Radha Gobinda Bhuin
Dr. Amitava Srimany (also worked as Institute PDF)
Dr. Ananya Baksi (also worked as Institute PDF)
Dr. Balaji Sambandam (Till August 2015)
Dr. Tuhina Adit Maark (March-September 2015)
Dr. Jaseentha Rani (Till October 2015)
Dr. R. G. Hemalatha (Till November 2015)

Project Associates

Manoj Kumar Panwar
A. Anil Kumar
Ramesh Kumar
Vasanthanarayan Murugesan
A. A. Arokia Gnani Loyola

M.Sc. Students

Tripti Ahuja
Anindita Mahapatra
Esma Khatun
Pallab Basuri
Bibhuti Bhusan Rath

Project Students

Ananthu Mahendranath (BITS, Pilani)
Harvinder Singh Sindhu (Chem. Engg., IIT Madras)

Project Consultants

Hemanta R. Naik
Dr. J. Purushothaman
Adit Maark Yvon

Laboratory Managers

Dr. Vasudeva Bhat
Mr. T. K. Sunil (TUE In-Charge)

Visiting students

1. Jukka Hassinen, Aalto University, Finland (February 25 – March 4, 2015)
2. Michael Stanley Wleklinski, Purdue University, U.S.A (January 21 – April 8, 2015)
3. Han Soo Young, Hanyang University, Seoul, South Korea (January 15 – February 05, 2015)
4. Nishil Mohammed, University of Waterloo, Canada (October 2015 - April 2016)

Summer students

From left to right: Mr. Mohith M.M., BS-MS Dual Degree student, Department of Chemical Sciences, IISER Kolkata; Mr. Dheeraj Kumar, M.Sc student, University of Hyderabad**;** Ms. Liz George M.Sc Chemistry student, Stella Maris College, Chennai; Prof. T.Pradeep; Ms. Ann Candice Fernandez, M.Sc Chemistry student, Stella Maris College, Chennai; Mr. Raj Kumar, Integrated BS-MS student, IISER Kolkata**;** Ms. Sanchita Shah, M.Sc Chemistry student, Central University of Karnataka**;** Ms. Divya Rajendran, BE student, PES University**;** Ms. Ravneet Kaur, B.Tech Chemical Science student, IIT Patna and Ms. J. Tharini, Lecturer in Chemistry, Thiagarajar College, Madurai (not in the picture).

Publications

Journal papers*

1. Inter-cluster reactions between $Au_{25}(SR)_{18}$ and $Ag_{44}(SR)_{30}$, K. R. Krishnadas, Atanu Ghosh, Ananya Baksi, Indranath Chakraborty, Ganapati Natarajan and T. Pradeep, J. Am. Chem. Soc., (2015) (DOI: 10.1021/jacs.5b09401)

2. Carbon aerogels through organo-inorganic co-assembly and their application in water desalination by capacitive deionization, Rudra Kumar, Soujit Sen Gupta, Shishir Katiyar, V. Kalyan Raman, Siva Kumar Varigala, T. Pradeep and Ashutosh Sharma, Carbon, Carbon, 99 (2016) 375-383 (DOI: 10.1016/j.carbon.2015.12.004).

3. Metallic nanobrushes made using ambient droplet sprays, Depanjan Sarkar, M. K. Mahitha, Anirban Som, Anyin Li, Michael Wleklinski, R. G. Cooks and T. Pradeep, Adv. Mater., (2015) (DOI: 10.1002/adma.201505127) (In Press).

4. Defining switching efficiency of multi-level resistive memory with PdO as example, K. D. M. Rao, Abhay A. Sagade, Robin John, T. Pradeep and G. U. Kulkarni, Adv. Electron. Mater., (2015) (DOI: 10.1002/aelm.201500286) (In Press).

5. A profile of heavy metals in rice (Oryza sativa ssp. indica) landraces, Debal Deb, Soujit Sen Gupta and T. Pradeep, Curr. Sci., 109 (2015) 407-409.

6. A low cost approach to synthesize sand like AlOOH nanoarchitecture (SANA) and its application in defluoridation of water, Gaurab Saha, Shihabudheen M. Maliyekkal, P.C. Sabumon and T. Pradeep, J. Environ. Chem. Eng. 3 (2015) 1303-1311 (DOI: 10.1016/j.jece.2014.11.030).

7. A unified framework for understanding the structure and modifications of atomically precise monolayer protected gold clusters, Ganapati Natarajan, Ammu Mathew, Yuichi Negishi, Robert L. Whetten and T. Pradeep, J. Phys. Chem. C, 119 (2015) 27768−27785 (DOI: 10.1021/acs.jpcc.5b08193).

8. Anisotropic molecular ionization at 1 V from tellurium nanowires (Te NWs), Rahul Narayanan, Depanjan Sarkar, Anirban Som, Michael Wleklinski, R. G. Cooks and T. Pradeep, Anal. Chem., 87 (2015) 10792-10798 (DOI: 10.1021/acs.analchem.5b01596).

9. Cellulose derived graphenic fibers for capacitive desalination of brackish water, Nalenthiran Pugazhenthiran, Soujit Sen Gupta, Anupama Prabhath, Muthu Manikandan, Jakka Ravindran Swathy, V. Kalyan Raman and T. Pradeep, ACS Appl. Mater. Interfaces, 7 (2015) 20156-20163 (DOI: 10.1021/acsami.5b05510).

10. Efficient red luminescence from organic-soluble Au25 clusters by ligand structure modification, Ammu Mathew, Elizabeth Varghese, Susobhan Choudhury, Samir Kumar Pal and T. Pradeep, Nanoscale, 7 (2015) 14305-14315 (DOI: 10.1039/C5NR03457D).

11. Ambient preparation and reactions of gas phase silver cluster cations and anions, Michael Wleklinski, Depanjan Sarkar, Adam Hollerbach, T. Pradeep, and R. G. Cooks, Phys. Chem. Chem. Phys., 17 (2015) 18364-18373 (DOI: 10.1039/C5CP01538C).

12. Zero volt paper spray ionization and its mechanism, Michae Wleklinski, Yafeng Li, Soumabha Bag, Depanjan Sarkar, Rahul Narayanan, T. Pradeep and R. G. Cooks, Anal. Chem., 87 (2015) 6786-6793 (DOI: 10.1021/acs.analchem.5b01225).

13. Rapid detection of Fusarium wilt in Basil (Ocimum sp.) leaves by desorption electrospray ionization mass spectrometry (DESI MS) imaging, R. G. Hemalatha, Hemanta R. Naik, Vasundhara Mariappa and T. Pradeep, RSC Adv., 5 (2015) 50512–50522 (DOI: 10.1039/c4ra16706f).

14. Rapid synthesis of C-TiO2: Tuning the shape from spherical to rice grain morphology for visible light photocatalytic application, Balaji Sambandam, Anupama Surenjan, Ligy Philip and T. Pradeep, ACS Sustain. Chem. Eng., 3 (2015) 1321-1329 (DOI: 10.1021/acssuschemeng.5b00044).

15. Noble metal clusters protected with mixed proteins exhibit intense photoluminescence, Jyoti Sarita Mohanty, Ananya Baksi, Haiwon Lee and T. Pradeep, RSC Adv., 5 (2015) 48039-48045 (DOI:10.1039/c5ra06964e).

16. Simultaneous dehalogenation and removal of persistent halocarbon pesticides from water using graphene nanocomposites: A case study of lindane, Soujit Sen Gupta, Indranath Chakraborty, Shihabudheen M. Maliyekkal, Tuhina A. Maark, Dheeraj K. Pandey, Sarit K. Das and T. Pradeep, ACS Sustain. Chem. Eng., 3 (2015) 1155-1163 (DOI: 10.1021/acssuschemeng.5b00080).

17. Interaction of acetonitrile with water-ice: An infrared spectroscopic study, Radha Gobinda Bhuin, Rabin Rajan J. Methikkalam, Bhalamurugan Sivaraman and T. Pradeep, J. Phys. Chem. C, 119 (2015) 11524-11532 (DOI: 10.1021/jp512607v).

18. Ambient solid-state mechano-chemical reactions between functionalized carbon nanotubes, Mohamad A. Kabbani, Chandra Sekhar Tiwary, Pedro A. S. Autreto, Gustavo Brunetto, Anirban Som, K. R. Krishnadas, Sehmus Ozden, Ken Hackenberg, Yongi Gong, Douglas S. Galvao, Robert Vajtai, Ahmad T. Kabbani, T. Pradeep and Pulickel M. Ajayan, Nature Commun., 6 (2015) 7291 (DOI: 10.1038/ncomms8231).

19. Initial growth kinetics of luminescent quantum clusters of silver within albumin family protein templates, Kamalesh Chaudhari and T. Pradeep, J. Phys. Chem. C., 119 (2015) 9988-9994 (DOI: 10.1021/acs.jpcc.5b00496).

20. Translocation of uranium from water to foodstuff while cooking, Krishnapriya K. C., Ananya Baksi, Swathi Chaudhari, Soujit Sen Gupta and T. Pradeep, J. Haz. Mater., 297 (2015) 183-190 (DOI: 10.1016/j.jhazmat.2015.04.041).

21. In vitro co-localization of plasmonic nano-bio labels and biomolecules using plasmonic and Raman scattering microspectroscopy, Kamalesh Chaudhari and T. Pradeep, J. Biomed. Opt., 20 (2015) 046011 (DOI: 10.1117/1.JBO.20.4.046011).

22. Ambient ionization mass spectrometry imaging of rohitukine, a chromone anti-cancer alkaloid, during seed development in *Dysoxylum binectariferum* Hook. F (Meliaceae), Mohana Kumara P, Amitava Srimany, Ravikanth G, Uma Shaanker R and T. Pradeep, Phytochemistry, 116 (2015) 104-110 (DOI: 10.1016/j.phytochem.2015.02.031).

23. Size evolution of protein protected gold clusters in solution: A combined SAXS-MS investigation, Ananya Baksi, Anuradha Mitra, Jyoti Sarita Mohanty, Haiwon Lee, Goutam De and T. Pradeep, J. Phys. Chem. C., 119 (2015) 2148-2157 (DOI:10.1021/jp509332j).

* Some of these may appear in 2016

Editorial

1. Advancing the Use of Sustainability Metrics, D. T. Allen, B. J. Hwang, P. Licence, T. Pradeep and B. Subramaniam, ACS Sustainable Chem. Eng., 3 (2015) 2359–2360 (DOI: 10.1021/acssuschemeng.5b01026).

Lectures Delivered

1. Towards point-of-care mass spectrometry: New advances in ambient ionization methods, H3C (International conference of the Ohio State University), Taj Palace Hotel, Mumbai January 15-17, 2015.

2. Clean drinking water and inequality – Technological challenges, addressing economic inequality in India, International Centre for Human Development and National Institute of Advanced Studies, Bengaluru, 8-9 January 2015.

3. Affordable point-of-use water purification using nanomaterials, Plenary lecture at 150 years of BASF, Mumbai, January 23, 2015.

4. Affordable point-of-use water purification using nanomaterials, Nano India 2015 – Plenary lecture, Sastra, Thanjavur, January 29-30, 2015.

5. Understanding the evolution of atomically precise clusters using mass spectrometry, 29th ISMAS Symposium on Mass Spectrometry, Vivanta by Taj Hari Mahal, Jodhpur, February 2-6, 2015.

6. On the birth of metals, Emerging Frontiers of Materials Science, Opening lecture, Maris Stella College, Vijayawada, February 12, 2015.

7. Understanding cancer therapy using mass spectrometry and single particle plasmonics, International symposium on Nanotechnology and Cancer Theranostics, IIT Bombay, Mumbai, February 15-17, 2015.

8. Mass spectrometric imaging of living objects, AgriNANO-2015, Opening lecture, Institute of Frontier Technology, Regional Agricultural Research Station, Tirupati, March 11, 2015.

9. On the birth of metals, Thrust Areas in Chemistry, Govt. Arts College, Nandanam, Chennai March 12, 2015.

10. Atomically precise clusters of noble metals, MANA, Tsukuba, Japan, March 18, 2015.

11. Understanding cancer therapy using mass spectrometry and single particle plasmonics, Kovai Medical Center and Hospital April 25, 2015.

12. Safe water through advanced materials, CII-UNICEF CSR Conference and Exhibition on Swachh Bharat Abhiyan, Chennai May 12, 2015.

13. Optical sensors using synthetic nanostructures, IC-IMPACTS Summer Institute, University of Toronto, June 15, 2015.

14. Affordable clean water using nanomaterials, University of Waterloo, June 17, 2015.

15. Nanotechnology for clean water, University of Alberta, Edmonton, June 19, 2015.

16. Cluster reactions, International Symposium on Monolayer Protected Clusters 2015, Fuji area, Japan, July 13-16, 2015.

17. Affordable clean water using nanomaterials, Emerging Frontiers for Sustainable Water – A Trilateral Partnership, Africa-India-UK Johannesburg, August 3-5, 2015.

18. Affordable clean water using nanomaterials, Plenary lecture, BITRI, Gaborone, August 6, 2015.

19. Chemistry of Noble Metal Clusters, Department of Chemistry, Purdue University, August 19, 2015.

20. Chemistry of Noble Metal Clusters, Professor S. V. Anantakrishnan Memorial Lecture, MCC Chennai, August 28, 2015.

21. Chemistry of Nano molecules, Stella Maris College, Chennai, September 7, 2015.

22. Affordable clean water using nanomaterials, Indian Institute of Toxicology Research, Lucknow, Golden Jubilee Lecture, October 13, 2015.

23. Affordable clean water using nanomaterials, IWA Development Congress, Plenary lecture, Amman, Jordan, October 17, 2015.

24. Extraction of Silver by Glucose, International Toxicology Conclave, Indian Institute of Toxicology Research, November 5, 2015.

25. Clean water and materials, Indian Academy of Sciences Refresher Course, Madikeri, November 16-29, 2015.

26. Fundamental problems at ice surfaces, Indian Academy of Sciences Refresher Course, Madikeri, November 16-29, 2015.

27. Investigating ice surfaces with ions, Indian Academy of Sciences Refresher Course, Madikeri, November 16-29, 2015.

28. Chemistry of Atomically Precise Clusters of Noble Metals, Institute for Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany, November 24, 2015.

Students’ Activities

1. S. Vidhya visited Seoul National University, South Korea to work with Dr. Sung Jae Kim from 8th July to 5th October, 2015.

2. Avijit Baidya visited Aalto University, Finland to work with Prof. Robin Ras from 16th July to 9th October, 2015.

3. Gana Natarajan gave a talk at the Third International Symposium on Monolayer Protected Clusters, Japan, July 13-16, 2015.

Patents/Technology/Grants

Patents

Applications

- On-line water purifier for hand pumps, Design application, Application No. 271059, April 6, 2015.
- Method for colocalization of plasmonic nanoparticles and biomolecules with plasmonic and Raman scattering microspectroscopy, T. Pradeep and Kamalesh Choudhari, 1864/CHE/2015, April 09, 2015.
- Cellulose derived graphenic fibers for capacitive desalination of brackish water and preparation method of the electrode thereof, T. Pradeep, N. Pugazhenthiran, Soujit Sen Gupta, Anupama Prabhath and J R Swathy, 3951/CHE/2015, July 31, 2015
- Methods of making alloys of precise composition in solution by inter-cluster reactions in solution, T.Pradeep, K. R. Krishnadas, Atanu Ghosh, Ananya Baksi, Indranath Chakrabarti and Ganapathy Natarajan, Filed on December 14, 2015.
- Method for preparing crossed bilayer assembly of 1D nanowires using atomically precise clusters, T. Pradeep, Anirban Som, Indranath Chakraborty, Tuhina Adit Maark and Shridevi Bhat, Filed on December 28, 2015.
- Composition for sustained release of carbonate and a water purification device based on the same with enhanced biocidal activity, T.Pradeep, Swathy J.R. and Nalendhiran Pugazhenthiran, Filed on December 29, 2015.

Granted

- Gold and Silver quantum clusters in molecular containers, methods for their preparation and use, E. S. Shibu and T. Pradeep, US-8999717, Issued: April 7, 2015.

Technology development

- AMRIT hand-pump model commercialized; 330 units (serving ~100,000 people) were installed in the arsenic affected areas.


Photograph of an installation in a school

- Arsenic free drinking water technology developed by the lab and our incubated company, Inno Nano Research Pvt. Ltd. has been approved for nationwide implementation.

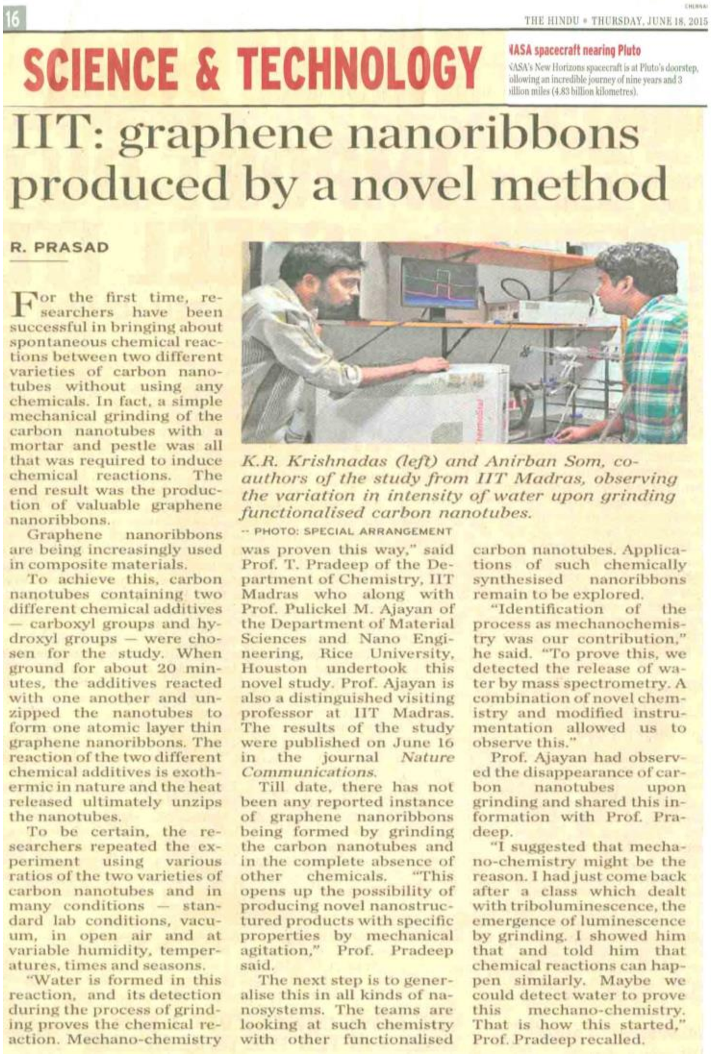
Technology receipts

- Technology licensing fee of $130,000 for some of our patents was received.
- Cumulative royalty receipts for the pesticide removal patent has crossed Rs. 150,00,000.

New grants

- Indo – UK GITA grant: Development of a novel combined arsenic filtration/monitoring system for community-scale water supplies amounting to Rs. 160,00,000 at the Indian side and £614,000 at the UK side.
- DST Grant: Arsenic free South 24 Parganas using Indian Technology, amounting to Rs. 460,00,000
- Indo-German grant: Cluster-composite nanofibre membranes for rapid, ultra-trace detection of waterborne contaminants, Rs. 200,00,000 at the Indian side and Euro 400,000 at the German side.

Media Reports (selected)



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CHENNAI

THE HINDU • THURSDAY, JUNE 18, 2015

SCIENCE & TECHNOLOGY

NASA spacecraft nearing Pluto

ASA's New Horizons spacecraft is at Pluto's doorstep, ollowing an incredible journey of nine years and 3 illion miles (4.83 billion kilometres).

IIT: graphene nanoribbons produced by a novel method

R. PRASAD

For the first time, researchers have been successful in bringing about spontaneous chemical reactions between two different varieties of carbon nanotubes without using any chemicals. In fact, a simple mechanical grinding of the carbon nanotubes with a mortar and pestle was all that was required to induce chemical reactions. The end result was the production of valuable graphene nanoribbons.

Graphene nanoribbons are being increasingly used in composite materials.

To achieve this, carbon nanotubes containing two different chemical additives — carboxyl groups and hydroxyl groups — were chosen for the study. When ground for about 20 minutes, the additives reacted with one another and unzipped the nanotubes to form one atomic layer thin graphene nanoribbons. The reaction of the two different chemical additives is exothermic in nature and the heat released ultimately unzips the nanotubes.

To be certain, the researchers repeated the experiment using various ratios of the two varieties of carbon nanotubes and in many conditions — standard lab conditions, vacuum, in open air and at variable humidity, temperatures, times and seasons.

"Water is formed in this reaction, and its detection during the process of grinding proves the chemical reaction. Mechano-chemistry was proven this way," said Prof. T. Pradeep of the Department of Chemistry, IIT Madras who along with Prof. Pulickel M. Ajayan of the Department of Material Sciences and Nano Engineering, Rice University, Houston undertook this novel study. Prof. Ajayan is also a distinguished visiting professor at IIT Madras. The results of the study were published on June 16 in the journal *Nature Communications*.

Till date, there has not been any reported instance of graphene nanoribbons being formed by grinding the carbon nanotubes and in the complete absence of other chemicals. "This opens up the possibility of producing novel nanostructured products with specific properties by mechanical agitation," Prof. Pradeep said.

The next step is to generalise this in all kinds of nanosystems. The teams are looking at such chemistry with other functionalised carbon nanotubes. Applications of such chemically synthesised nanoribbons remain to be explored.

"Identification of the process as mechanochemistry was our contribution," he said. "To prove this, we detected the release of water by mass spectrometry. A combination of novel chemistry and modified instrumentation allowed us to observe this."

Prof. Ajayan had observed the disappearance of carbon nanotubes upon grinding and shared this information with Prof. Pradeep.

"I suggested that mechano-chemistry might be the reason. I had just come back after a class which dealt with triboluminescence, the emergence of luminescence by grinding. I showed him that and told him that chemical reactions can happen similarly. Maybe we could detect water to prove this mechano-chemistry. That is how this started," Prof. Pradeep recalled.

K.R. Krishnadas (left) and Anirban Som, co-authors of the study from IIT Madras, observing the variation in intensity of water upon grinding functionalised carbon nanotubes.

-- PHOTO: SPECIAL ARRANGEMENT

Centre approves nationwide use of IIT-M water purifier

A nanotechnology-based water purifier developed by Indian Institute of Technology, Madras that provides arsenic-free water at an affordable cost will soon be installed in all arsenic-affected regions of the country.

TNN | 15 December 2015, 7:35 AM IST

Chennai: A nanotechnology-based water purifier developed by Indian Institute of Technology, Madras that provides arsenic-free water at an affordable cost will soon be installed in all arsenic-affected regions of the country.

The purifier is already providing arsenic-free water to more than four lakh people in West Bengal at a cost of less than 5 paise per litre.

The Union ministry of drinking water and sanitation has recommended the replication

BITRI Hosts the 7th Public Seminar

AUGUST 18, 2015

The Botswana Institute for Technology Research and Innovation (BITRI) held the 7th Public Seminar on Thursday August 6, 2015 at the **Avani Gaborone Hotel and Casino** main conference room.

The guest speaker for the Seminar was Professor Thalappil Pradeep, a renowned Professor of Chemistry at the Indian Institute of Technology in Madras and a leading expert on the development of affordable technologies for drinking water purification, some of which have been commercialised.

The topic for the seminar "*Affordable point-of-use water purification using nanomaterials*" could have not been more relevant since availability and quality of potable is a topical issue in Botswana, and indeed the whole globe.

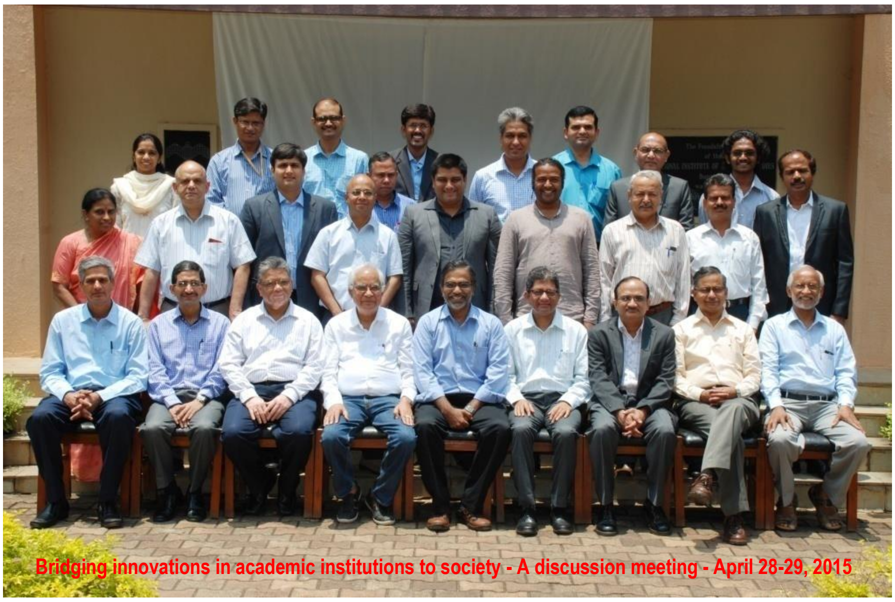
Professor Thalappil Pradeep presented technical information on nanotechnology and demonstrated the limitless capabilities that

BITRI Hosts Seminar on Open Data
DECEMBER 14, 2015

BITRI Sets Up Centre for Material Science
DECEMBER 14, 2015

Service

- Associate Editor of the journal, *ACS Sustainable Chemistry & Engineering*
- Member, India-Japan Council of the Department of Science and Technology
- Member, Nanoscience Advisory Committee, Nano Mission, Department of Science and Technology
- Member, Proof of Concept Expert Committee, Nano Mission, Department of Science and Technology
- Member, Executive Committee, Neutron Scattering Society of India
- Vice President of the Indian Society for Mass Spectrometry
- Member of the Council of Materials Research Society of India
- Member, Bureau of Indian Standards – on drinking water products
- Member, Board of studies of the Department of Atomic and Molecular Physics, Manipal University
- Member, Board of School of Life Sciences, Ahmedabad University
- Coordinator, Interdisciplinary programme, IIT Madras
- Organised a two-day discussion meeting on Bridging innovations in academic institutions to society, National Institute of Advanced Studies, Bangalore, April 28-29, 2015



Bridging innovations in academic institutions to society - A discussion meeting - April 28-29, 2015

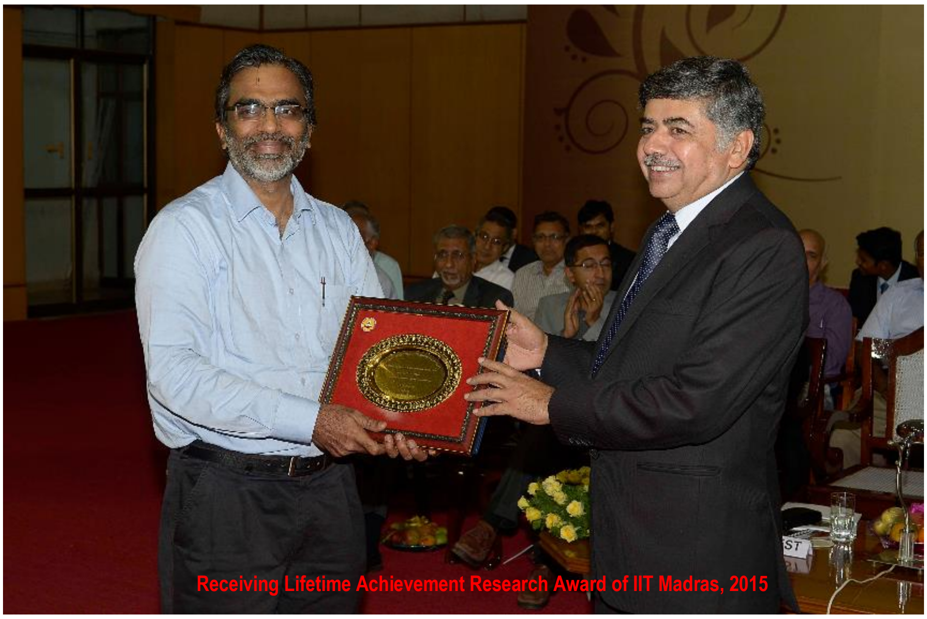
- Conducted the 3rd International Conference on Emerging Technologies for Clean Water in collaboration with Royal Society of Chemistry and Pan Africa Network, UK Science & Innovation Network India, National Research Foundation & Department of Water and Sanitation, South Africa, Department of Science and Technology, in collaboration with Department of Applied

Chemistry, Institute of Nanotechnology and Water, University of Johannesburg, August 3-6, 2015

Awards and Recognitions

T. Pradeep

- J. C. Bose National Fellowship
- Appointed to the Graduate Faculty, Purdue University
- Lifetime Achievement Research Award of IIT Madras and named as, 'Institute Professor'
- Elected fellow of The National Academy of Sciences
- Elected fellow of the Indian National Science Academy
- Member, Editorial Board of the journal, Scientific Reports (Nature Group)
- Member, Editorial board of the journal, International Journal of Water and Wastewater Treatment



Receiving Lifetime Achievement Research Award of IIT Madras, 2015

Students

- Rahul Narayanan received the Royal Society of Chemistry poster prize at the 17th Chemical Research Society of India Symposium held at National Chemical Laboratory, Pune, 2015.

Alumni News

- Indranath Chakraborty joined as a post-doctoral fellow at Department of Chemistry, University of Illinois at Urbana–Champaign, United State.

- Indranath Chakraborty was awarded Alexander von Humboldt Postdoctoral Fellowship, July 2015.

- Anupama Prabhath, joined as a PhD student in Institute for Regenerative Engineering, University of Connecticut Health Center, Farmington, CT, USA.

- Ammu Mathew was awarded Prof. Langmuir Prize for the best thesis in Ph.D Chemistry [Physical & Theoretical Chemistry], 2015.
- Kamalesh Chaudhari joined as a post-doctoral fellow at Department of Chemical and Materials Engineering, University of Alberta, Edmonton, Canada.
- Soumabha Bag joined as a post-doctoral fellow at Department of Chemistry, University of Hawaii at Manoa, Honolulu, Hawai, USA.
- Rajeev Kumar V. R. joined as Ad-hoc Lecturer at School of Nano Science and Technology National Institute of Technology, Calicut
- E Shibu received Madam Marie Curie Fellowship 2015-2017, currently working as a post-doctoral fellow at Institute of Optics Graduate School, University of Bordeaux Talence, France.
- C Subramaniam appointed as associate editor for RSC Advances published by the Royal Society of Chemistry.
- A. Sreekumaran Nair joined as Senior Manager (R&D) of Advanced Design and Materials Group at MRF Limited, Chennai.
- R Selvan was awarded 2015 - Team Award from Sai Life Sciences for Drug Metabolism and Pharmacokinetics Department.

Graduation

PhD

- Indranath Chakraborty, Department of Chemistry, IIT Madras, 2015

An Investigation into the formation, functionalization and applications of atomically precise silver clusters

- Radha Gobinda Bhuin, Department of Chemistry, IIT Madras, 2015

Understanding molecules of interstellar relevance by optical spectroscopies

- Amitava Srimany, Department of Chemistry, IIT Madras, 2015

Investigations of molecular signatures of plants and cells by ambient mass spectrometry

- Ananya Baksi, Department of Chemistry, IIT Madras, 2015

Interaction of proteins and sugars with noble metals: Adducts, Clusters and Dissolution

M.Sc.

- Manisha Samanta$^{\$}$ Department of Chemistry, IIT Madras, 2015

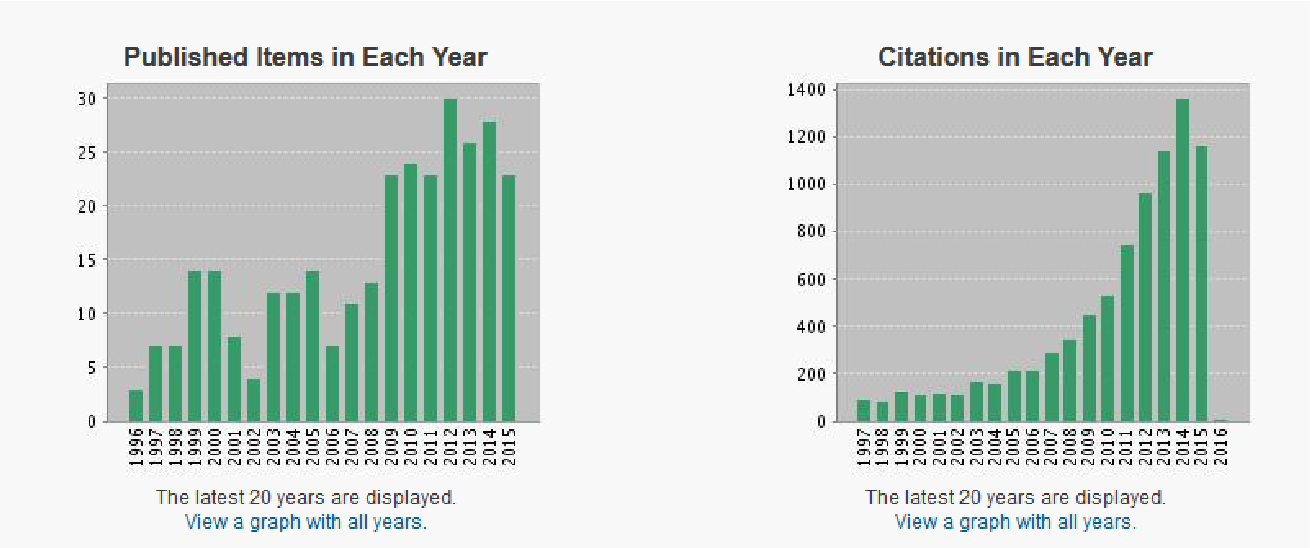
  Separation of Isomers of $Au_{25}SR_{118-n}SR_{2n}$ Cluster Using HPLC

- Abhijit Nag* Department of Chemistry, IIT Madras, 2015
- Biswajit Mondal*, Department of Chemistry, IIT Madras, 2015

$Joined as PhD student at JNCASR, Bangalore *joined as Integrated PhD students, in the group

Publication Analysis

Source: Web of science, Dec26, 2015



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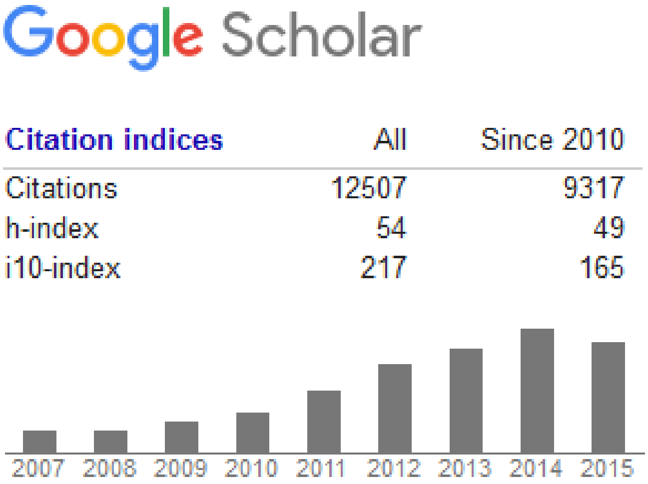


Google Scholar

Citation indices	All	Since 2010
Citations	12507	9317
h-index	54	49
i10-index	217	165

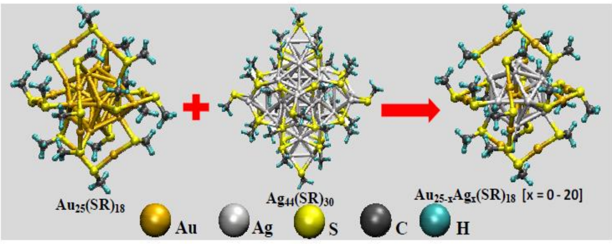
Abstracts of Journal Papers

Inter-cluster reactions between $Au_{25}(SR)_{18}$ and $Ag_{44}(SR)_{30}$

K. R. Krishnadas, Atanu Ghosh, Ananya Baksi, Indranath Chakraborty, Ganapati Natarajan, and Thalappil Pradeep

J. Am. Chem. Soc. **DOI:** 10.1021/jacs.5b09401

Abstract



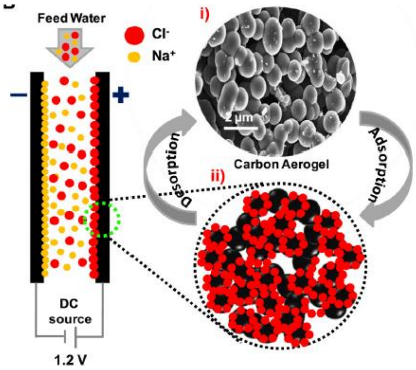
We present the first example of inter-cluster reactions between atomically precise, monolayer protected noble metal clusters usingAu$_{25}$(SR)$_{18}$ and Ag$_{44}$(SR)$_{30}$ (RS- = alkyl/aryl thiolate) as model compounds. These clusters undergo spontaneous reaction in solution at ambient conditions. Mass spectrometric measurements both by electrospray ionization and matrix assisted laser desorption ionization show that the reaction occurs through the exchange of metal atoms and protecting ligands of the clusters. Inter-cluster alloying is demonstrated to be a much more facile method for heteroatom doping into Au$_{25}$(SR)$_{18}$, as observed by doping up to twenty Ag atoms. We investigated the thermodynamic feasibility of the reaction using DFT calculations and a tentative mechanism has been presented. Metal core-thiolate interfaces in these clusters play a crucial role in inducing these reactions and also affect rates of these reactions. We hope that our work will help accelerate activities in this area to establish chemistry of monolayer protected clusters.

Carbon aerogels through organo-inorganic co-assembly and their application in water desalination by capacitive deionization

Rudra Kumar, Soujit Sen Gupta, Shishir Katiyar, V. Kalyan Raman, Siva Kumar Varigala, T. Pradeep and Ashutosh Sharma

Carbon, **DOI**:1016/j.carbon.2015.12.004

Abstract



We report the preparation of a carbon aerogel (CA) material utilizing the simultaneous co-assembly of organic and inorganic precursors, having a high Brunauer–Emmet–Teller surface area of 2600 m^2/g, through a one step sol–gel process. This CA was characterized using different spectroscopic and microscopic techniques. The as-synthesized CA with its tunable porosity, high mechanical strength, transport property and electrical conductivity was found to be a suitable candidate for water desalination via capacitive deionization (CDI). The optimum working potential for CDI was in the range of 1.2–1.4 V. The material was tested for the removal of different ions of varying charges and the experiment was performed for multiple cycles. The result showed high adsorption capacity of 10.54 mg/g for Cl− in laboratory batch experiments compared to 3–4 mg/g reported for most of the CDI materials. The materials were also characterized after adsorption/desorption cycles. Adsorption was physical in nature and the ions desorbed completely after reversing the polarity. The result showed that the material can be used for multiple cycles without any change in its spectroscopic and adsorption properties.

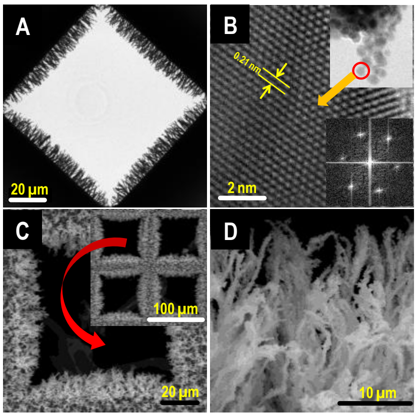
Metallic nanobrushes made using ambient droplet sprays

Depanjan Sarkar, Maheswari Kavirajan Mahitha, Anirban Som, Anyin Li, Michael Wleklinski, Robert Graham Cooks and Thalappil Pradeep

Adv. Mater. DOI: DOI: 10.1002/adma.201505127

Abstract

We report an ambient solution-state method of making uniform nanobrushes composed of oriented one-dimensional silver nanowires (NW) with aspect ratios of $10^2 – 10^4$. These structures can be grown over large (cm^2) areas over conducting surfaces. The assemblies of NWs form nanobrush structures with remarkable uniformity, which can capture micron-sized objects, such as bacteria and particulate matter, demonstrating potential applications of these materials.

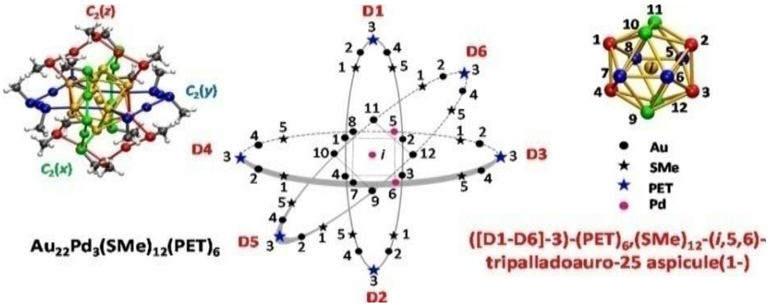


A Unified Framework for Understanding the Structure and Modifications of Atomically Precise Monolayer Protected Gold Clusters

Ganapati Natarajan, Ammu Mathew, Yuichi Negishi, Robert L. Whetten and T. Pradeep

J. Phys. Chem. C, ***DOI:*** *10.1021/acs.jpcc.5b08193*

Abstract



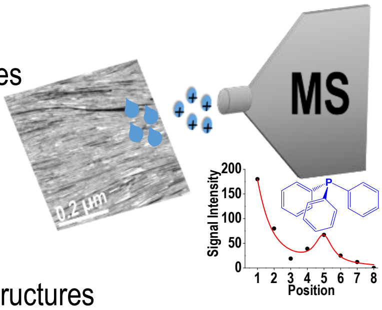
Atomically precise mono-layer protected clusters are molecules comprising a few -atom cluster core of a noble metal, typically Au or Ag, surrounded by a pro- tective layer of ligands, exhibiting many special optical, electrical, catalytic, and magnetic properties, and are emerging as important materials in biology, medicine, catalysis, energy conversion and storage, and sensing. The structural diversity of these clusters or aspicules, as we definitively term them, meaning shielded molecules, combining the Greek word *aspis* (shield) with molecule, is rapidly increasing due to new compositions and modification routes such as ligand-exchange, alloying, or supramolecular functionalization. We present a structural analysis of the most stable cluster of this kind, $Au_{25}(SR)_{18}$, and propose a Borromean rings diagram for the cluster, showing its topological configuration of three interlocked (Au_8S_6)-rings. This simplified two-dimensional diagram is used to represent its structure and modifications via ligand or metal atom substitution uniquely. We enumerate and name its isomers with two-ligand or metal atom substituents. Among the several structural insights obtained, the identification of the Borromean rings-interlocked configuration in $Au_{25}(SR)_{18}$ may explain its high geometric stability and indicate a possible general unified structural viewpoint for these clusters without the division between core and staple motifs. On the basis of our structural analysis, we developed a structure-based nomenclature system that can be applied to both describe and understand the structure and modifications of gold thiolate clusters, $Au_M(SR)_N$, and is adaptable to the general case of $M_M(X)_N$ (M, metal and X, ligand). The application of structural analysis and diagrams to $Au_{38}(SR)_{24}$ and $Au_{102}(SR)_{44}$, revealing the possible formation of the cluster core by stacking or growth of rings of metal atoms, is also presented.

Anisotropic Molecular Ionization at 1 V from Tellurium Nanowires (Te NWs)

Rahul Narayanan, Depanjan Sarkar, Anirban Som, Michael Wleklinski, R. Graham Cooks and T. Pradeep

Anal. Chem. **DOI:** 10.1021/acs.analchem.5b01596

Abstract



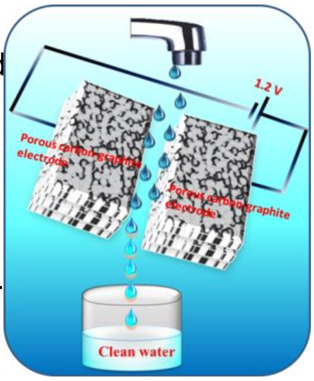
Ionization of molecular species from one-dimensional (1D) tellurium nanowires (Te NWs) has been achieved at 1 V. Molecules with a range of chemical functional groups gave quality mass spectra with high signal/noise ratios and no fragment ions. Experiments suggest the possibility of emission of microdroplets of solution due to the intense fields at the ends or interfaces of nanostructures. It appears that electrolytic conduction of the solution wetting of the nanostructures and not the electronic conduction of the nanostructures themselves is involved in the ionization event. Anisotropy was seen when twodimensionally aligned Te NWs were used for ionization. The orientation effect of aligned Te NWs on molecular ion intensity is demonstrated for many analytes including organic molecules and amino acids with experiments done using a silicon substrate having aligned Te NWs. These measurements suggest the possibility of creating a MS source that extends the applicability of mass spectrometry. Analysis of a variety of analytes, including amino acids, pesticides, and drugs, in pure form and in complex mixtures, is reported. These experiments suggest that 1D nanostructures in general could be excellent ionization sources

Cellulose Derived Graphenic Fibers for Capacitive Desalination of Brackish Water

Nalenthiran Pugazhenthiran, Soujit Sen Gupta, Anupama Prabhath, Muthu Manikandan, Jakka Ravindran Swathy, V. Kalyan Raman and T. Pradeep

ACS Appl. Mater. Interfaces, **DOI:** 10.1021/acsami.5b05510

Abstract



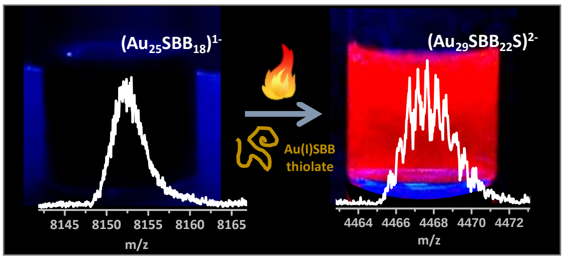
We describe a simple and inexpensive cellulose-derived and layer-by-layer stacked carbon fiber network electrode for capacitive deionization (CDI) of brackish water. The microstructure and chemical composition were characterized using spectroscopic and microscopic techniques; electrochemical/electrical performance was evaluated by cyclic voltammetry and 4-probe electrical conductivity and surface area by Brunauer−Emmett−Teller analysis, respectively. The desalination performance was investigated using a laboratory batch model CDI unit, under fixed applied voltage and varying salt concentrations. Electro-adsorption of NaCl on the graphite reinforced-cellulose (GrC) electrode reached equilibrium quickly (within 90 min) and the adsorbed salts were released swiftly (in 40 min) back into the solution, during reversal of applied potential. X-ray photoelectron spectroscopic studies clearly illustrate that sodium and chloride ions were physisorbed on the negative and positive electrodes, respectively during electro-adsorption. This GrC electrode showed an electro-adsorption capacity of 13.1 mg/g of the electrode at a cell potential of 1.2 V, with excellent recyclability and complete regeneration. The electrode has a high tendency for removal of specific anions, such as fluoride, nitrate, chloride, and sulfate from water in the following order: Cl− > NO3− > F− > SO42−. GrC electrodes also showed resistance to biofouling with negligible biofilm formation even after 5 days of incubation in Pseudomonas putida bacterial culture. Our unique cost-effective methodology of layer-by-layer stacking of carbon nanofibers and concurrent reinforcement using graphite provides uniform conductivity throughout the electrode with fast electro-adsorption, rapid desorption, and extended reuse, making the electrode affordable for capacitive desalination of brackish water.

Efficient red luminescence from organic-soluble Au_{25} clusters by ligand structure modification

Ammu Mathew, Elizabeth Varghese, Susobhan Choudhury, Samir Kumar Pal and T. Pradeep

Nanoscale, **DOI:** 10.1039/C5NR03457D

Abstract



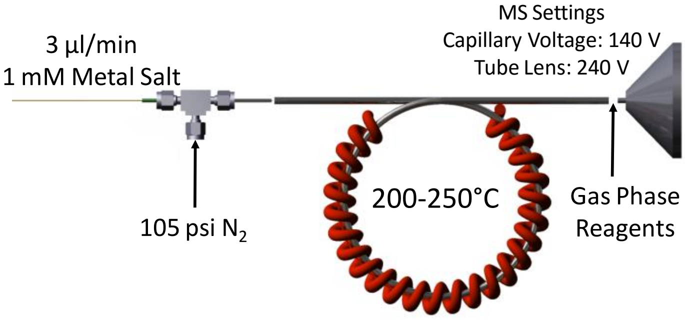
An efficient method to enhance visible luminescence in a visibly non-luminescent organic-soluble 4-(tert butyl)benzyl mercaptan (SBB)-stabilized Au_{25} cluster has been developed. This method relies mainly on enhancing the surface charge density on the cluster by creating an additional shell of thiolate on the cluster surface, which enhances visible luminescence. The viability of this method has been demonstrated by imparting red luminescence to various ligand-protected quantum clusters (QCs), observable to the naked eye. The bright red luminescent material derived from $Au_{25}SBB_{18}$ clusters was characterized using UV-vis and luminescence spectroscopy, TEM, SEM/EDS, XPS, TG, ESI and MALDI mass spectrometry, which collectively proposed an uncommon molecular formula of $Au_{29}SBB_{24}S$, suggested to be due to different stapler motifs protecting the Au_{25} core. The critical role of temperature on the emergence of luminescence in QCs has been studied. The restoration of the surface ligand shell on the Au_{25} cluster and subsequent physicochemical modification to the cluster were probed by various mass spectral and spectroscopic techniques. Our results provide fundamental insights into the ligand characteristics determining luminescence in QCs.

Ambient preparation and reactions of gas phase silver cluster cations and anions

Michael Wleklinski, Depanjan Sarkar, Adam Hollerbach, T. Pradeep and R. G. Cooks

Phys. Chem. Chem. Phys, **DOI:** 10.1039/C5CP01538C

Abstract



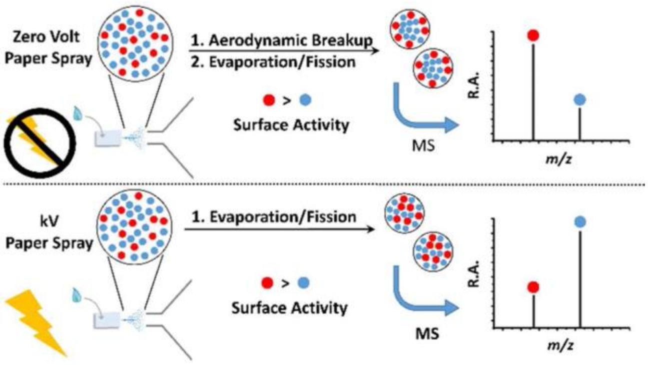
Electrospray ionization of metal salt solutions followed by ambient heating transforms the resulting salt clusters into new species, primarily naked metal clusters. This is done by passing the clusters through a heated coiled loop outside the mass spectrometer which releases the counter anion while generating the anionic or cationic naked metal clusters. The nature of the anion in the starting salt determines the type of metal cluster observed. For example, silver acetate upon heating generates only positive silver clusters, Ag_n^+, but silver fluoride upon heating generates both positive and negative silver clusters, $Ag_n^{+/-}$ (3< n <20). Both unheated and heated metal salts display ions with characteristic geometric and electronic magic numbers. There is also a strong odd/even effect in the cationic and anionic silver clusters. Thermochemical control is suggested as the basis for favored formation of the observed clusters, with anhydride elimination occurring from the acetates and F_2 elimination from the fluorides to give cationic and anionic clusters, respectively. Data on the intermediates observed as the temperature of the heater is ramped support this. The naked metal clusters react with gaseous reagents in the open air, including methyl substituted pyridines, hydrocarbons, common organic solvents, ozone, ethylene, and propylene. Argentation of hydrocarbons, including saturated hydrocarbons, is shown to occur and serves as a useful method of ionization. This new methodology allows for the investigation of ligand-metal binding and of reactions of industrial importance, such as olefin epoxidation. The potential use of this ion source in ion soft landing is demonstrated by reproducing the mass spectra of heated salts using a custom surface science instrument.

Zero volt paper spray ionization and its mechanism

Michael Wleklinski, Yafeng Li, Soumabha Bag, Depanjan Sarkar, Rahul Narayanan, T. Pradeep and R. G. Cooks

Anal. Chem., **DOI:** 10.1021/acs.analchem.5b01225

Abstract



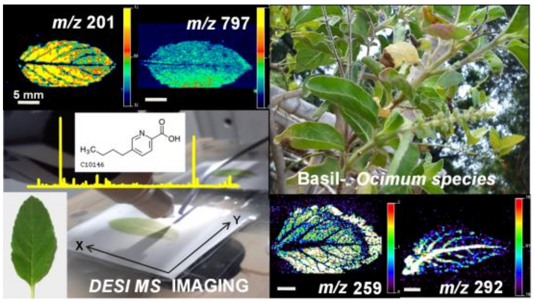
The analytical performance and a suggested mechanism for zero volt paper spray using chromatography paper are presented. A spray is generated by the action of the pneumatic force of the mass spectrometer (MS) vacuum at the inlet. Positive and negative ion signals are observed, and comparisons are made with standard kV paper spray (PS) ionization and nanoelectrospray ionization (nESI). While the range of analytes to which zero volt PS is applicable is very similar to kV PS and nESI, differences in the mass spectra of mixtures are interpreted in terms of the more significant effects of analyte surface activity in the gentler zero volt experiment than in the other methods due to the significantly lower charge. The signal intensity of zero volt PS is also lower than in the other methods. A Monte Carlo simulation based on statistical fluctuation of positive and negative ions in solution has been implemented to explain the production of ions from initially uncharged droplets. Uncharged droplets first break up due to aerodynamics forces until they are in the 2−4 μm size range and then undergo Coulombic fission. A model involving statistical charge fluctuations in both phases predicts detection limits similar to those observed experimentally and explains the effects of binary mixture components on relative ionization efficiencies. The proposed mechanism may also play a role in ionization by other voltage-free methods.

Rapid detection of *Fusarium* wilt in Basil (Ocimum sp.) leaves by desorption electrospray ionization mass spectrometry (DESI MS) imaging

R. G. Hemalatha, Hemanta R. Naik, Vasundhara Mariappa and T. Pradeep

RSC Adv., ***DOI:*** *10.1039/c4ra16706f*

Abstract



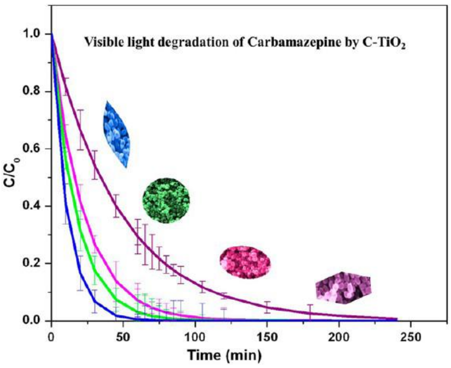
Basil (*Ocimum* sp.), a medicinal herb is used fresh and/or dry in various (culinary, cosmetic and pharmaceutical) preparations. Fusarium wilt caused by the fungus *Fusarium oxysporum* f. sp. *basilic*i is limiting basil cultivation in many countries. Since the leaf is the edible part in basil, new approaches are required to identify, and to prevent the spread of Fusarium pathogens. Desorption electrospray ionization mass spectrometry (DESI MS) was used for imaging thin layer chromatography (TLC) –imprints of leaves of three different species of basil (*Ocimum basilicum* L., *O. tenuiflorum* L., and *O.gratissimum* L.), and the molecular manifestations during *Fusarium* contamination are recorded. DESI MS images showed the chemotaxonomic differences of basil species and the changes in metabolite ion peaks during pathogen infection. Besides easy detection of reported toxic metabolite(s) of the pathogen(s), the results include molecular images showing spatial distribution of all coexisting surface bound metabolites in plant leaves, their fragment ions, and the transient changes in their spatial distribution during *Fusarium* attack under natural conditions. Demonstration of the same protocol to image seedling, young/mature leaves, basil/other related plant (Patchouli – *Pogostemon cablin* (Blanco) Benth.), wilt/other disease symptoms shows that prior knowledge of the metabolite profile of the plant/pathogen is not required. This rapid detection method can be tailored to large scale screening programs for plant diseases suggesting potential implications in agriculture and quarantine requirements.

Rapid synthesis of C-TiO_2: Tuning the shape from spherical to rice grain morphology for visible light photocatalytic application

Balaji Sambandam, Anupama Surenjan, Ligy Philip and T. Pradeep

ACS Sustain. Chem. Eng., **DOI:** 10.1021/acssuschemeng.5b00044

Abstract



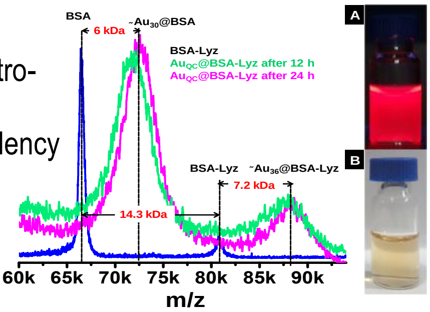
Visible light-active carbon-loaded anatase TiO_2 (C-TiO_2) nanocrystals of spherical, distorted spherical, rice grain and hexagonal morphologies , with a particle size range of 50-70 nm have been synthesized by a rapid microwave-assisted route in the solution state. The morphology of these materials is greatly tuned at low concentrations of the precursors used. The absorption band gaps (E_{gap}) are shifted to the visible region due to C loading, and the distorted spherical C-TiO_2 exhibits a maximum energy shift relative to pure TiO_2. Carbon gets deposited predominantly on the surface as graphitic carbon, in the preparative conditions, as confirmed by X-ray photoelectron, SEM elemental mapping and Raman spectroscopic studies. The rapid degradation of an endocrine disrupting agent and a persistent pollutant in wastewater, carbamazepine, by the rice grain shaped C-TiO_2 is attributed to the large surface area (229 m^2/g) of the particles and co-exposure of the high surface energy and more reactive {001} facets along with the low energy and thermodynamically stable {101} facets.

Noble metal clusters protected with mixed proteins exhibit intense photoluminescence

Jyoti Sarita Mohanty, Ananya Baksi, Haiwon Lee and T. Pradeep

RSC Adv., **DOI**:10.1039/c5ra06964e

Abstract



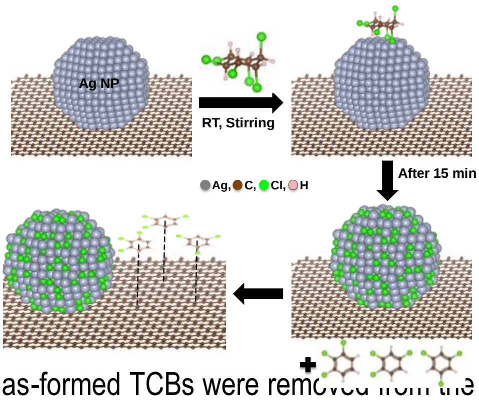
Here we report the synthesis and detailed mass spectrometric and spectroscopic characterization of highly luminescent gold and silver clusters protected with mixed proteins. Taking advantage of the aggregation tendency of the protein, lysozyme (Lyz), we could make an inter-protein conjugate from a physical mixture of the two proteins, bovine serum albumin (BSA) and Lyz. Based on the matrix assisted laser desorption ionization mass spectrometry (MALDI MS) data, the new cluster is assigned as ~Au_{36}@BSA-Lyz. This specific system showed very high red luminescence and the calculated quantum yield was 42% which is highest till date for such cluster systems. A similar study on silver system showed the formation of ~Ag_{35}@BSA-Lyz when similar metal and protein concentration was used. By varying the concentration of the silver precursor, different compositions of the cluster protected by the mixed protein have been achieved. Such a system with high quantum yield can be used for various applications such as sensors for ultralow levels of analytes, fluorescent tags and for tracking biomolecules in real systems.

Simultaneous dehalogenation and removal of persistent halocarbon pesticides from water using graphene nanocomposites: A case study of lindane

Soujit Sen Gupta, Indranath Chakraborty, Shihabudheen M. Maliyekkal, Tuhina A. Maark, Dheeraj K. Pandey, Sarit K. Das and T. Pradeep

ACS Sustain. Chem. Eng., **DOI**: 10.1021/acssuschemeng.5b00080

Abstract



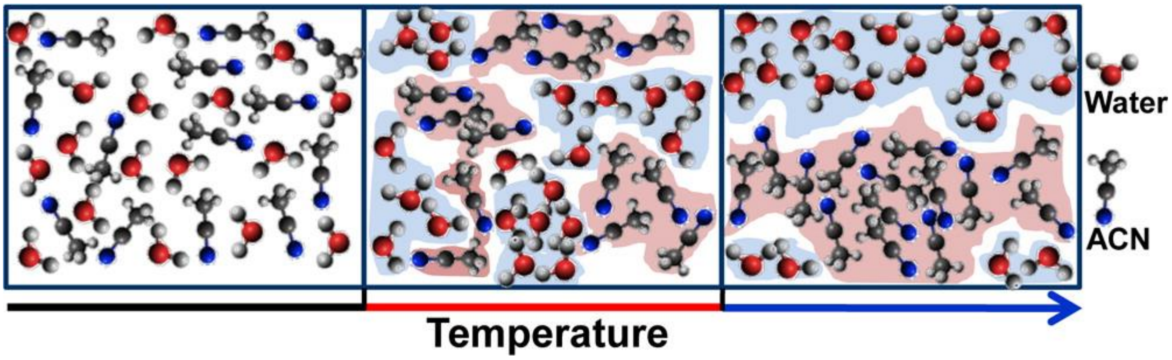
This paper describes an unusual chemical reaction that takes place on a graphene composite in a concerted fashion. The reaction shows the conversion of a persistent organochlorine pesticide, lindane ($C_6H_6Cl_6$), present in water, to different isomers of trichlorobenzenes (TCBs, $C_6H_3Cl_3$) on the surface of reduced graphene oxide-silver composites (RGO@Ag). The reaction is unique to the composite and does not occur on RGO and nanoparticles of Ag separately. The products of the reaction were isolated and extensively characterized using analytical techniques such as GC-MS, ESI-MS, IR and NMR, which unequivocally confirmed their identity. The as-formed TCBs were removed from the aqueous medium by adsorption on the same composite. Adsorption of lindane is physical in nature, but that of TCBs is through π-π interactions. The study reveals the unusual chemical reactivity of graphene-metal composites and their potential for water treatment. The uniqueness of the reaction on RGO@Ag is due to the simultaneous removal of three HCl molecules leading to the formation of aromatic compounds and concomitant formation of silver chloride. Recycling capacity and effect of diverse species present in natural waters were tested for potential applications in sustainable water treatment.

Interaction of acetonitrile with water-ice: An infrared spectroscopic study

Radha Gobinda Bhuin, Rabin Rajan J. Methikkalam, Bhalamurugan Sivaraman and T. Pradeep

J. Phys. Chem. C, **DOI:** 10.1021/jp512607v

Abstract



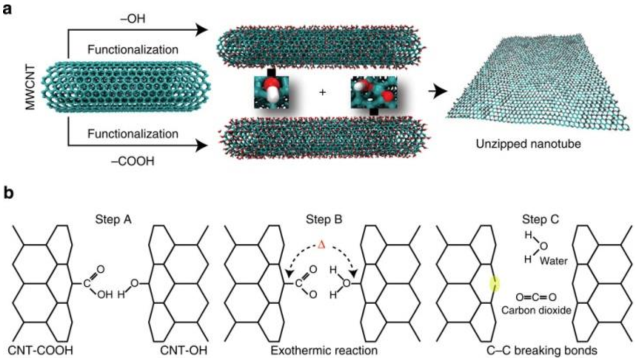
Interaction of water-ice and acetonitrile has been studied at low temperatures in their co-deposited mixtures, in ultrahigh vacuum conditions. They interact strongly at low temperatures (in the temperature range of 40–110 K), which was confirmed from the new features manifested in the reflection absorption infrared spectra of the mixtures. This interaction was attributed to strong hydrogen bonding which weakens upon warming as the acetonitrile molecules phase segregate from water-ice. Complete phase separation was observed at 130 K prior to desorption of acetonitrile from the water-ice matrix. Such a hydrogen-bonded structure is not observed when both the molecular solids are deposited as water on acetonitrile or acetonitrile on water overlayers. A quantitative analysis shows that in a 1:1 co-deposited mixture, more than 50% acetonitrile molecules are hydrogen bonded with water-ice at low temperatures (40–110 K).

Ambient solid-state mechano-chemical reactions between functionalized carbon nanotubes

Mohamad A. Kabbani, Chandra Sekhar Tiwary, Pedro A. S. Autreto, Gustavo Brunetto, Anirban Som, K. R. Krishnadas, Sehmus Ozden, Ken Hackenberg, Yongi Gong, Douglas S. Galvao, Robert Vajtai, Ahmad T. Kabbani, T. Pradeep and Pulickel M. Ajayan

Nature Commun., **DOI:** 10.1038/ncomms8231)

Abstract



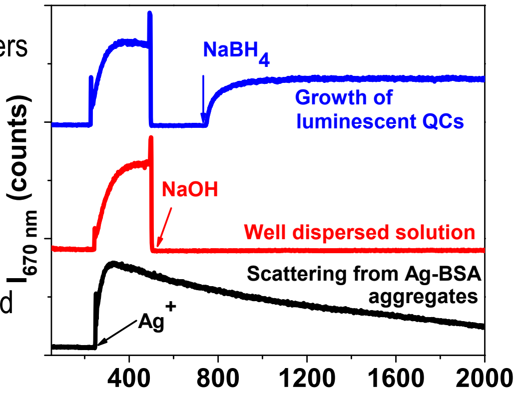
Carbon nanotubes can be chemically modified by attaching various functionalities to their surfaces, although harsh chemical treatments can lead to their break-up into graphene nanostructures. On the other hand, direct coupling between functionalities bound on individual nanotubes could lead to, as yet unexplored, spontaneous chemical reactions. Here we report an ambient mechano-chemical reaction between two varieties of nanotubes, carrying predominantly carboxyl and hydroxyl functionalities, respectively, facilitated by simple mechanical grinding of the reactants. The purely solid-state reaction between the chemically differentiated nanotube species produces condensation products and unzipping of nanotubes due to local energy release, as confirmed by spectroscopic measurements, thermal analysis and molecular dynamic simulations.

Initial growth kinetics of luminescent quantum clusters of silver within albumin family protein templates

Kamalesh Chaudhari and T. Pradeep

J. Phys. Chem. C, **DOI:** 10.1021/acs.jpcc.5b00496

Abstract



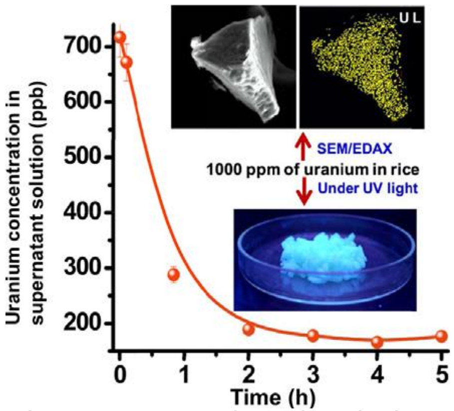
We probed the initial growth kinetics of luminescent quantum clusters of silver (AgQCs) within two albumin family proteins, bovine serum albumin (BSA) and ovalbumin (Ova). Shorter time scale (seconds to minutes) growth of AgQCs monitored using real time photoluminescence spectroscopy has shown that at lower concentrations of Ag^+, only unstable QCs were formed. The major role of basic pH in the synthesis was not only to facilitate Ag^+-BSA conjugation but also to provide well dispersed medium for controlled nucleation of QCs. Increase in the concentration of $NaBH_4$ affects growth kinetics greatly and leads to increase in the growth rate of AgQCs; but for $NaBH_4$ concentrations higher than the optimum value, growth rate becomes constant. Precise measurements have shown that excitation and emission of AgQCs exhibit linear red-shift with the increasing concentration of $NaBH_4$ whereas protein excitation remains constant. Similar results were observed for both the proteins, Ova and BSA. We believe that various insights provided by this study will be helpful for further improvements in the synthetic methodology and applications of protein protected AgQCs.

Translocation of uranium from water to foodstuff while cooking

Krishnapriya K. C., Ananya Baksi, Swathi Chaudhari, Soujit Sen Gupta and T. Pradeep

J. Haz. Mater., **DOI:** 10.1016/j.jhazmat.2015.04.041

Abstract



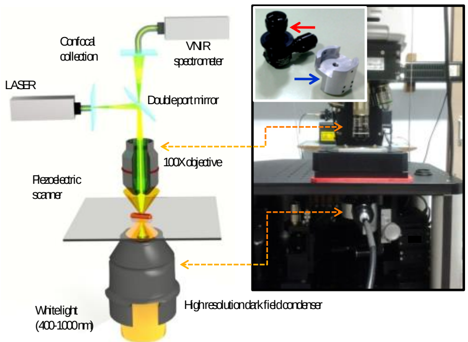
The present work report the unusual uranium uptake by foodstuff, especially those rich in carbohydrates like rice when they are cooked in water, contaminated with uranium. The major staple diet in South Asia, rice, was chosen to study its interaction with UO_2^{2+}, the active uranium species in water, using inductively coupled plasma mass spectrometry. Highest uptake limit was checked by cooking rice at very high uranium concentration and it was found to be good scavenger of uranium. To gain insight into the mechanism of uptake, direct interaction of UO_2^{2+} with monosaccharides was also studied, using electrospray ionization mass spectrometry taking mannose as a model. The studies have been done with dissolved uranium salt, uranyl nitrate hexahydrate ($UO_2(NO_3)_2 \cdot 6H_2O$), as well as the leachate of a stable oxide of uranium, $UO_2(s)$, both of which exist as UO_2^{2+} in water. Among the eight different rice varieties investigated, Karnataka Ponni showed the maximum uranium uptake whereas unpolished Basmati rice showed the minimum. Interaction with other foodstuffs (potato, carrot, peas, kidney beans and lentils) with and without NaCl affected the extent of chemical interaction but was not consistent with the carbohydrate content. Uranium interaction with d-mannose monitored through ESI–MS, under optimized instrumental parameters, identified the peaks corresponding to uranyl adduct with mannose monomer, dimer and trimer and the species were confirmed by MS/MS studies. The product ion mass spectra showed peaks illustrating water loss from the parent ion as the collision energy was increased, an evidence for the strong interaction of uranium with mannose. This study would constitute the essential background for understanding interaction of uranium with various foods. Extension of this work would involve identification of foodstuff as green heavy metal scavengers.

In vitro co-localization of plasmonic nano-bio labels and biomolecules using plasmonic and Raman scattering microspectroscopy

Kamalesh Chaudhari and T. Pradeep

J. Biomed. Opt., ***DOI:*** *10.1117/1.JBO.20.4.046011*

Abstract



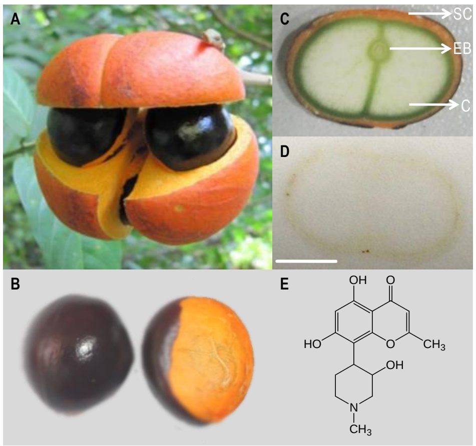
An insight into the intracellular fate of theranostics is important for improving their potential in biological applications. *In vivo* efficacy of plasmonic theranostics depend on our ability to monitor temporal changes in their size, shape, state of aggregation and identification of molecules adsorbed on their surfaces. We develop a technique which combines plasmonic and Raman scattering microspectroscopy to co-localize plasmonic scattering from metallic nanoparticles with the Raman signatures of biomolecules adsorbed on the surface of the former. Using this technique, we have co-localized biomolecules with the plasmonic scattering from silver nanoparticles in the vicinity of *Escherichia coli* bacteria. To prove the applicability of this set-up for the measurements on mammalian cells, imaging of HEK293 cells treated with gold nanoparticles was performed. We discuss the importance of such correlated measurements over individual techniques, the latter may lead to misinterpretation of results. Finally, with the above mentioned examples, we have given criteria to improve the specificity of theranostics. We believe that this methodology will be considered as a prime development in the assessment of theranostics..

Ambient ionization mass spectrometry imaging of rohitukine, a chromone anti-cancer alkaloid, during seed development in *Dysoxylum binectariferum* Hook. F (Meliaceae)

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

Phytochemistry, **DOI:** 10.1016/j.phytochem.2015.02.031

Abstract



Rohitukine, a chromone alkaloid, possesses anti-inflammatory, anti-cancer and immuno-modulatory properties. It has been reported from four species, belonging to the families, Meliaceae and Rubiaceae. Stem bark of *Dysoxylum binectariferum* (Meliaceae) accumulates the highest amount of rohitukine (3–7% by dry weight). In this study, we examine the spatial and temporal distribution of rohitukine and related compounds during various stages of seed development in *D. binectariferum* using desorption electrospray ionization mass spectrometry imaging (DESI MSI). Rohitukine (m/z 306.2) accumulation increased from early seed development to seed maturity stage. The spatial distribution of rohitukine was largely restricted to the cotyledonary tissue followed by the embryo and least in the seed coat. Besides rohitukine, rohitukine acetate (m/z 348.2) and glycosylated rohitukine (m/z 468.2) were also detected, both through mass fragmentation and exact mass analysis through Orbitrap mass spectrometry. These results indicate a dynamic pattern of chromane alkaloid accumulation through seed development in *D. binectariferum.*

Size evolution of protein protected gold clusters in solution: A combined SAXS-MS investigation

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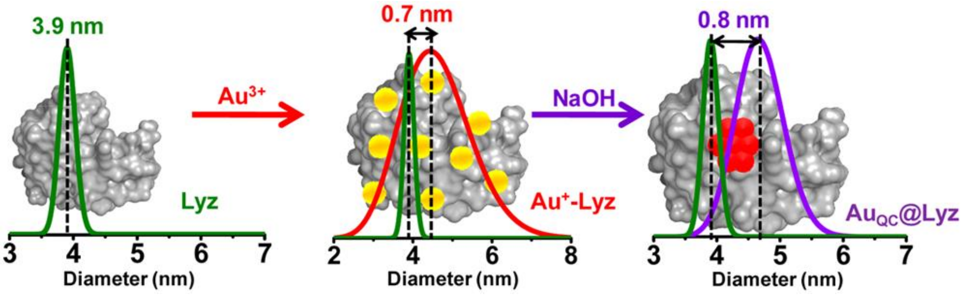
J. Phys. Chem. C, **DOI:**10.1021/jp509332j

Abstract



We report a combined small-angle X-ray scattering (SAXS) and mass spectrometric (MS) study of the growth of gold clusters within proteins, in the solution state. Two different proteins, namely, lysozyme (Lyz) and bovine serum albumin (BSA), were used for this study. SAXS study of clusters grown in Lyz shows the presence of a 0.8 nm gold core, which is in agreement with the Au_{10} cluster observed in MS. Dynamic light scattering suggests the size of the cluster core to be 1.2 nm. For BSA, however, a bigger core size was observed, comparable to the Au_{33} core obtained in MS. Concentration- and time-dependent data do not show much change in the core size in both SAXS and MS investigations. When metal−protein adducts were incubated for longer time in solution, nanoparticles were formed and protein size decreased, possibly due to the fragmentation of the latter during nanoparticle formation. The data are in agreement with dynamic light scattering studies. This work helps to directly visualize cluster growth within protein templates in solution.

Glimpses of 2015

With R. G. Cooks and C. N. R. Rao, JNCASR, January 27, 2015

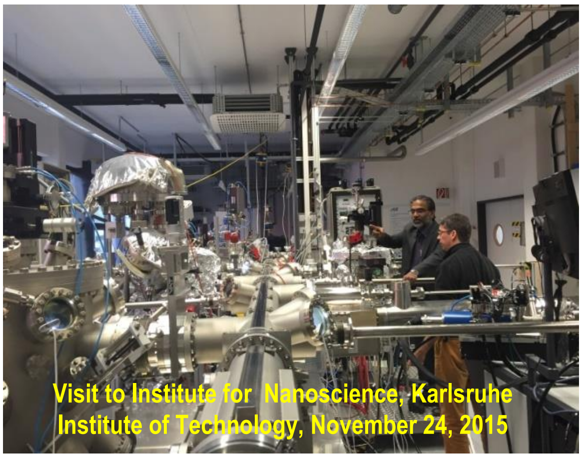
Nano Holdings team with the Director, August 11, 2015

Group photograph, July 2015

With scientists of BITRI, Botswana, August 7, 2015

At a lecture, Maris Stella College, Vijayawada, February 12, 2015

Visit of Korean Delegates to ARCI, IITM Research Park, November 28, 2015



Visit to Institute for Nanoscience, Karlsruhe Institute of Technology, November 24, 2015

Outside view of the new TUE building, to be inaugurated in January 2016

Acknowledgements

Collaborators and Students

Funding

सत्यमेव जयते

Department of Science and Technology, Government of India