An Institute of Eminence

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Since 1959

Emerging Frontiers in Sustainable Materials and Microdroplet Mechanochemistry

Thalappil Pradeep

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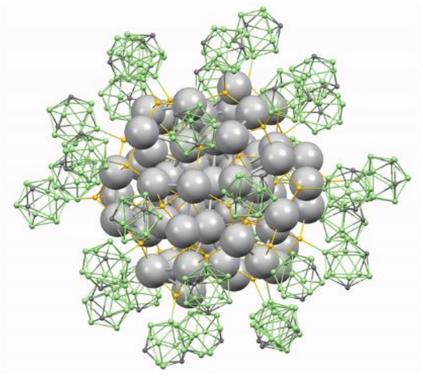
https://pradeepresearch.org

Co-founder

InnoNano Research Pvt. Ltd.
InnoDI Water Technologies Pvt. Ltd.
VayuJAL Technologies Pvt. Ltd.
Aqueasy Innovations Pvt. Ltd.
Hydromaterials Pvt. Ltd.
EyeNetAqua Solu
DeepS ovations Pvt. Ltd.



Associate Editor

ACS Sustainable Resource Management

Professor-in-charge

ICCW INTERNATIONAL CENTRE FOR CLEAN WATER

International Centre for Clean Water

https://iccw.world

pradeep RESEARCH GROUP

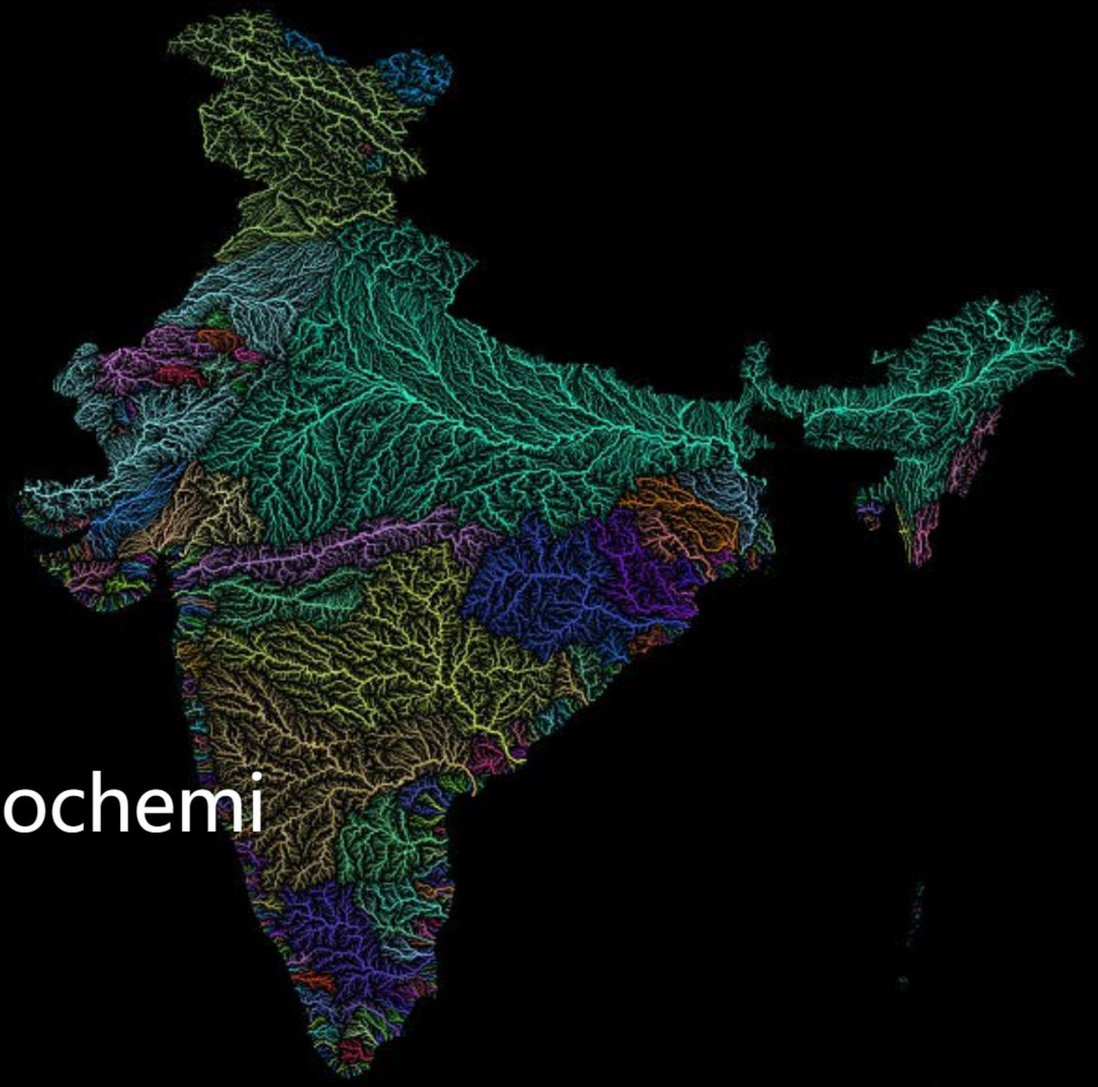
THEMATIC UNIT OF EXCELLENCE

Tsinghua Shenzhen International Graduate School, Shenzhen, November 10, 2025

Using ChatGP
T

Water is the most important inheritance of our p
lanet

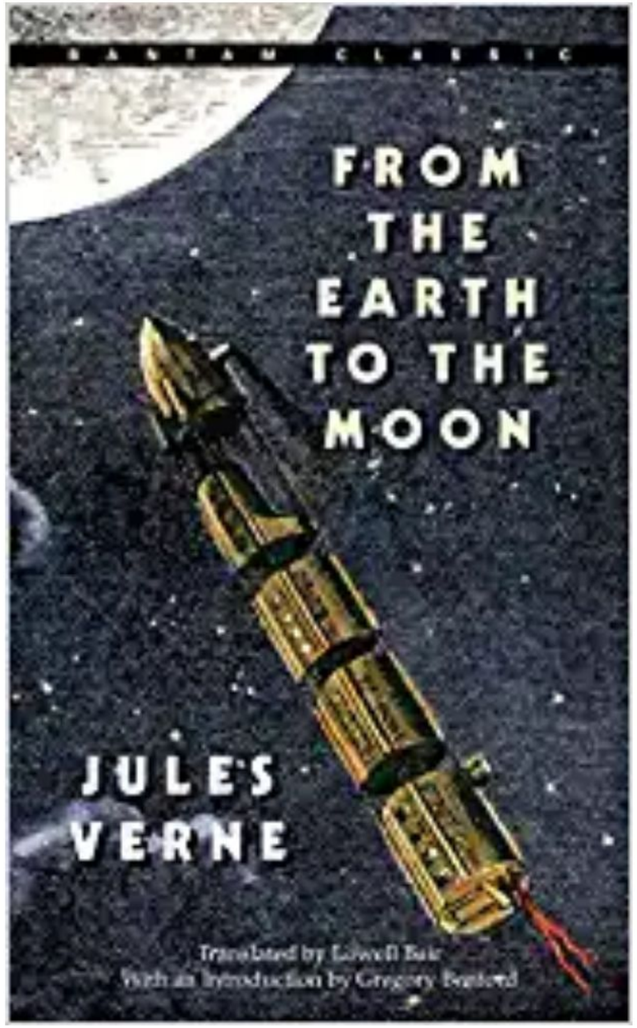
Advanced materials
Clean Water for all
Microdroplet mechanochemistry
Chemistry of ice



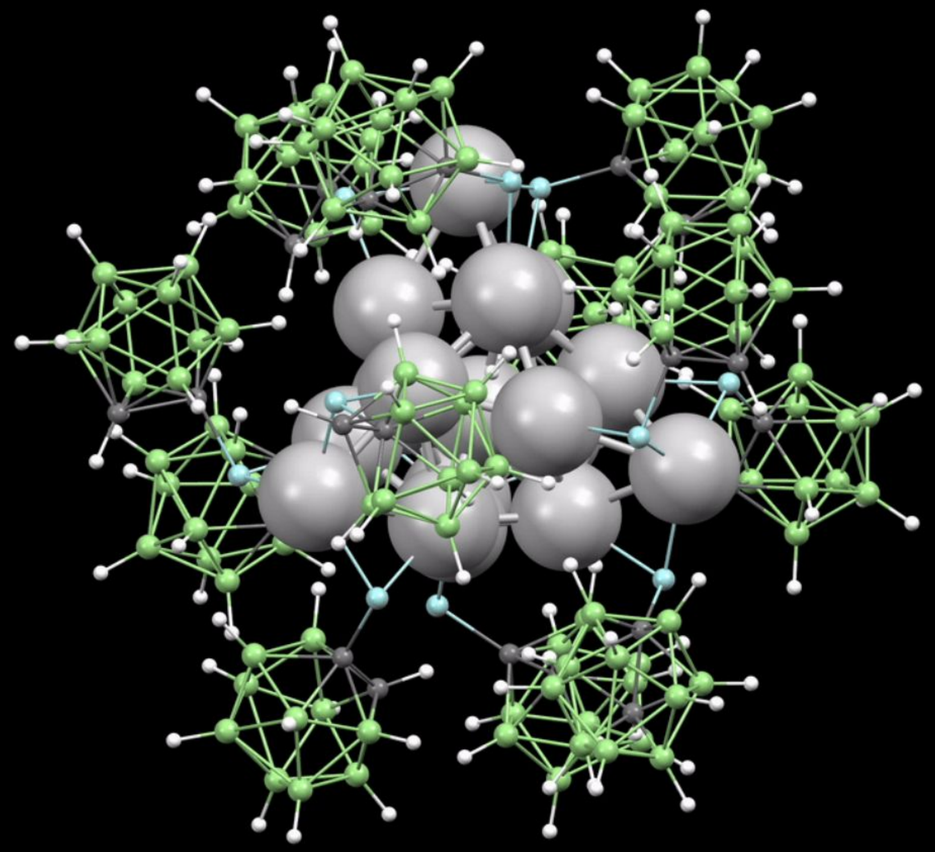
© Robert Szucs/Grasshopper Geography

From S. Vishwanath

Our dreams become reality with materials



But, matter is becomin
g
ATOMICALLY PRECISE



Vivek Yadav, et. al. *Nature Communications* 2
025

Organic and inorganic matter too are becoming atomically p
recise


HSB 148

World’s first nanochemistry-based water purifier

RSC | Advancing the Chemical Sciences

Chemistry World

Pesticide filter debuts in India

20 April 2007

Kilugudi Jayaraman/Bangalore, India

A domestic water filter that uses metal nanoparticles to remove dissolved pesticide residues is about to enter the Indian market. Its developers at the Indian Institute of Technology (IIT) in Chennai (formerly Madras) believe it is the first product of its kind in the world to be commercialised.

Mumbai-based Eureka Forbes Limited, a company that sells water purification systems, is collaborating with IIT and has tested the device in the field for over six months. Jayachandra Reddy, a technical consultant to the company, expects the first 1000 units to be sold door-to-door from late May.

'Our pesticide filter is an offshoot of basic research on the chemistry of nanoparticles,' Thalappil Pradeep who led the team at IIT Chennai told Chemistry World. He and his student Sreekumaran Nair discovered in 2003 that halocarbons such as carbon tetrachloride (CCl_4) completely break down into metal halides and amorphous carbon upon reaction with gold and silver nanoparticles[1].

Pradeep said this prompted them to extend their study to include organochlorine and organophosphorous pesticides, whose presence in water is posing a health risk in rural India. In research funded by the Department of Science and Technology in New Delhi, his team found[2,3] that gold and silver nanoparticles loaded on alumina were indeed able to completely remove endosulfan, malathion and chlorpyrifos - three pesticides that have been found at elevated levels in Indian water supplies.

Use and recycle

The mechanism of removal is 'adsorption followed by catalytic destruction', Pradeep explained. 'The chemistry occurs in a wide concentration range of environmental significance.' He added that tests proved silver particles from the

The pesticide-

[redacted]

A plant to make supported nanomaterials for water purification; with capacity of 4.5 tons per month,

[redacted]

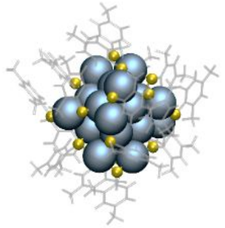
Indian patent 200767

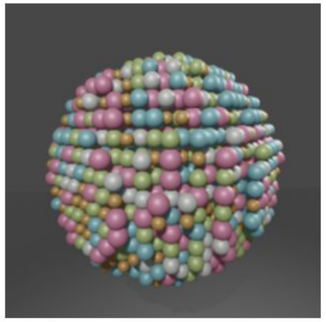
US 7,968,493

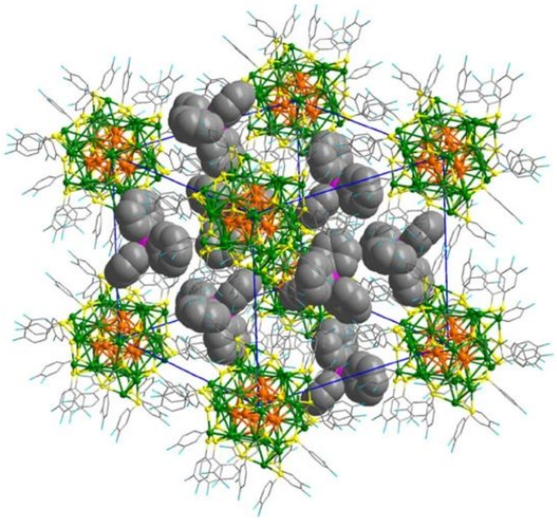
EP 17,15,947

Product is marketed now by a Eureka Forbes Ltd

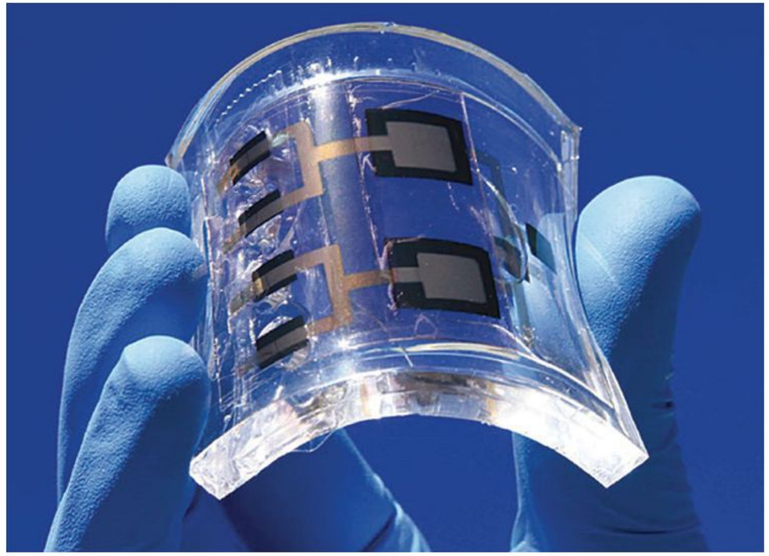
Based on the work of: R. W. Murray, Robert L. Whetten, Uzi Landman, Tatuya Tsukuda, Yuichi Negishi, Konishi, Hannu Hakkinen, Rongchao Jin, Nanfeng Zheng, Terry Bigioni, Osman Bakr, Kornberg, Jianping Xie, C. M. Aikens, Thomas Buergi, Stefan Wajda, Amala Dass, Christopher Ackerson, Kenneth L. Knappenberger, Rodolphe Antoine, Noelia Barrabes, Joanna Olesiak-Banska, Rajesh Sardar, George C. Schatz, Robert W. J. Scott, Kevin Stamplecoskie, Marcus Tofanelli, Jie Zheng, Gangli Wang, Julia Laskin, De-en Jiang, Robin Ras, Olli Ikkala, María Francisca Matus, Nonappa, Manfred Kappes, Stefanie Dehen, Stacy Copp, Andre Clayborne, Anindita Das, Ignacio Garzon, Lasse Jensen, Chris Johnson, Chen-Wei Liu, Dongil Lee, Di Sun, Quan-Ming Wang, Manzhou Zhu, Taeghawan Hyeon, Jian He, Yan Zhu, Meng Zhou, Wenwu Xu, Man-Bo Li, Shuang Quan Zang, Yongbo Song, Huan Yan, Zhikun Wu, Chuanhao Yao, Jinbin Liu, Hai-Long Jiang, Gao Li, Shaowei Chen, Sukhendu Mandal, Indranath Chakraborty, E. S. Shibu, Ananya Baksi, Amitav Pat



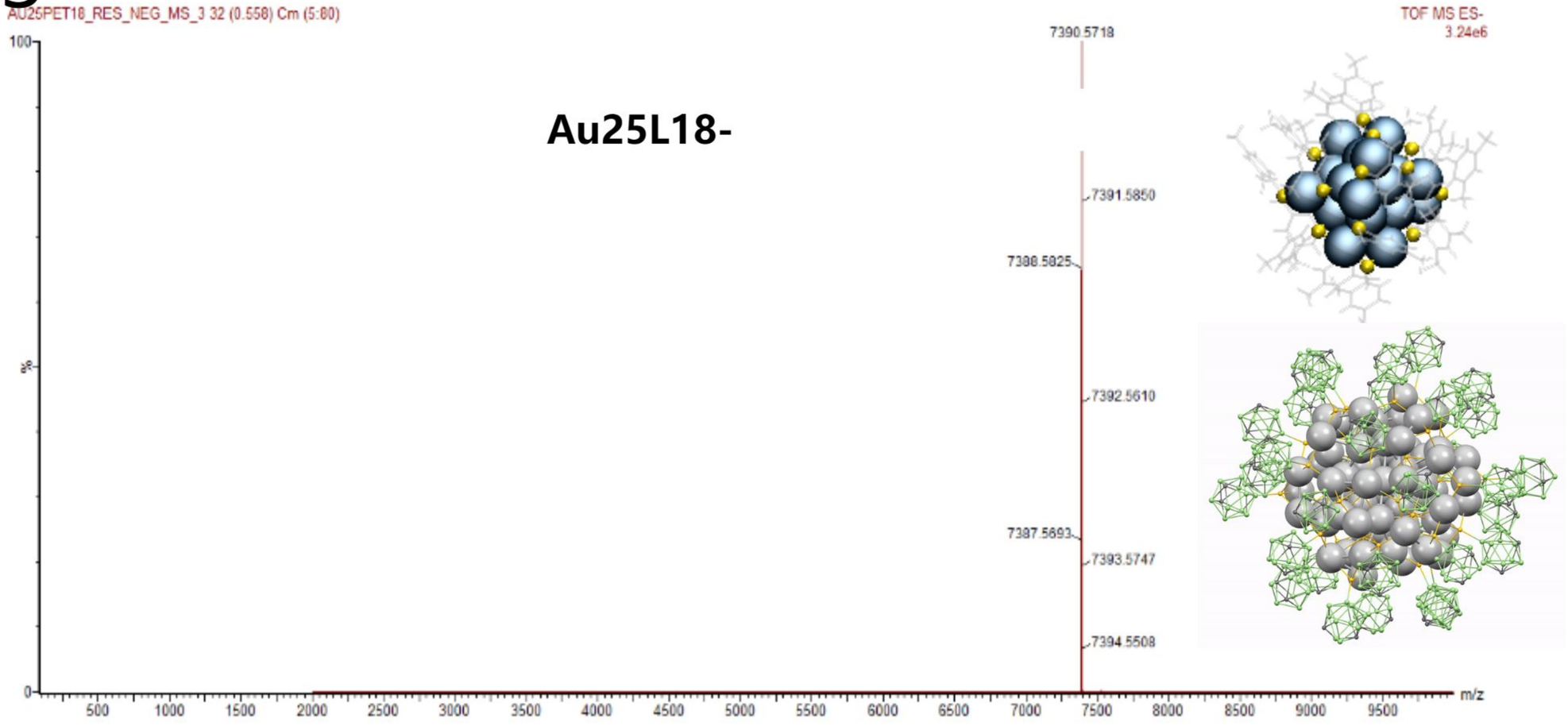




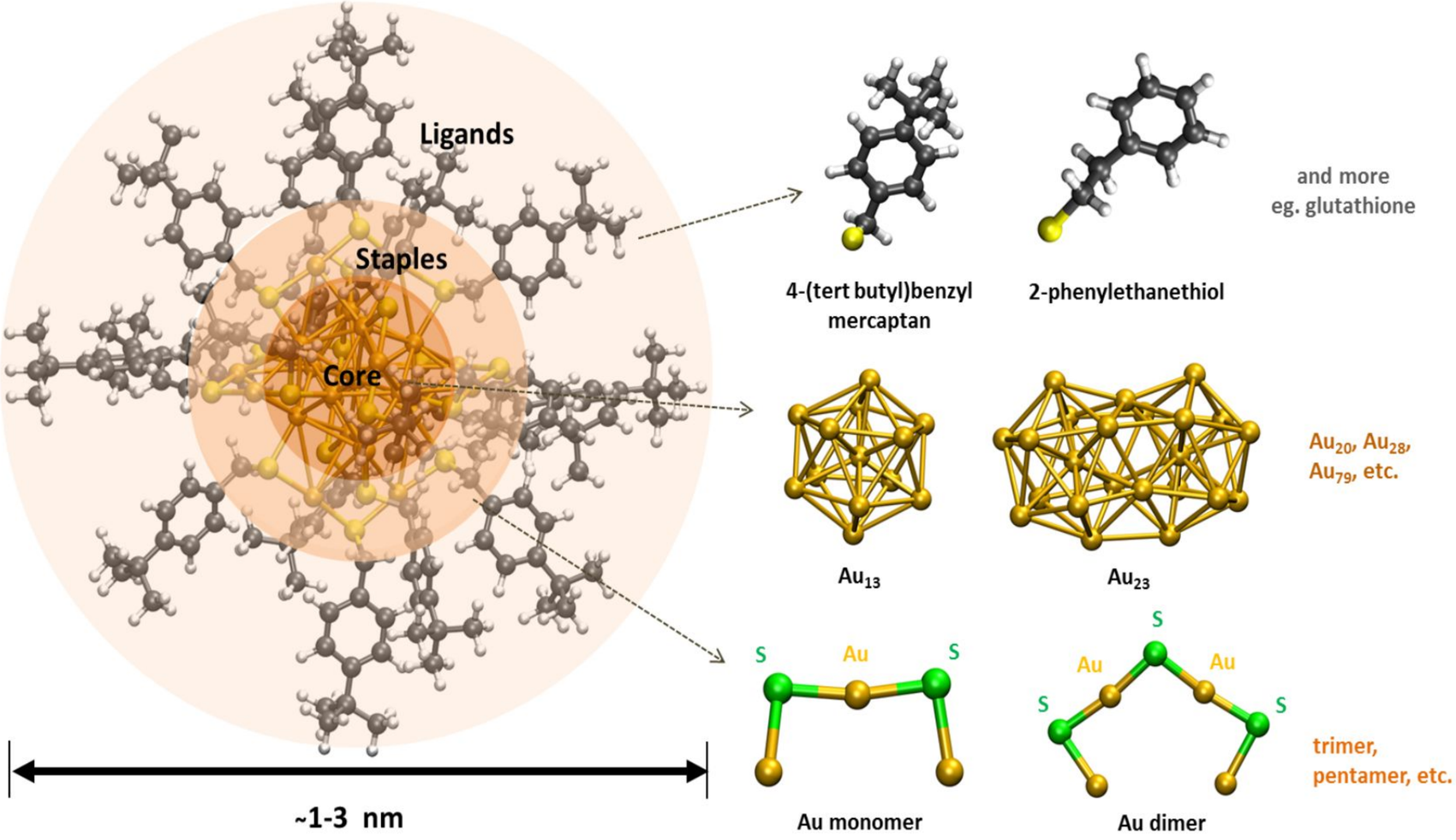
Chasing the ‘Cluster’ Dr
eams



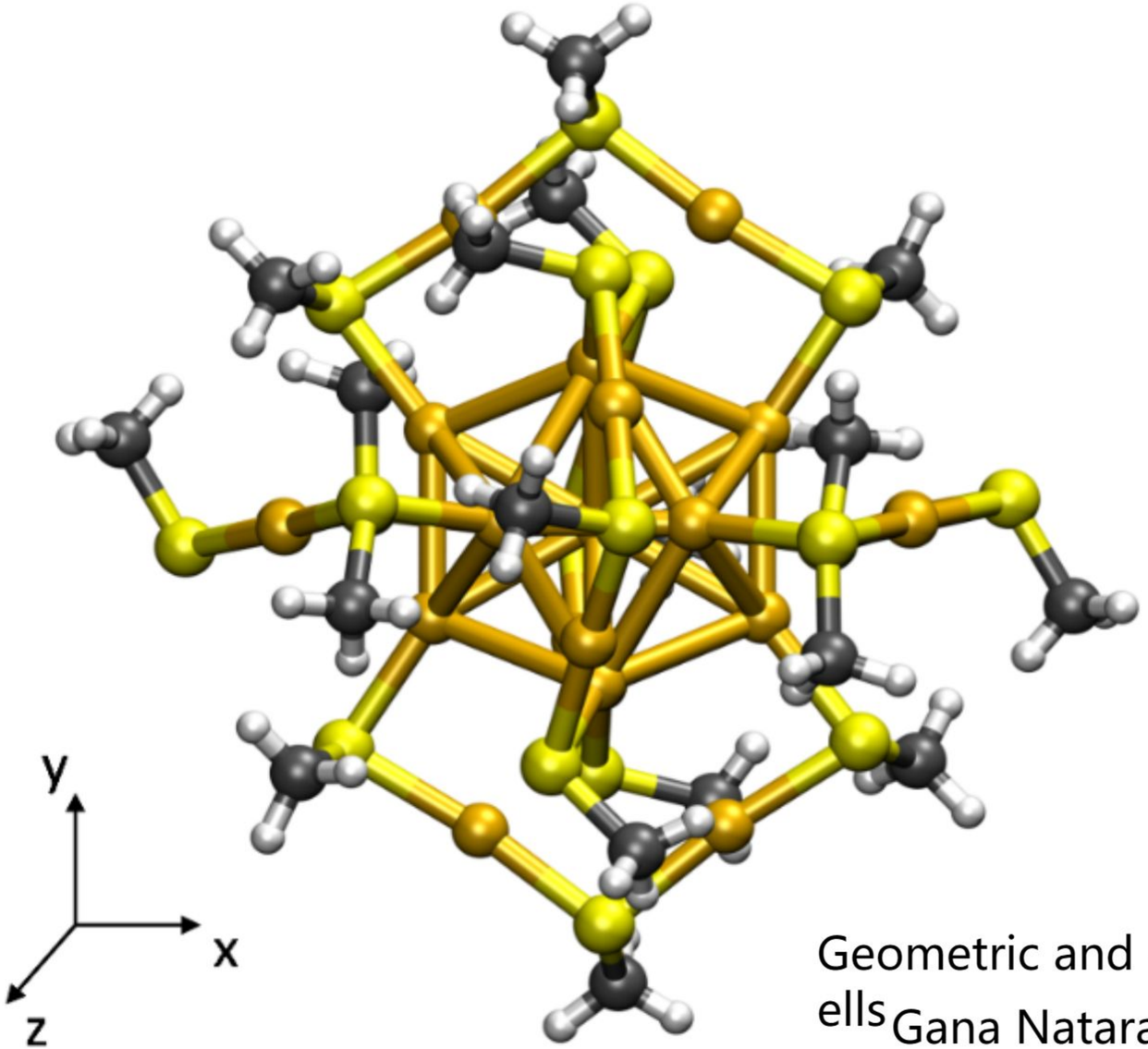
Molecular formula, Molecular weight



T. Pradeep et. al. *Acc. Chem. Res.* 2018; 2019.

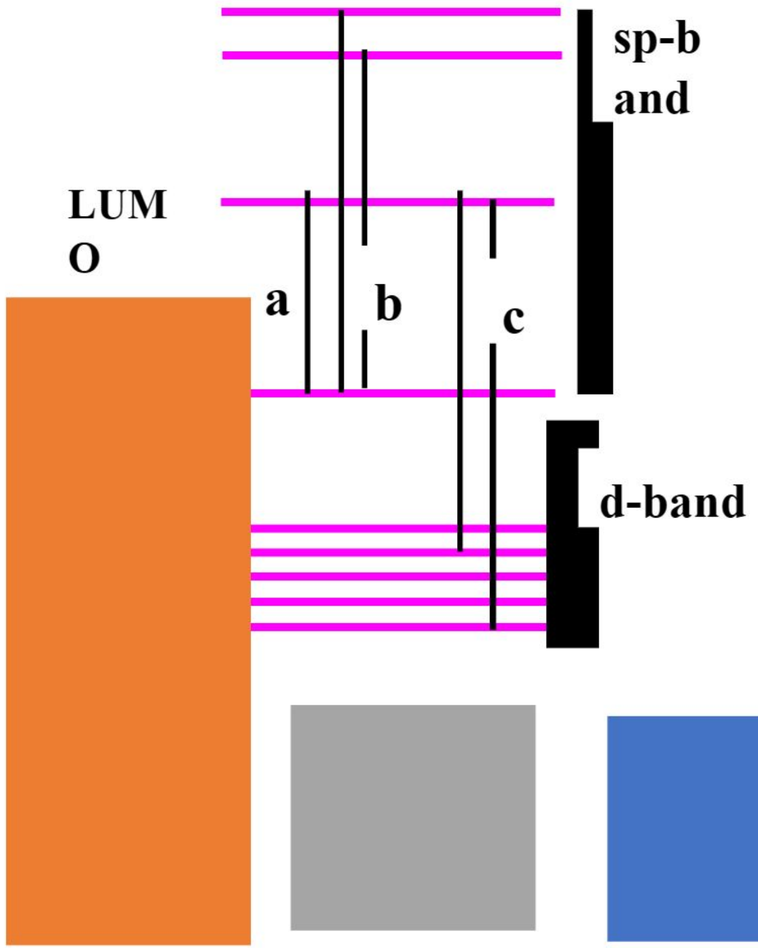

Ligands
Staples
Core
~1-3 nm
4-(tert butyl)benzyl mercaptan
2-phenylethanethiol
and more
eg. glutathione
Au_{13}
Au_{23}
Au_{20}, Au_{28}, Au_{79}, etc.
S
Au
S
Au monomer
S
Au
Au
S
S
Au dimer
trimer, pentamer, etc.

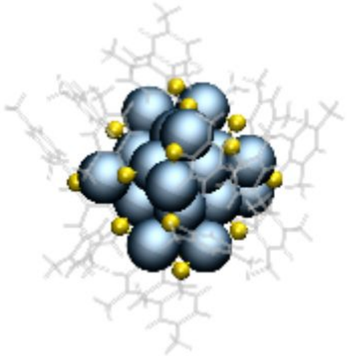
Molecular structure



Geometric and electronic shells

Gana Natarajan

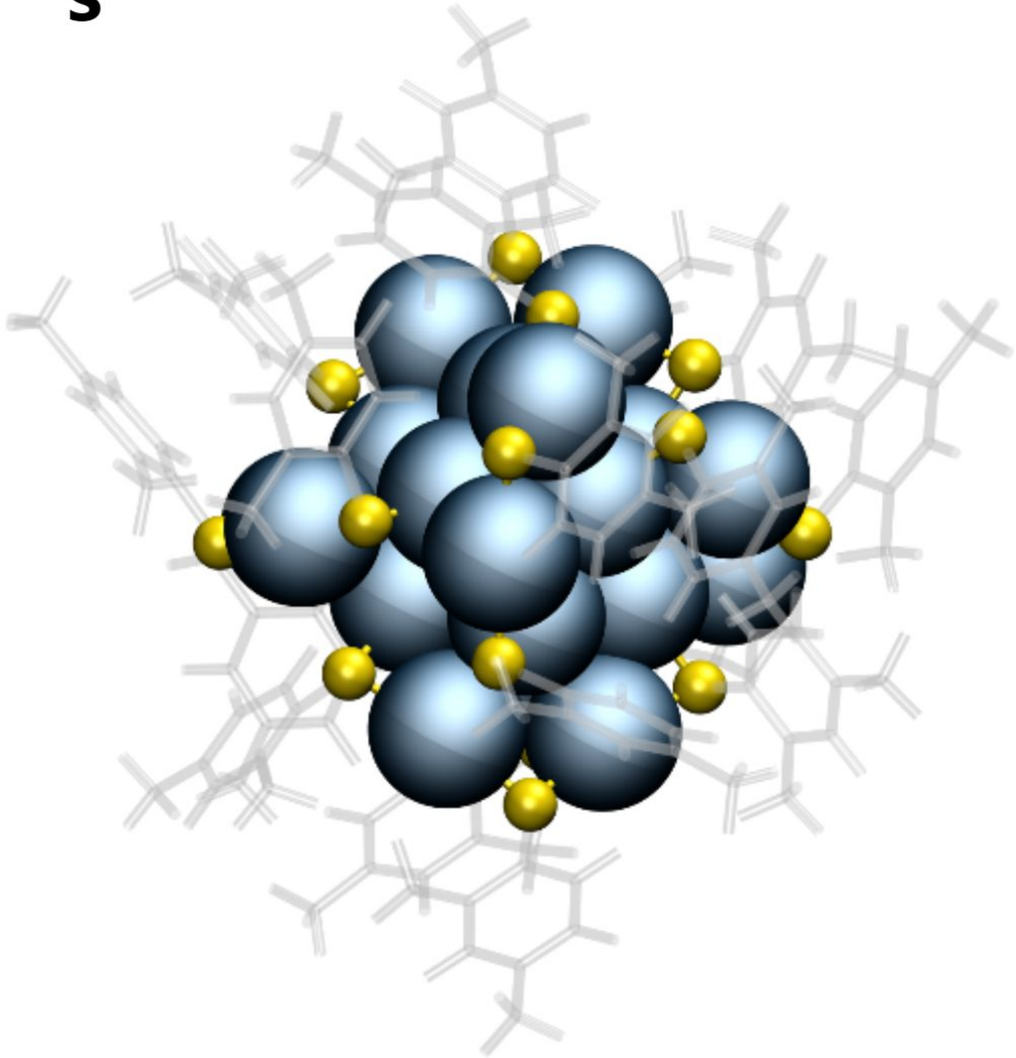




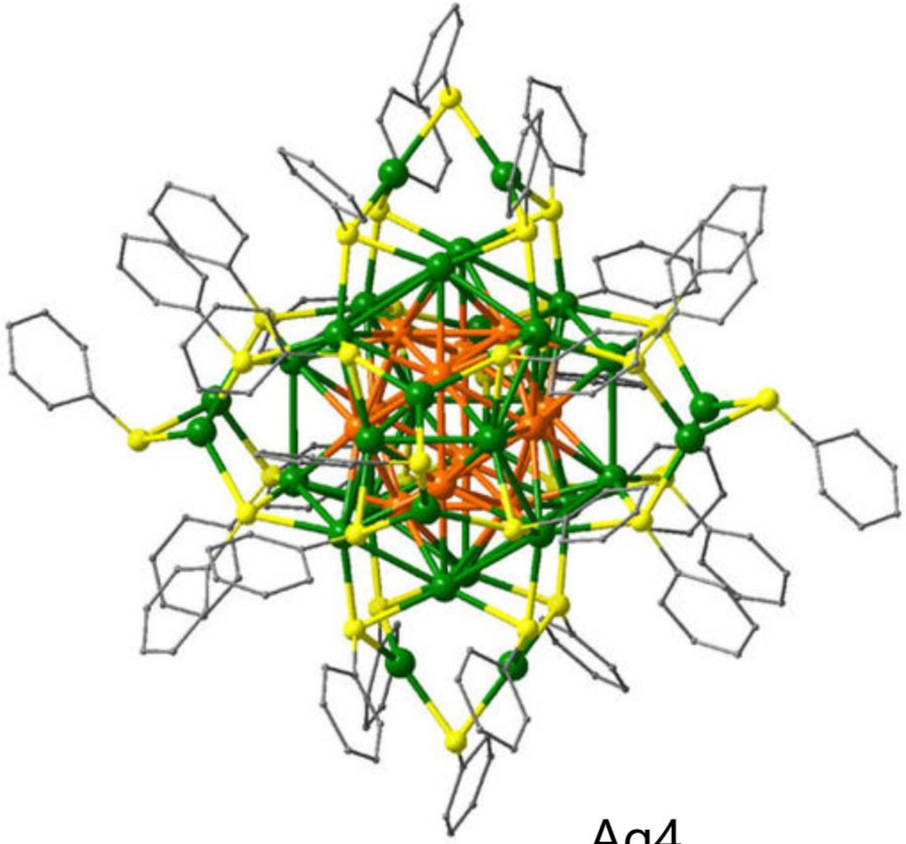
Jobin et. al. CPL, 2004

Shibu et. al. J. Phys. Chem. 200
8

New molecules



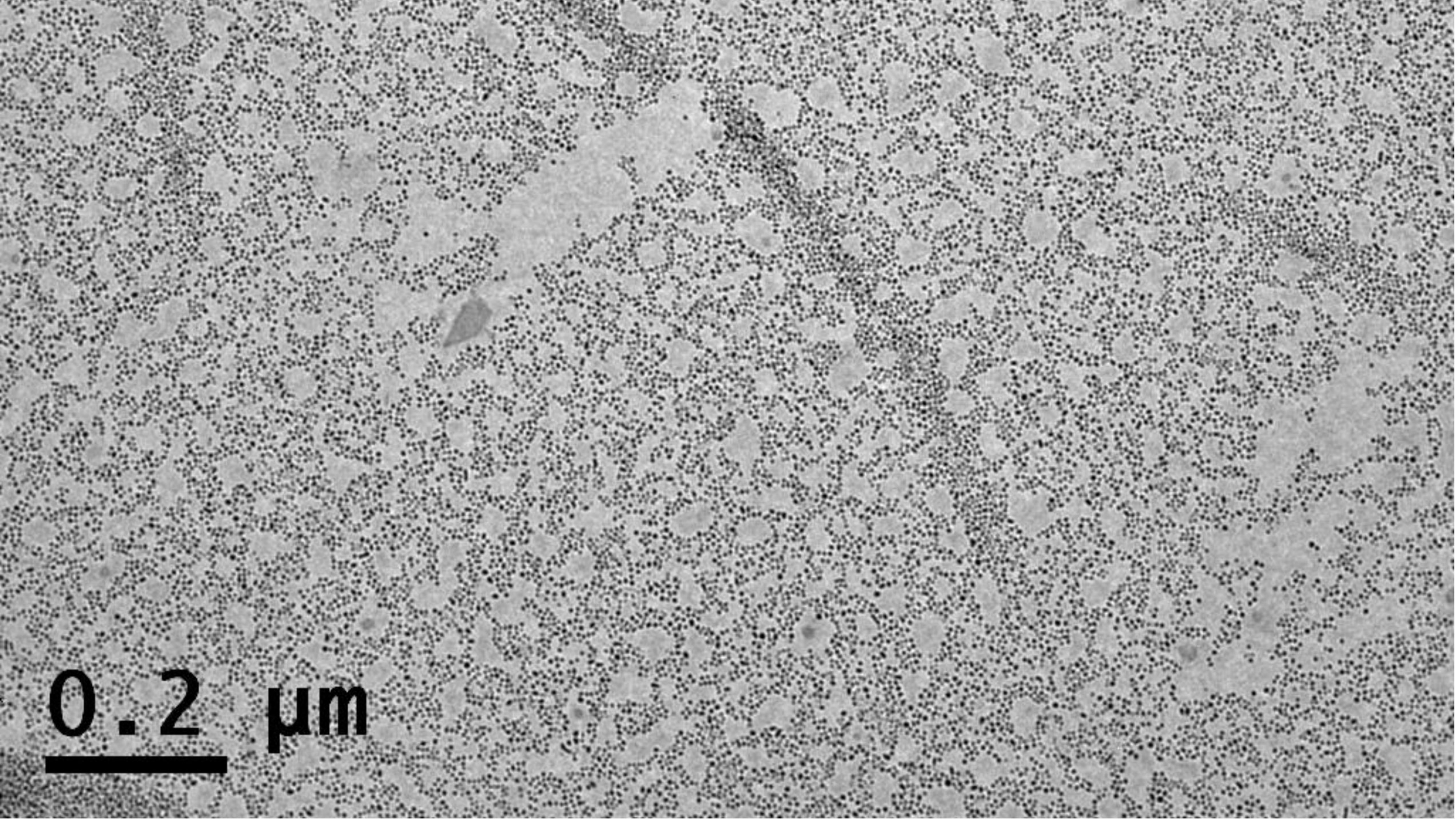
Au25, Ag25, Ag29



Ag44

Nanfeng Zheng et al. *Nature Communications*, 2013

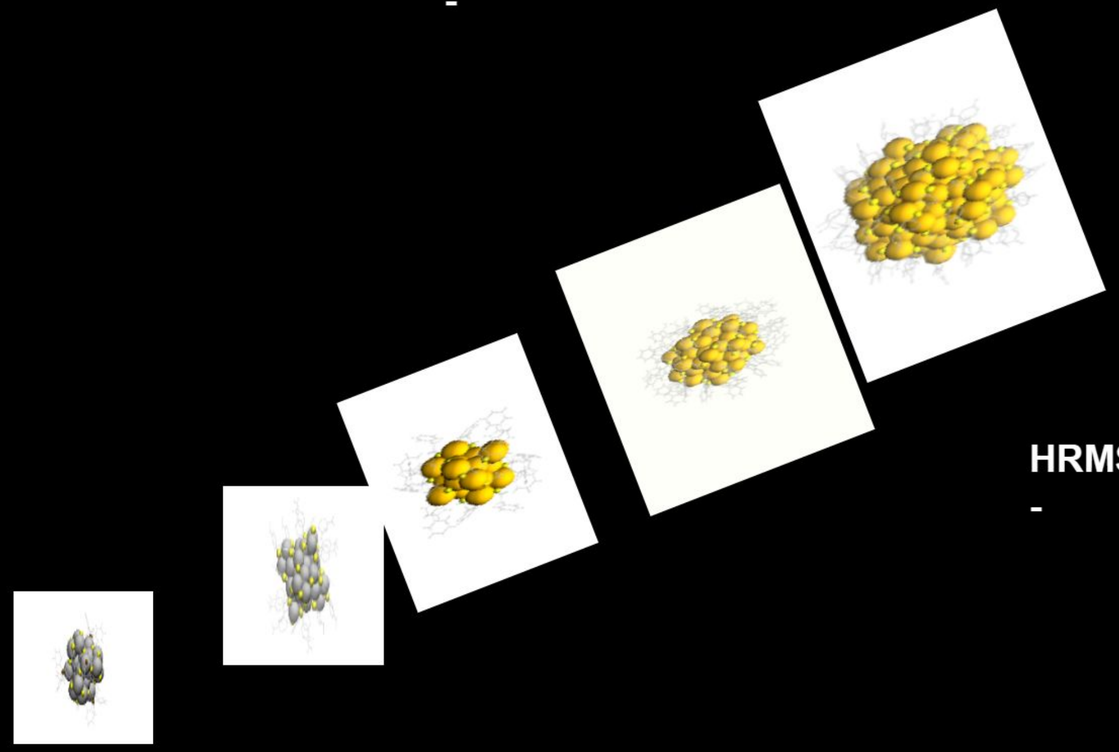
Terry Bigioni et al. *Nature* 2013


0.2 μm

Ag29(BDT)123-

Ag25(DMBT)18-

Au25(PET)18-



HRMS of Au25(PET)18-

m/z

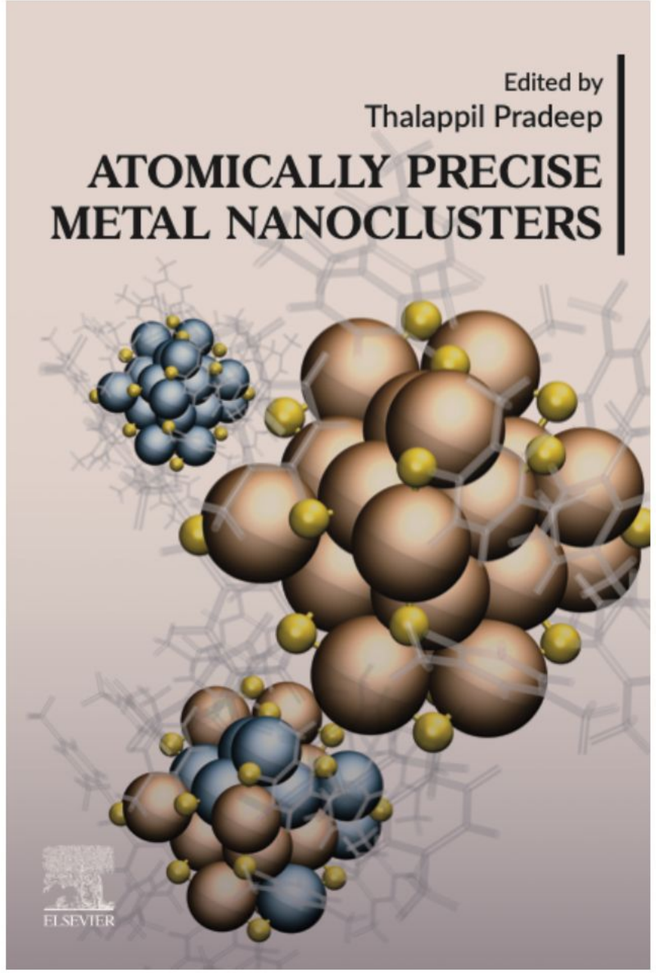
Molecular materials

Molecules and their properti es

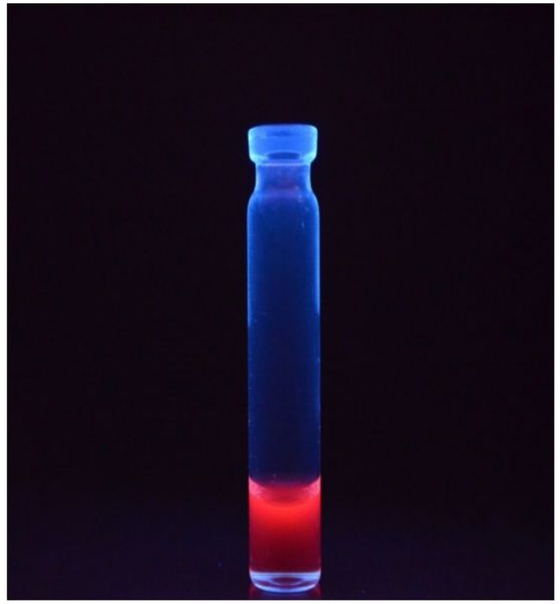
Chemical formula	H_2O
Molecular weight	18.0148
Critical temperature	373.91°C
Critical pressure	22.05 MPa
Critical density	315.0 kg/m^3
Triple point temperature	0.01°C
Triple point pressure	615.066 Pa
Normal boiling point	100.0°C
Normal freezing point	0.0°C
Density of ice at normal melting point	918.0 kg/m^3
Maximum density, 3.98°C	999.973 kg/m^3
Viscosity, 25°C	0.889 mN s/m^2
Surface tension, 25°C	72 mN/m
Heat Capacity, 25°C	4.1796 kJ/kg.K
Enthalpy of vaporisation, 100°C	2,257.7 kJ/kg
Enthalpy of fusion, 0°C	333.8 kJ/kg
Velocity of sound, 0°C	1.403 km/s
Dielectric constant, 25°C	78.40
Electrical conductivity, 25°C	8 μS/m
Refractive index, 25°C	1.333
Liquid compressibility, 10°C	480. × 10^{-12}m^2/N
Coefficient of thermal expansion, 25°C	256.32 × 10^{-6} K^{-1}
Thermal Conductivity, 25°C	0.608 W/m.K

Molecular formula
Molecular weight
Molecular structure
Molecular absorption and e mission
Molecular reactions
Molecular assembly
Molecular co-crystals

Phases - phase transitions
Physical properties
Electrical, magnetic
Mechanical properties
Electrochemical properties
Future?



Molecular reactio
ns



Reactions on clusters

Reactions between cluste
rs

Inter-cluster reactio
ns

JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
Article
pubs.acs.org/JACS

Intercluster Reactions between $Au_{25}(SR)_{18}$ and $Ag_{44}(SR)_{30}$

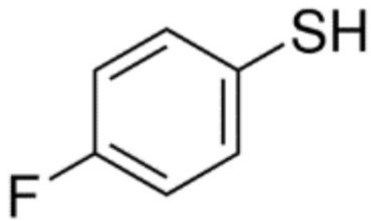
K. R. Krishnadas, Atanu Ghosh, Ananya Baksi, Indranath Chakraborty,[†] Ganapati Natarajan, and Thalappil Pradeep*

DST Unit of Nanoscience (DST UNS) and Thematic Unit of Excellence, Department of Chemistry, Indian Institute of Technology Madras, Chennai, 600 036, India

Supporting Information

A + B □ C + D

Au25(FTP)18 + Ag44(FTP)3[redacted] Au25-xAgx(FTP)18 + Ag44-xAu x(FTP)30



Energies for the substitution reaction of (A) Au in Ag44(SR)30, (B) Ag in Au25 (SR)18 and (C) the overall reaction energies (in eV) as a function of their positions in product clusters, Au*x*Ag44-*x*(SR)30 and Au25-*x*Ag*x*(SR)18 for x=1

Ag25-Au25 experiments

K. R. Krishnadas et al. *Nature Commun.* 20
16

Reaction between Au25(PET)18 and Ag25(DMBT)18

DMBT

PE
T

[Ag25(DMBT)18+Au25(PET)18]2-

DMBT

PE
T

Ag25(DMBT)
18

[Ag25(DMBT)18+Au25(PET)1
8]2-

Au25(PET)
18

Evolution of alloy clusters from the dianionic adduct, [Ag25Au25(DMBT)18(PET)18]2-

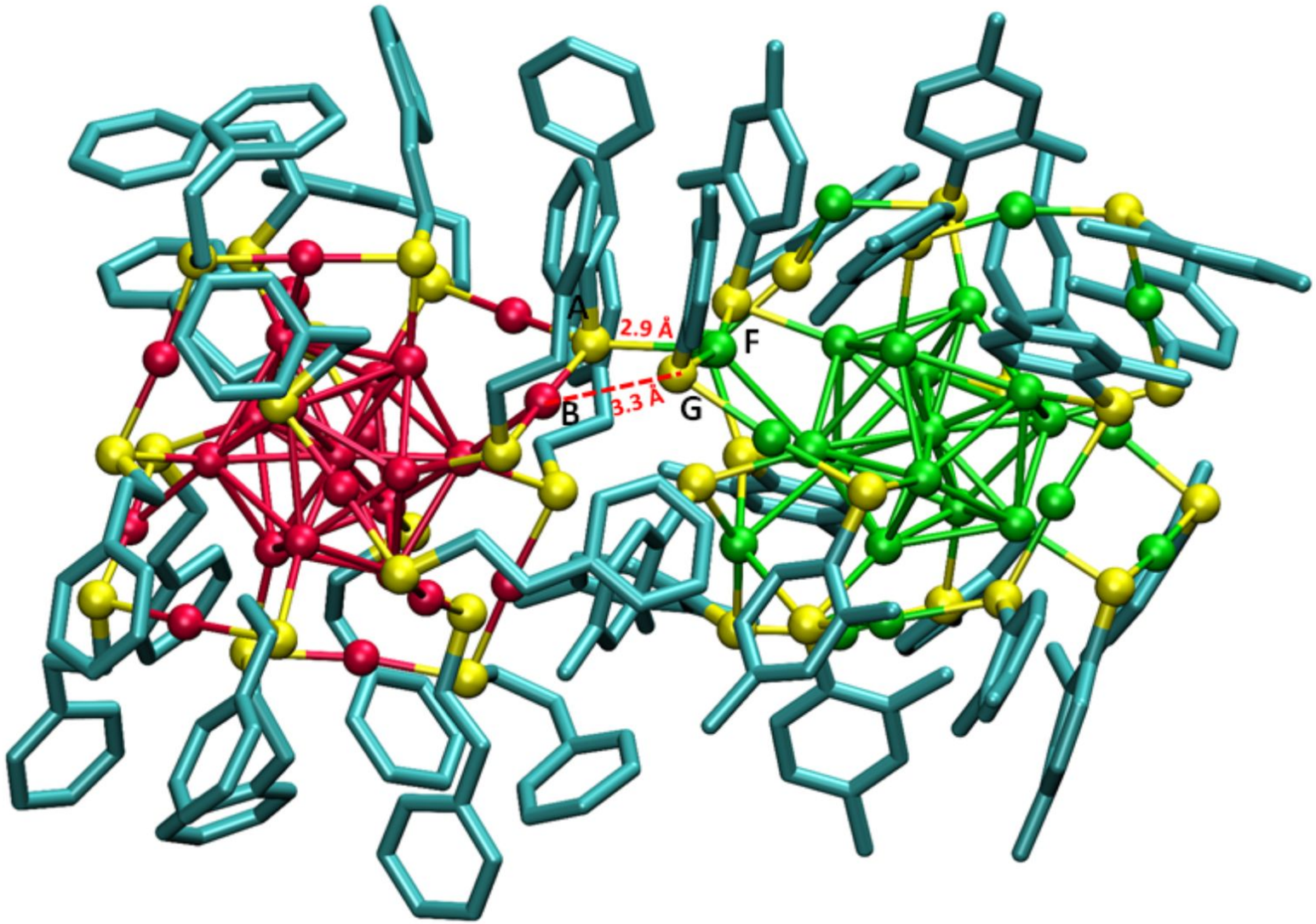
within 5 min

Ag25(DMBT)18:Au25(PET)18

0.3:1.0

within 2 min

Optimized structure of [Ag25Au25(DMBT)18(PET)18]2-



How do we comprehend th
is?

Nomenclatu
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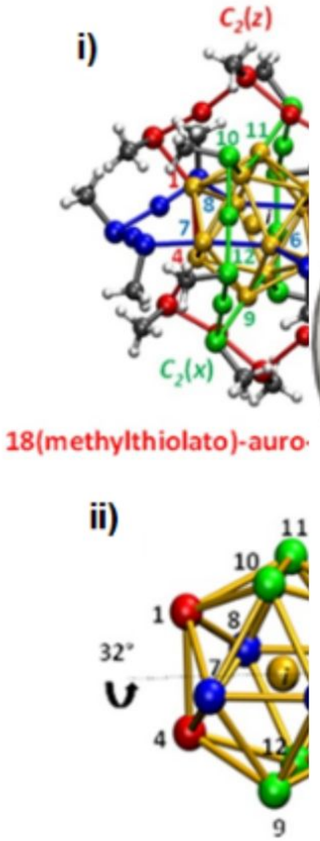
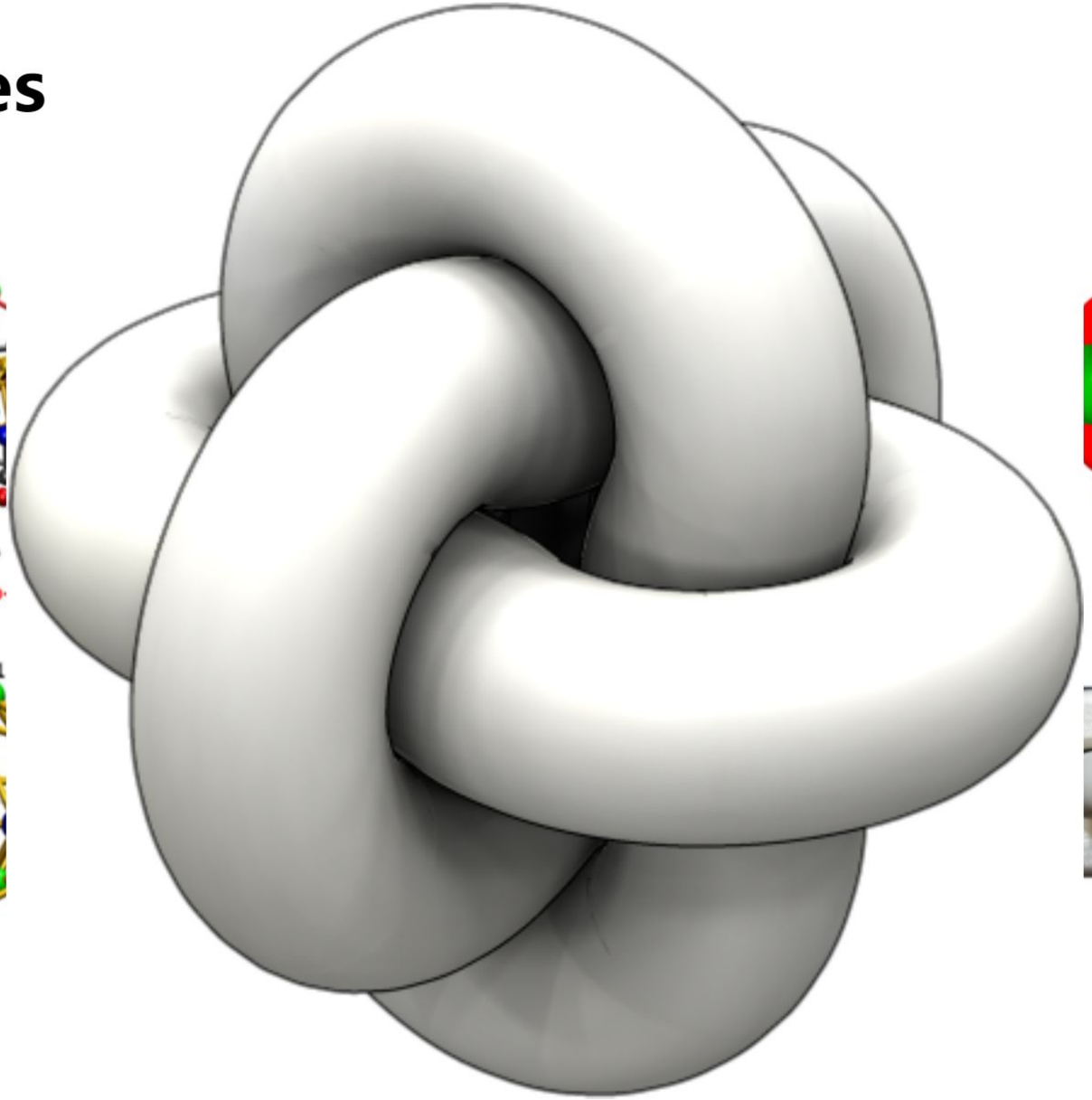
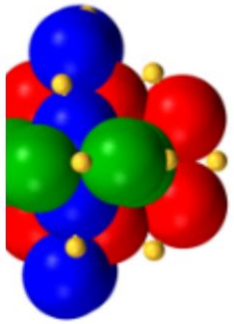
Aspicules

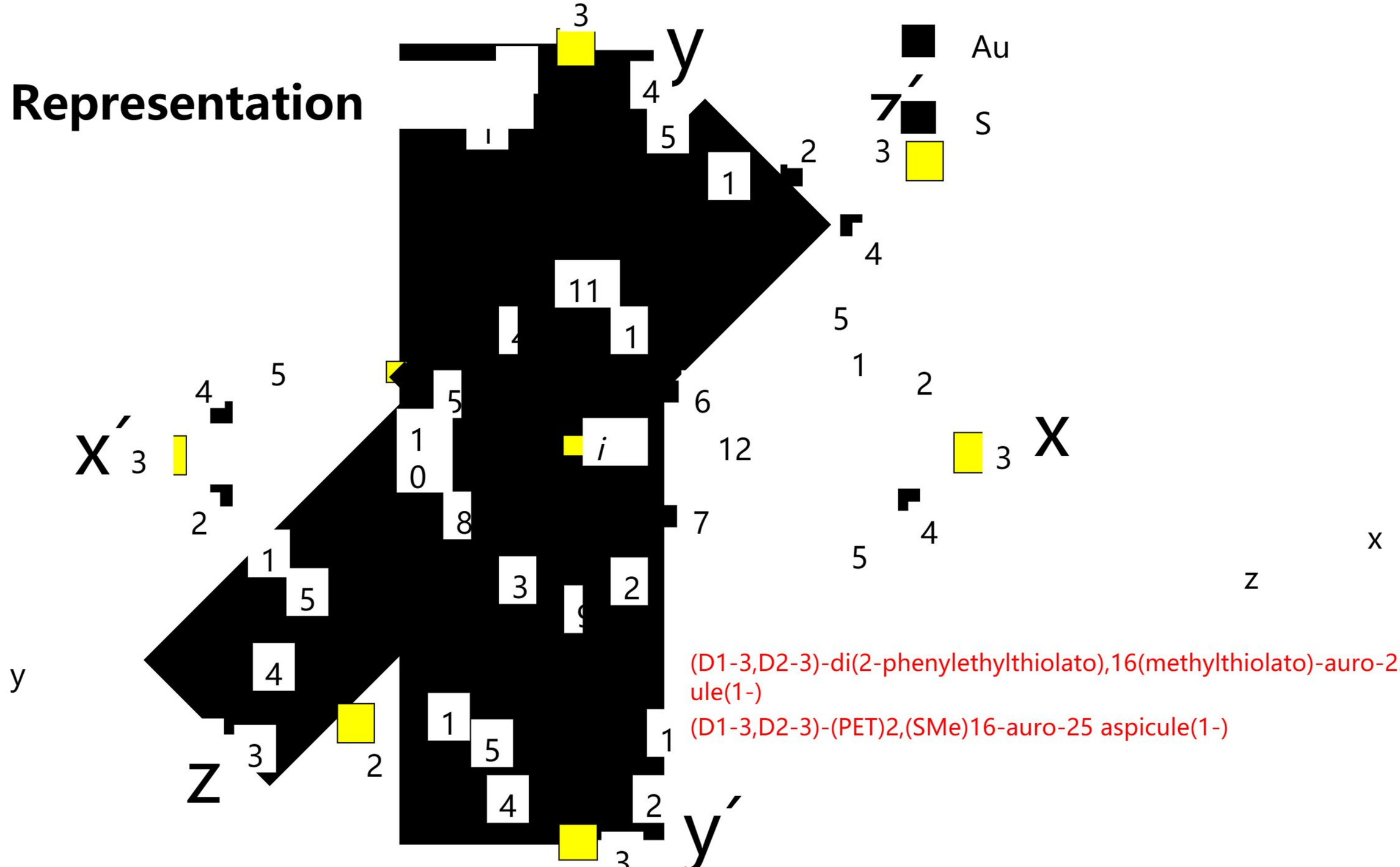






Gana Natarajan et. al. *JPC C* 2015

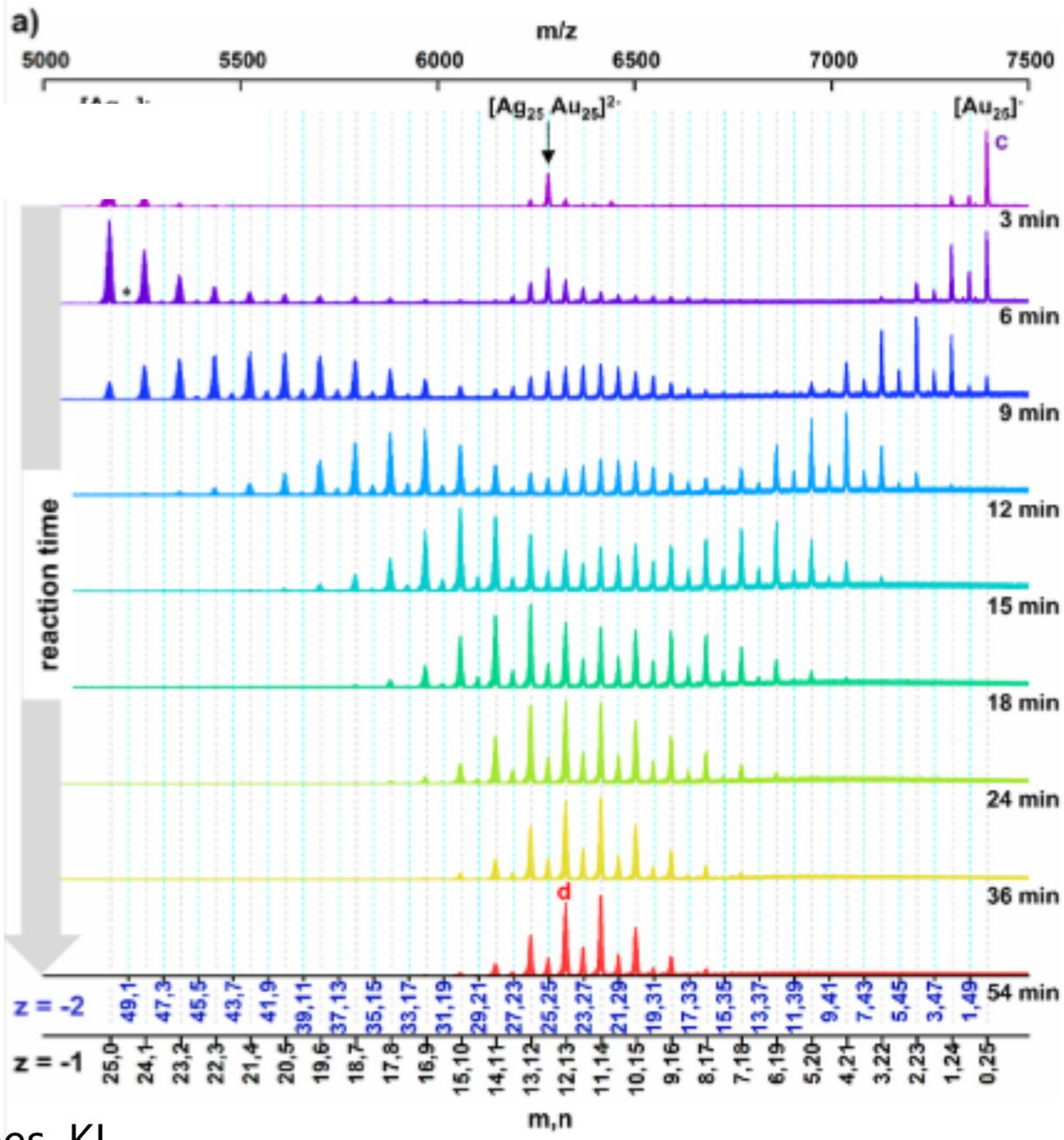
Representation



(D1-3,D2-3)-di(2-phenylethylthiolato),16(methylthiolato)-auro-25 aspicule(1-)

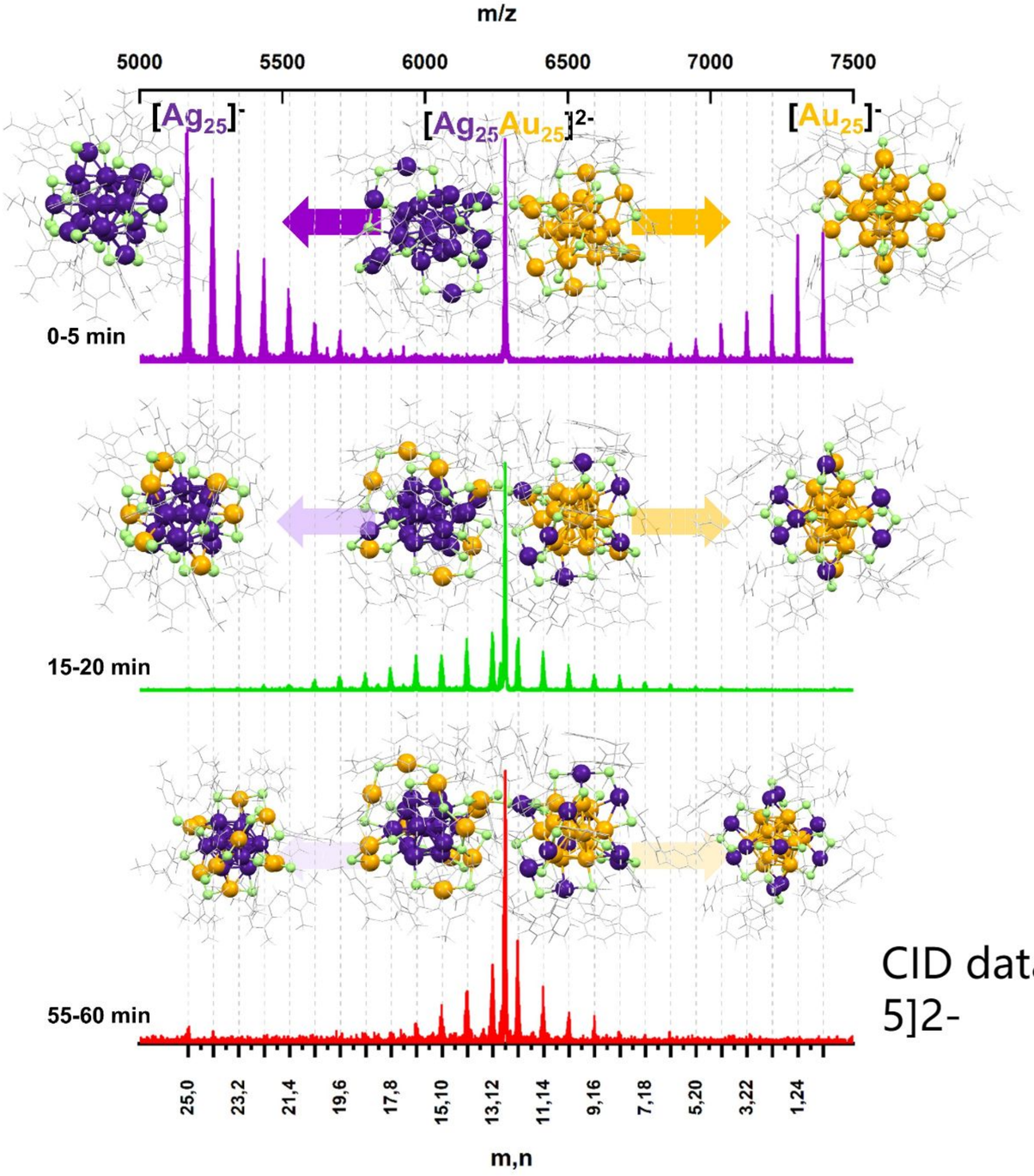
(D1-3,D2-3)-(PET)2,(SMe)16-auro-25 aspicule(1-)

Complexities



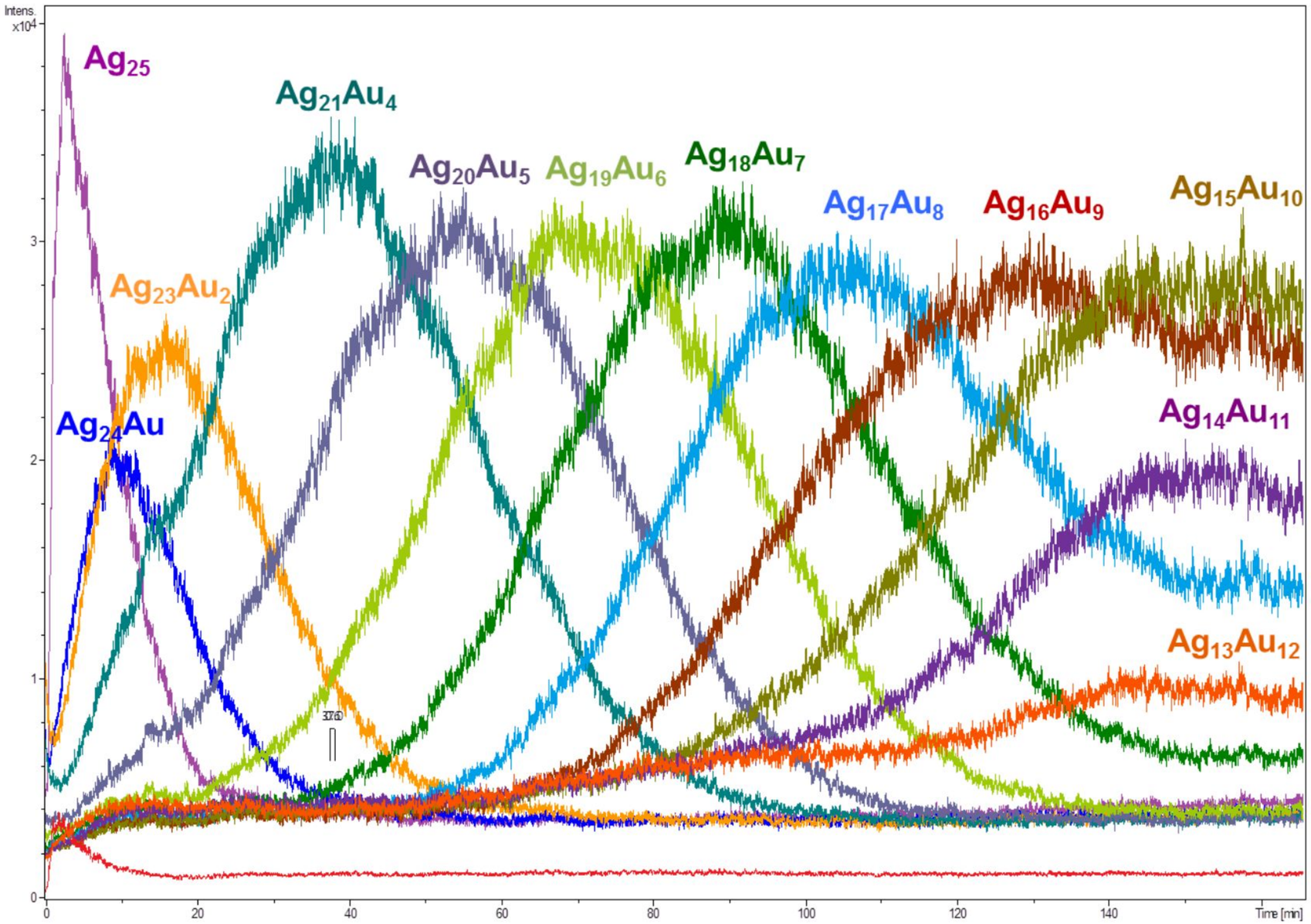
Manfred Kappes, KIT

M. Neumaier, A. Baksi, et. al., *JACS* 2021

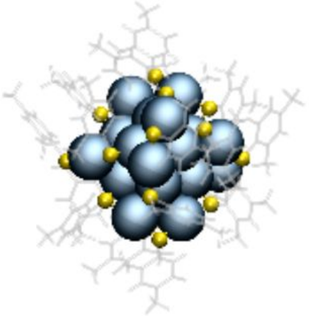


CID data of [Au25Ag25]2-

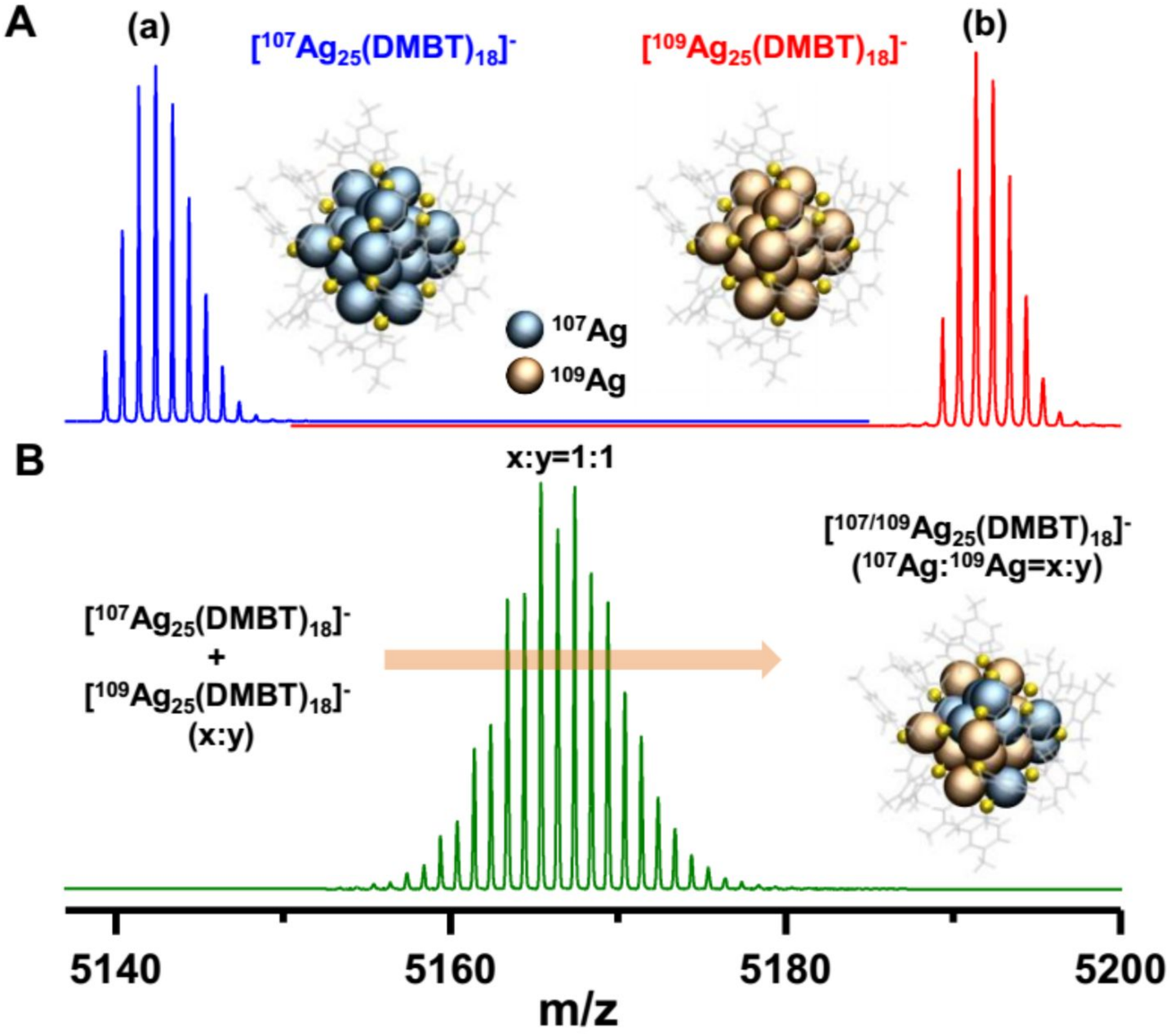
Kinetics of the exchange (monitored on the Ag25 sid e)

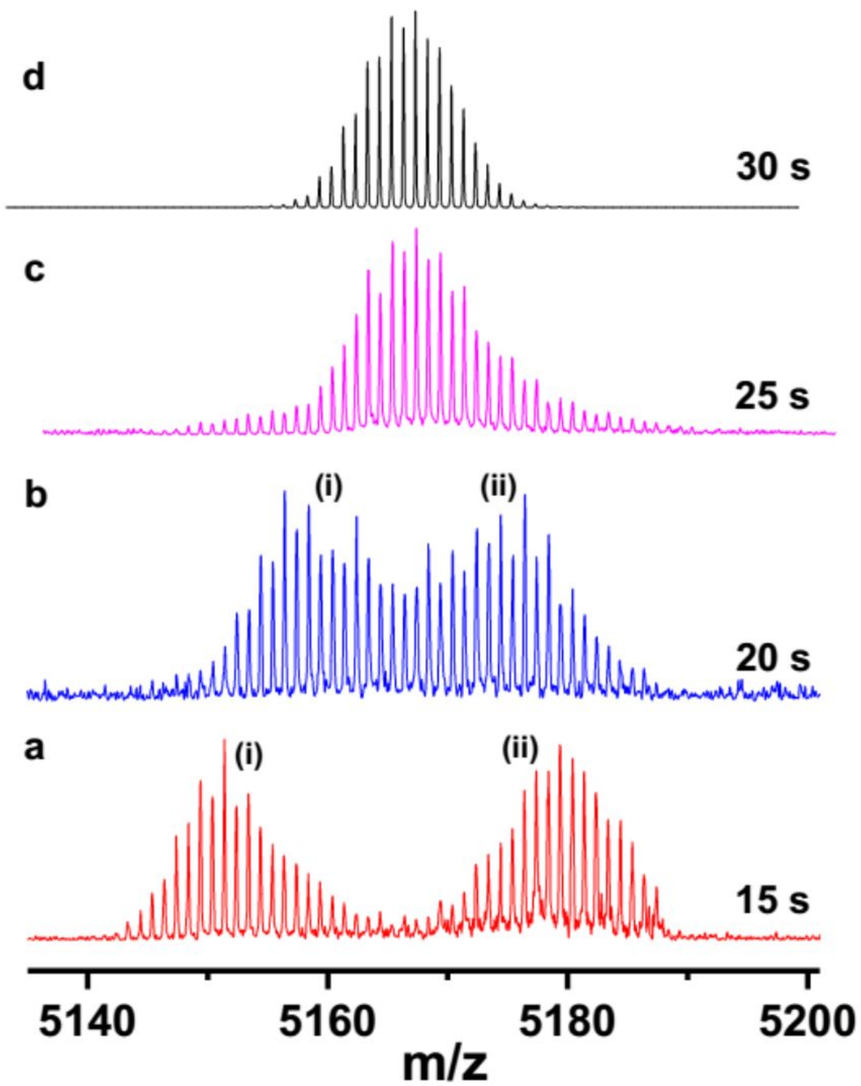


Coulomb adduc

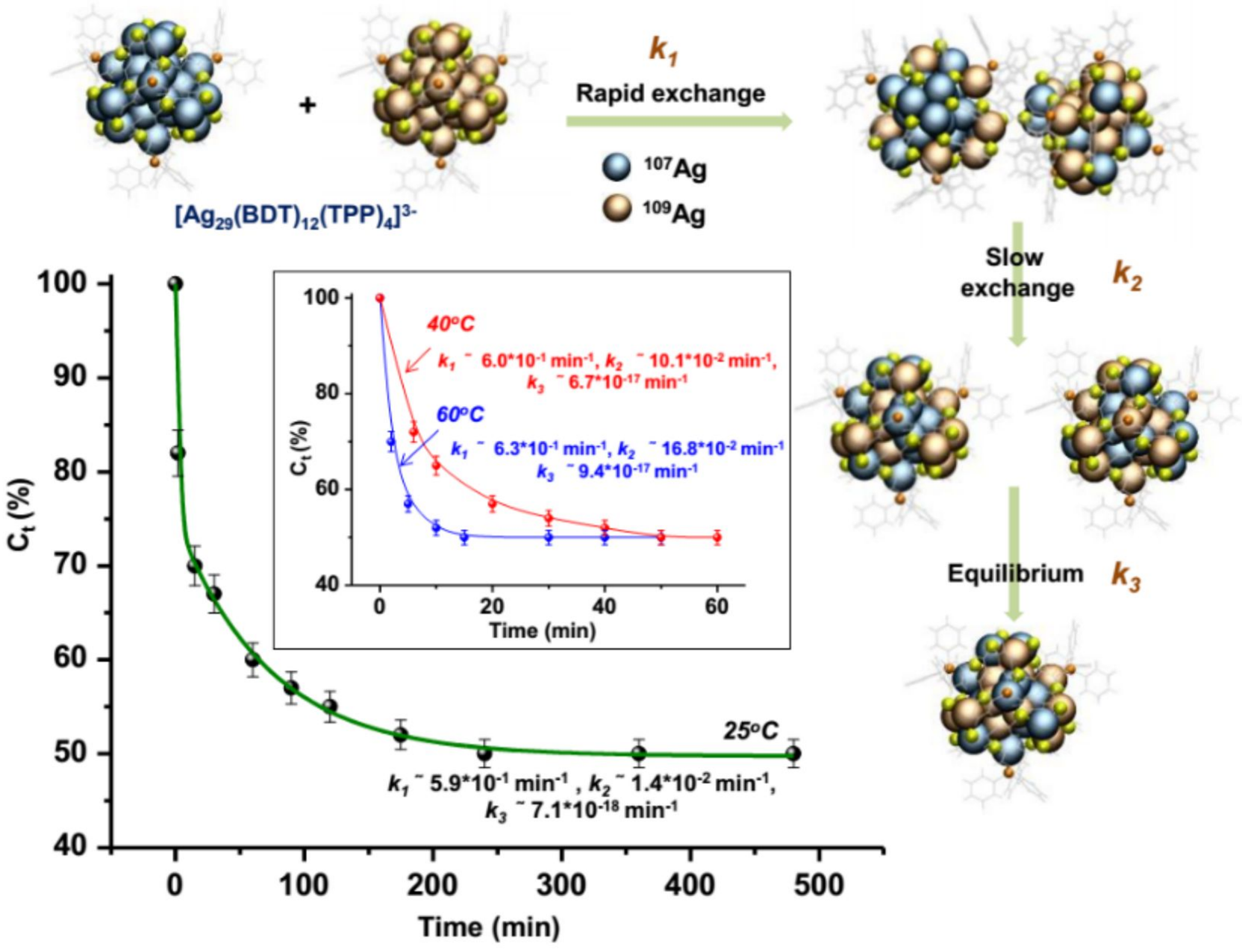


ESI MS of **A)** 107Ag25(DMBT)18 and **B)**109Ag25(DMBT)18. Insets shows the respective isotope patte rns.


A
(a)
[107Ag25(DMBT)18]-
[109Ag25(DMBT)18]-
(b)
107Ag
109Ag
B
x:y=1:1
[107/109Ag25(DMBT)18]-
(107Ag:109Ag=x:y)
[107Ag25(DMBT)18]-
+
[109Ag25(DMBT)18]-
(x:y)
5140
5160
5180
5200
m/z

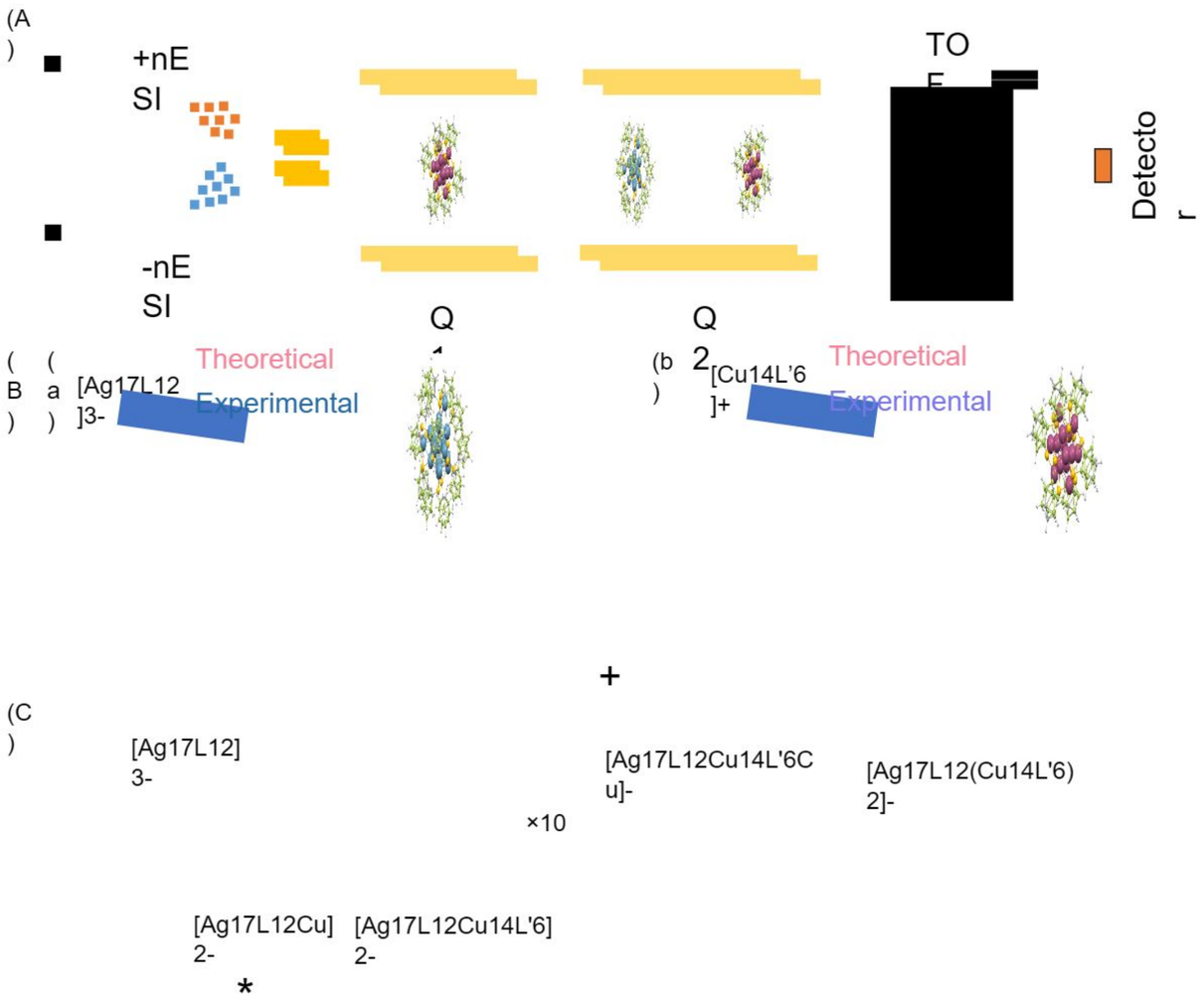


Papri Chakraborty, et. al. *Science Advances* 2019


$[Ag_{29}(BDT)_{12}(TPP)_4]^{3-}$
+
k_1
Rapid exchange
^{107}Ag
^{109}Ag
Slow exchange
k_2
Equilibrium
k_3
C_t (%)
Time (min)
25°C
k_1 ~ 5.9*10^{-1} min^{-1} , k_2 ~ 1.4*10^{-2} min^{-1},
k_3 ~ 7.1*10^{-18} min^{-1}
40°C
k_1 ~ 6.0*10^{-1} min^{-1}, k_2 ~ 10.1*10^{-2} min^{-1},
k_3 ~ 6.7*10^{-17} min^{-1}
60°C
k_1 ~ 6.3*10^{-1} min^{-1}, k_2 ~ 16.8*10^{-2} min^{-1}
k_3 ~ 9.4*10^{-17} min^{-1}


thermoscientific
ThermoFisher
SCIENTIFIC

Coulombic adducts



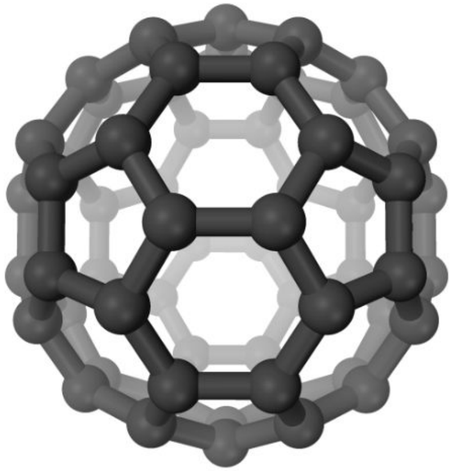
(A) Schematic representation of gas phase ion-ion reaction of atomically precise nanoclusters in an MS trap cell. Atomically precise nanoclusters (B) (a) [Ag17(o1-CBT)12]3- and (b) [Cu14(o9,12-CBDT)6]+ forming (C) Columbic adducts.

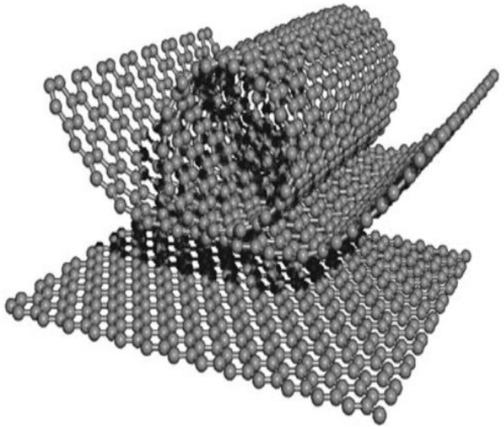
With Scott McLuckey and De-en Jiang

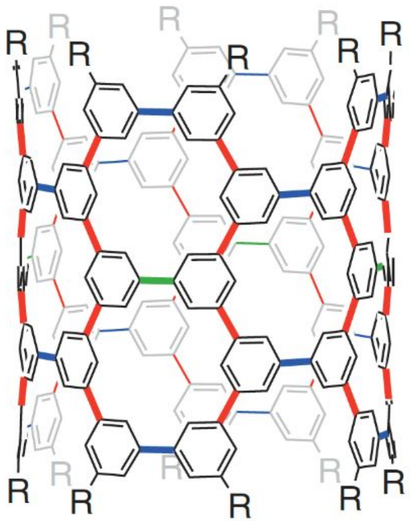
Power of chemistry - Anything can be made

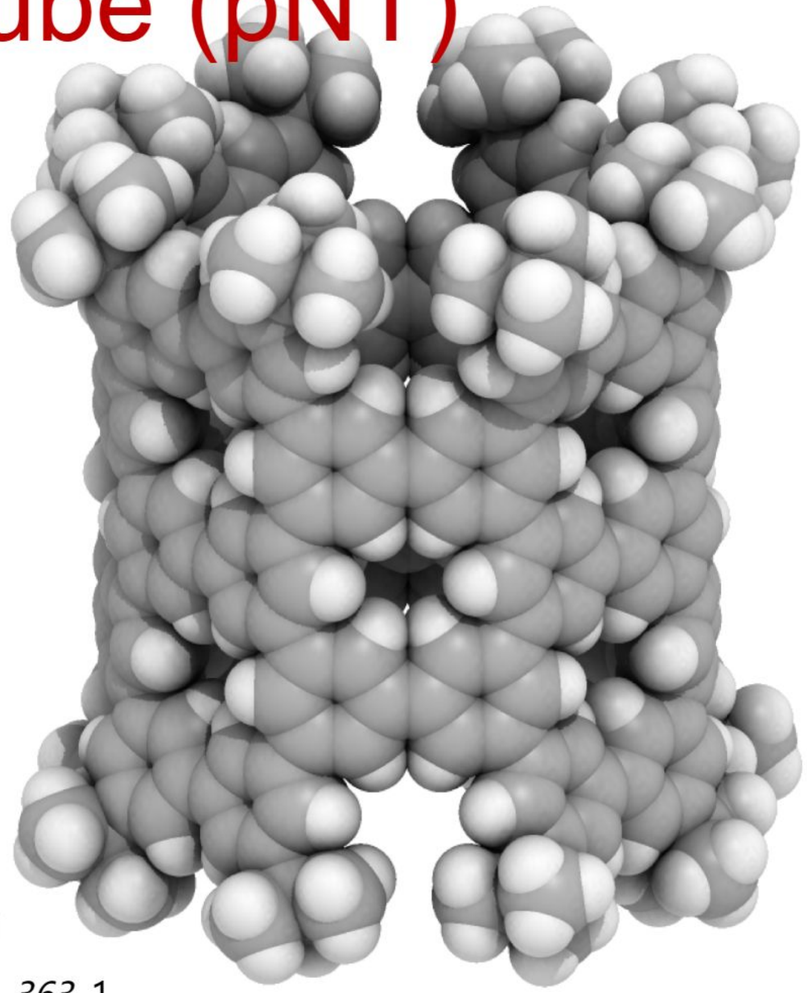
Phenine nanotube (pNT)

Precision is at another le
vel









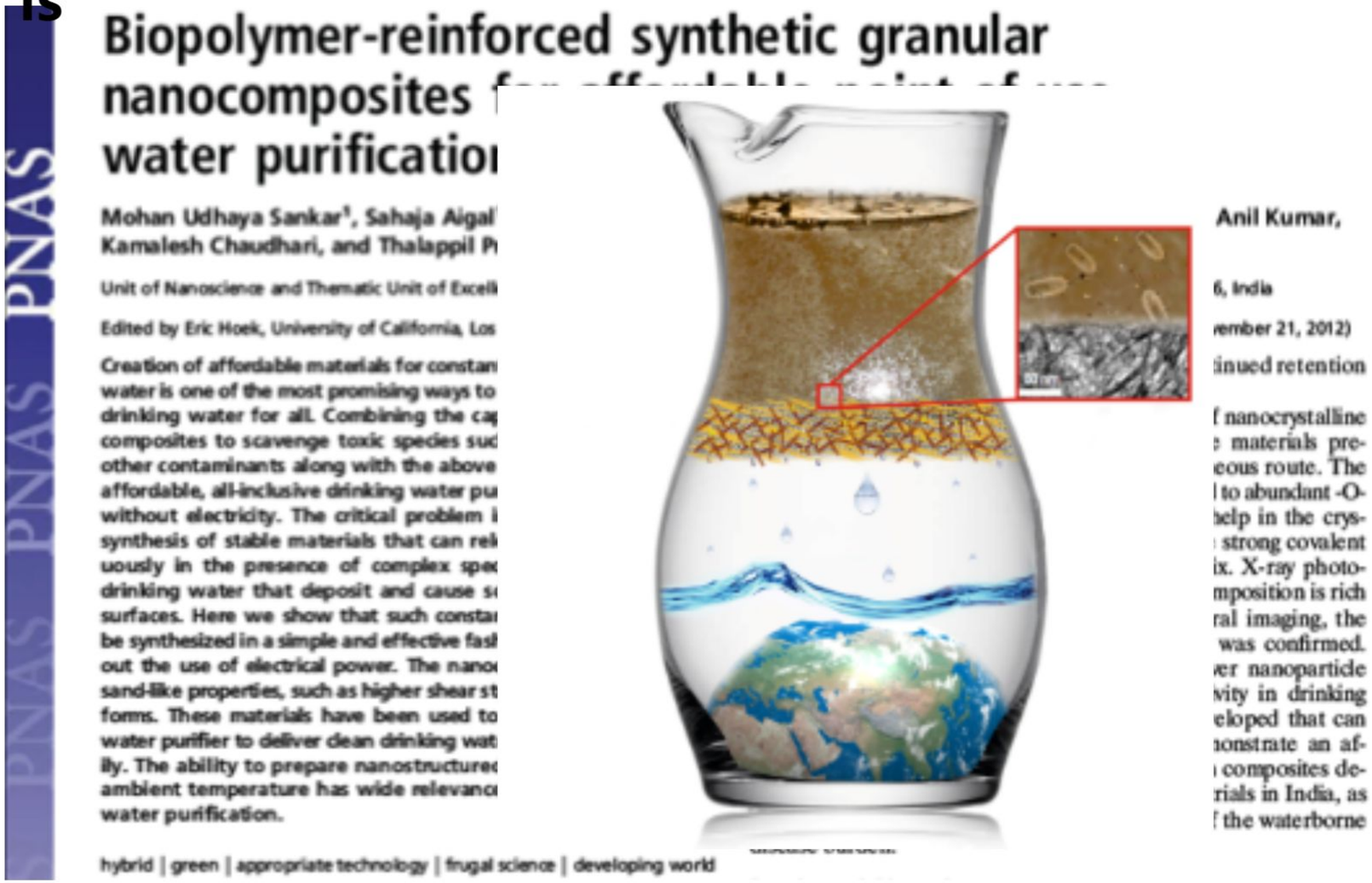
— Yamamoto coupling
— Suzuki-Miyaura coupling
— Bäurle/Yamago/Isobe coupli
ng

H. Isobe *et al. Science* **2019**, *363*, 1
51

Clean water for all

ACS Sustainable Chemistry & Engineering Editorial, December 2016

Water positive materials



PNAS

Biopolymer-reinforced synthetic granular nanocomposites for affordable point-of-use water purification

Mohan Udhaya Sankar[1], Sahaja Aigal
Kamalesh Chaudhari, and Thalappil P
Anil Kumar,

Unit of Nanoscience and Thematic Unit of Excell
6, India

Edited by Eric Hoek, University of California, Los
vember 21, 2012)

Creation of affordable materials for constan
water is one of the most promising ways to
drinking water for all. Combining the ca
composites to scavenge toxic species suc
other contaminants along with the above
affordable, all-inclusive drinking water pu
without electricity. The critical problem i
synthesis of stable materials that can rel
uously in the presence of complex spe
drinking water that deposit and cause s
surfaces. Here we show that such consta
be synthesized in a simple and effective fas
out the use of electrical power. The nano
sand-like properties, such as higher shear st
forms. These materials have been used to
water purifier to deliver clean drinking wat
ily. The ability to prepare nanostructure
ambient temperature has wide relevanc
water purification.

hybrid | green | appropriate technology | frugal science | developing world

inued retention

f nanocrystalline
materials pre-
eous route. The
to abundant -O-
help in the crys-
strong covalent
ix. X-ray photo-
mposition is rich
ral imaging, the
was confirmed.
er nanoparticle
vity in drinking
eloped that can
onstrate an af-
composites de-
rials in India, as
f the waterborne

M. Udhaya Sankar, et. al. *Proc. Natl. Acad. Sci.,* 110 (2013) 8459-8464.

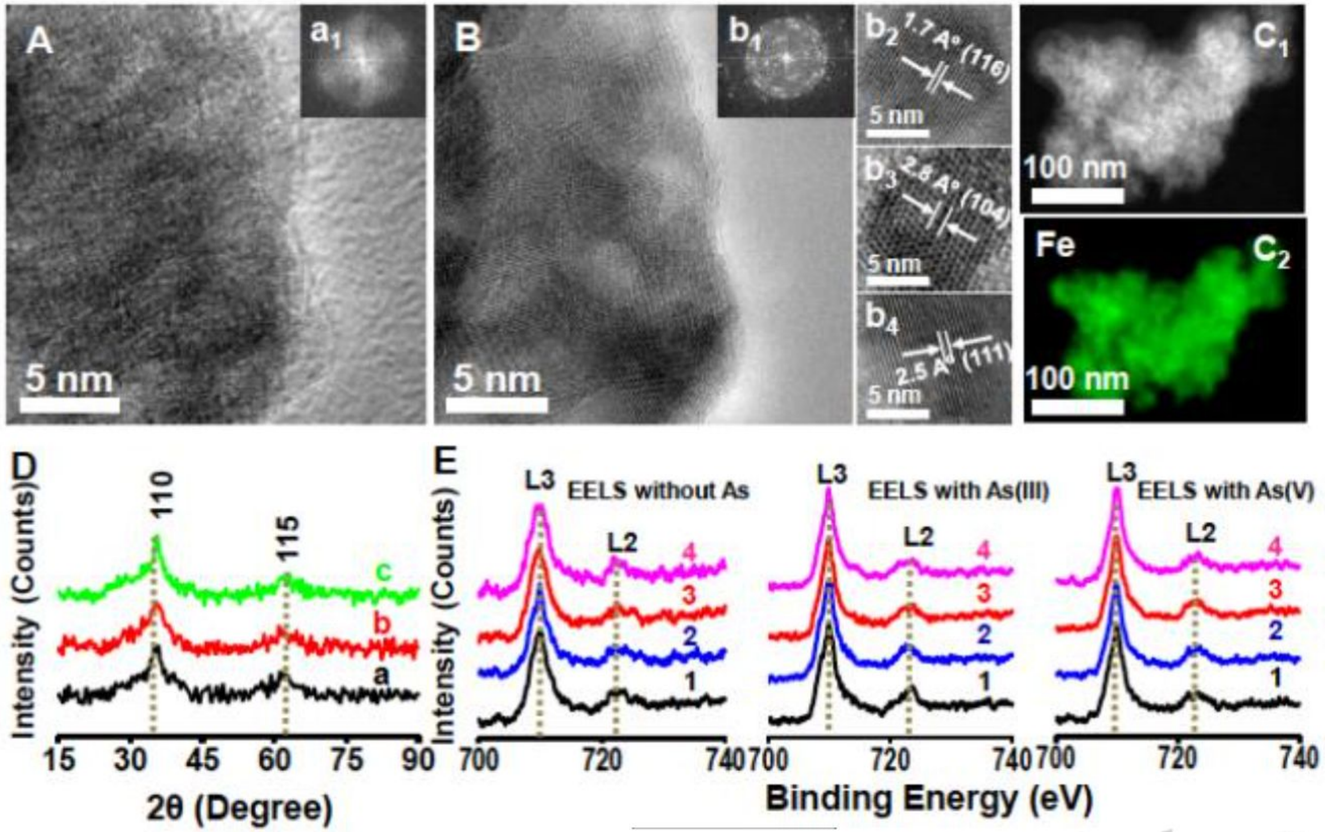
How to make?

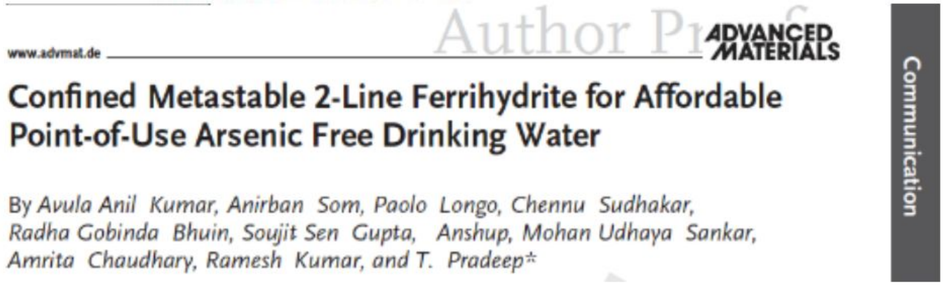
What is special?

Live/dead staining experiments

No nanotoxicity

Variety of materials




www.advmat.de

ADVANCED MATERIALS

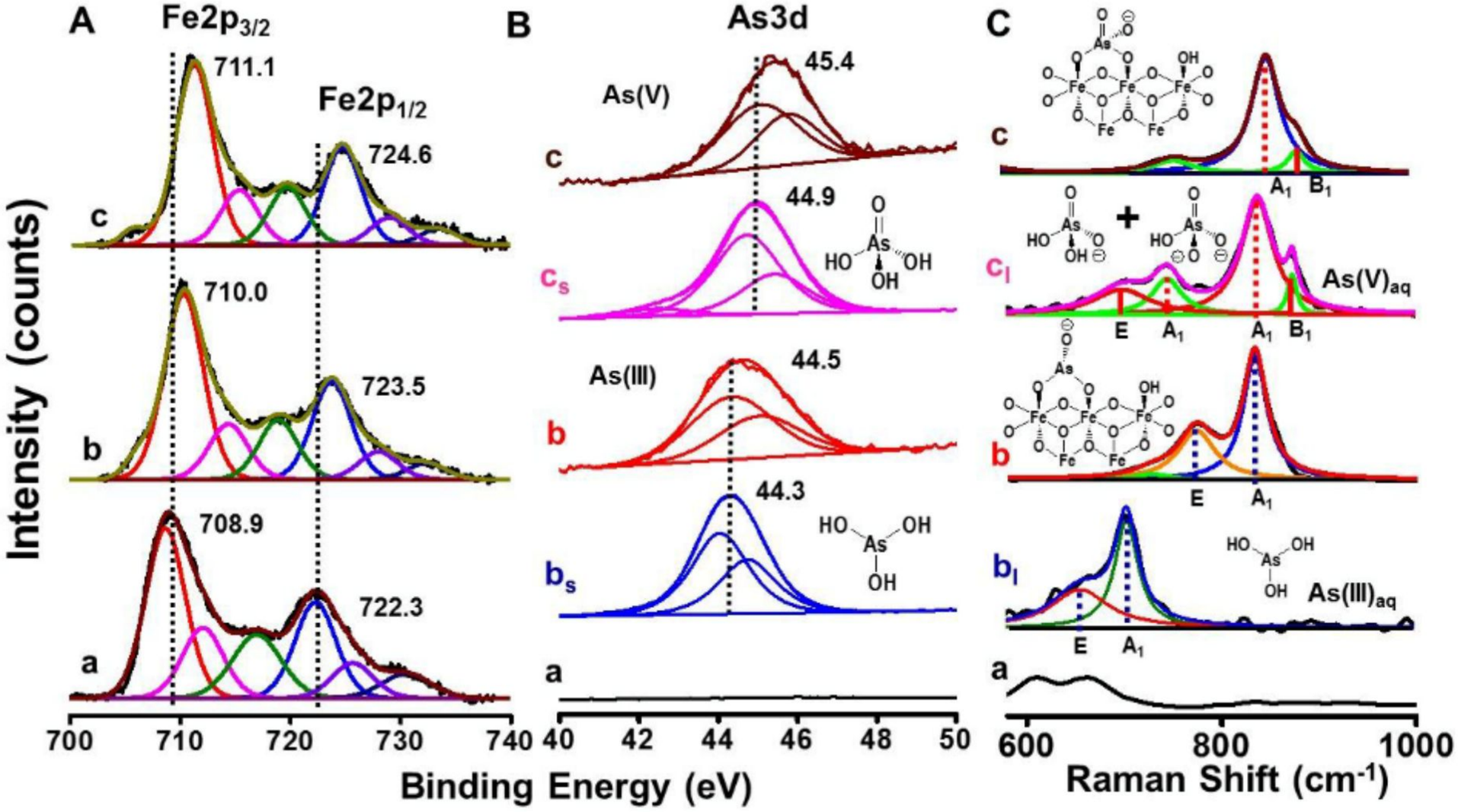
Communication

Confined Metastable 2-Line Ferrihydrite for Affordable Point-of-Use Arsenic Free Drinking Water

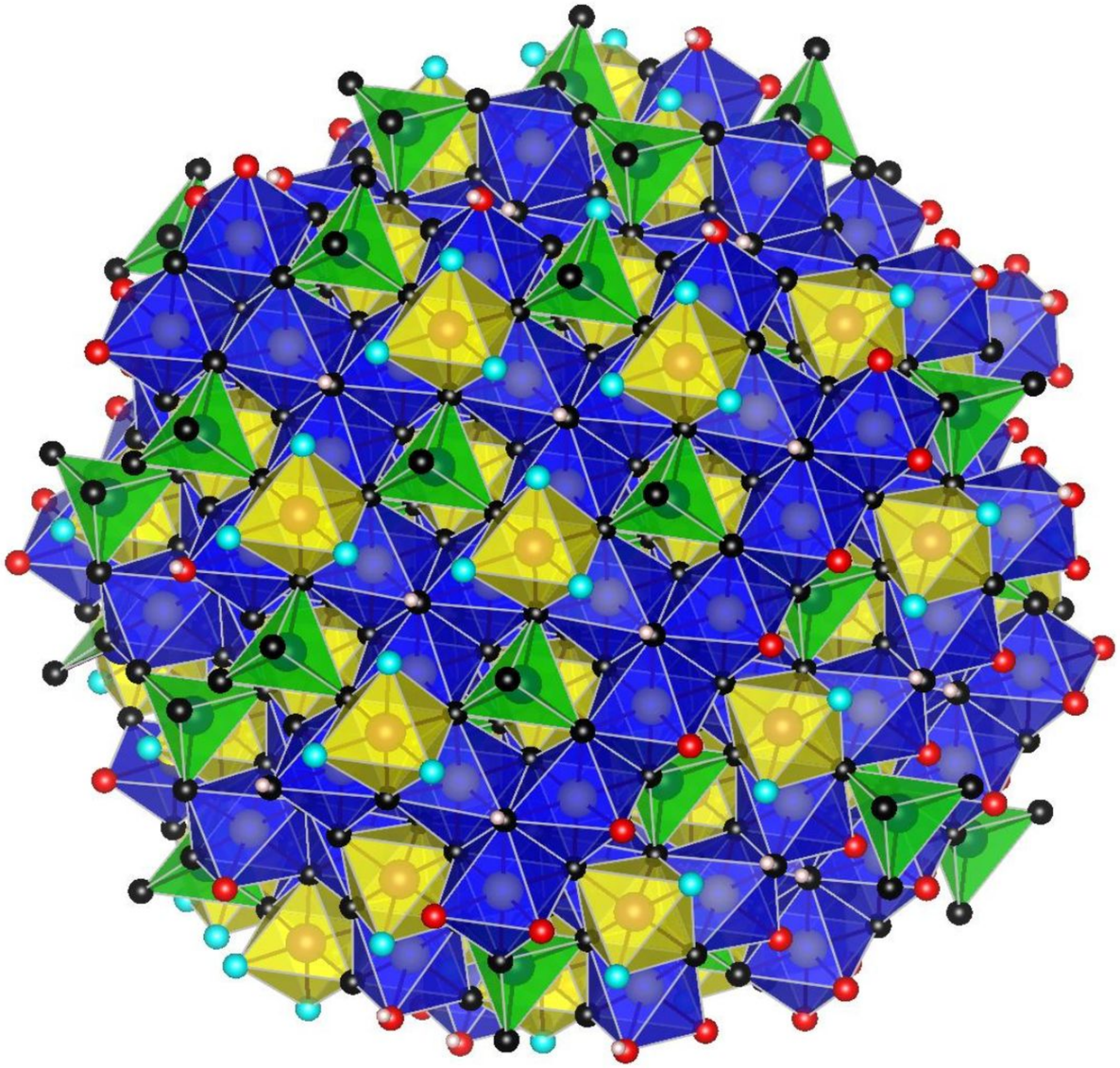
By Avula Anil Kumar, Anirban Som, Paolo Longo, Chennu Sudhakar, Radha Gobinda Bhuin, Soujit Sen Gupta, Anshup, Mohan Udhaya Sankar, Amrita Chaudhary, Ramesh Kumar, and T. Pradeep*

A. Anil Kumar, et. al. *Adv. Mater.*, 29 (2016) 16042

Mechanism – molecular too ls

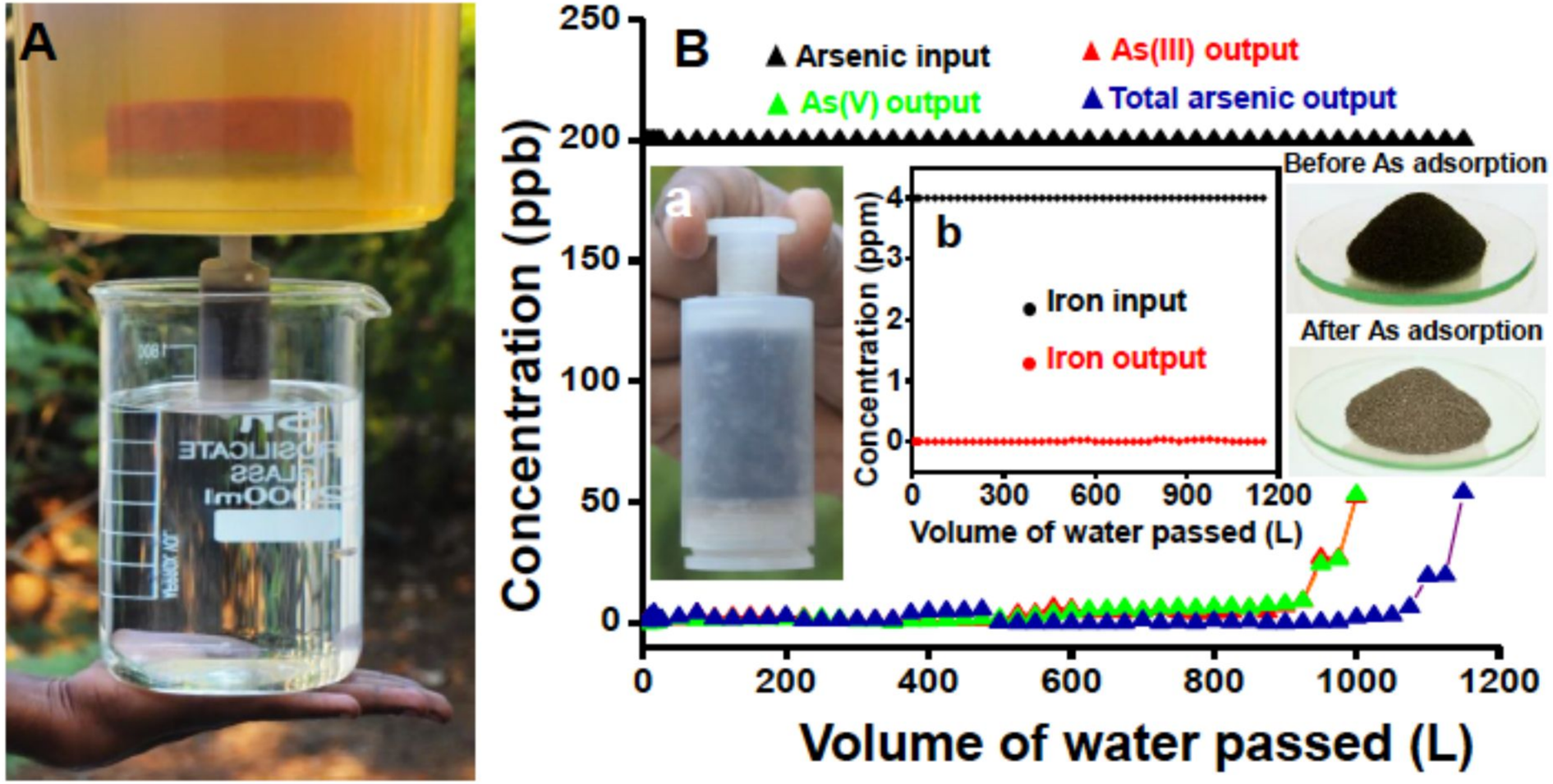


Modeling surfaces



Chennu Sudhakar, et al. *ACS Sustainable Chemistry & Engineering*, 6 (2018) 9990-10000.

Lab studies



A. Anil Kumar, et. al. *Adv. Mater.*, 29 (2016) 16042
60.

Initial pilot studies

Larger pilot studies

Implementation - From 25 KLD to 1 MLD

Large water supply schemes

Capacity: above 1 MLD

5 schemes in use across India

Retrofitted Water Purification Plant

Capacity: 0.1-1 MLD

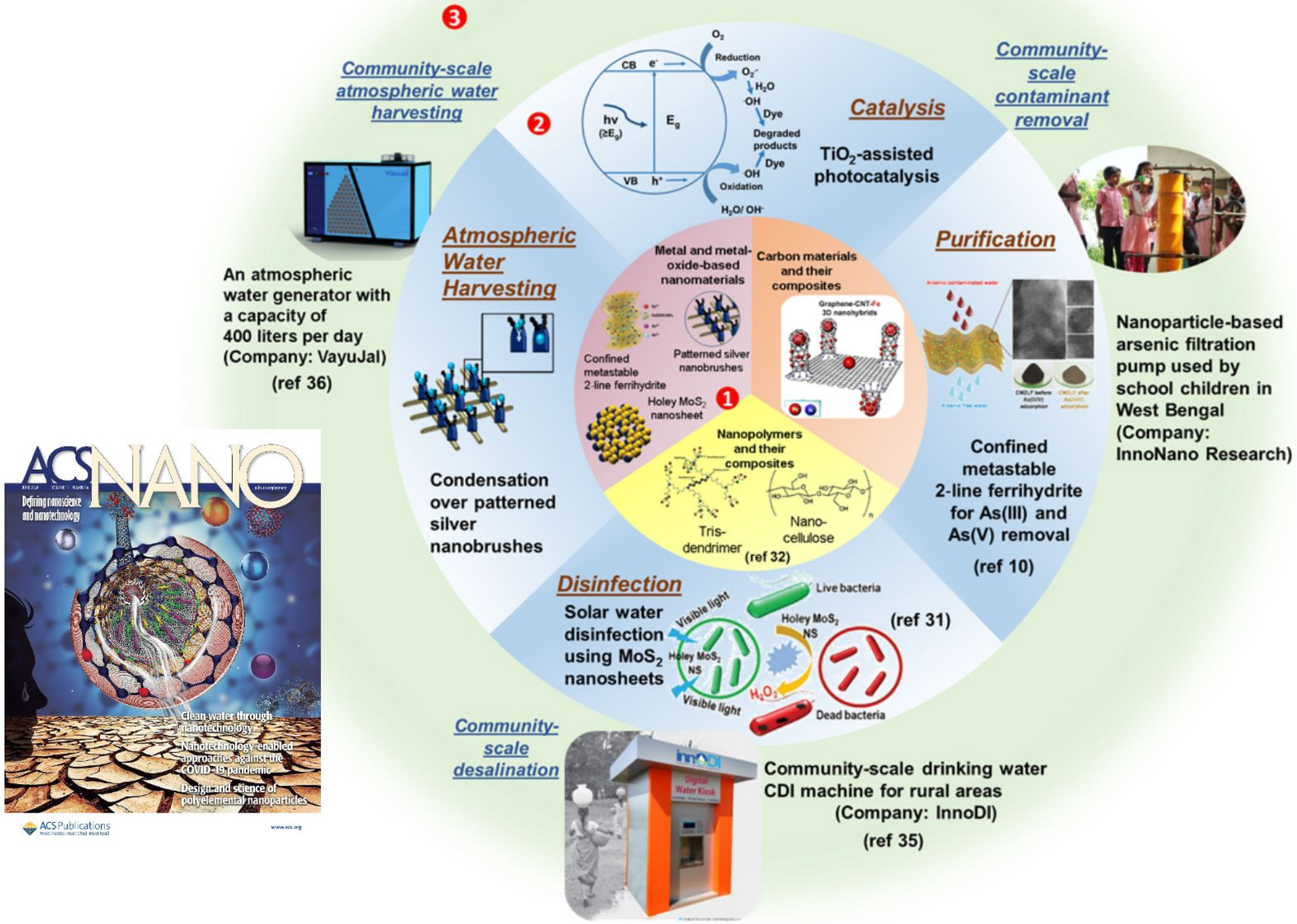
Over 180 units in use across India

Now they are across the countr y

Smart water purifiers and big data

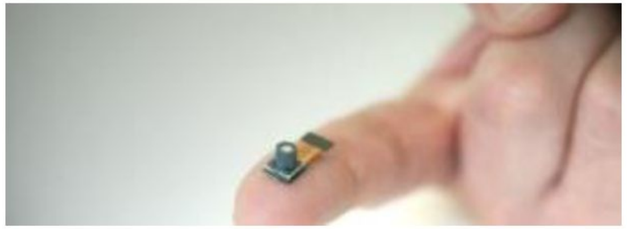
Ankit Nagar and T. Pradeep 14(2020). *ACS Nano*, 6420-6435

Evolution of materials to products



Ankit Nagar and T. Pradeep, *ACS Nano* 14 (2020) 6420-6435.

Sensors and new opportunities



Water quality measurement – In the pipe line

Cluster-based metal ion sensing

Decrease in the absorption of Au15 as a biofilm is dipped into the cluster soluti on. Inset: Free standing quantum cluster loaded film in visible light and UV light

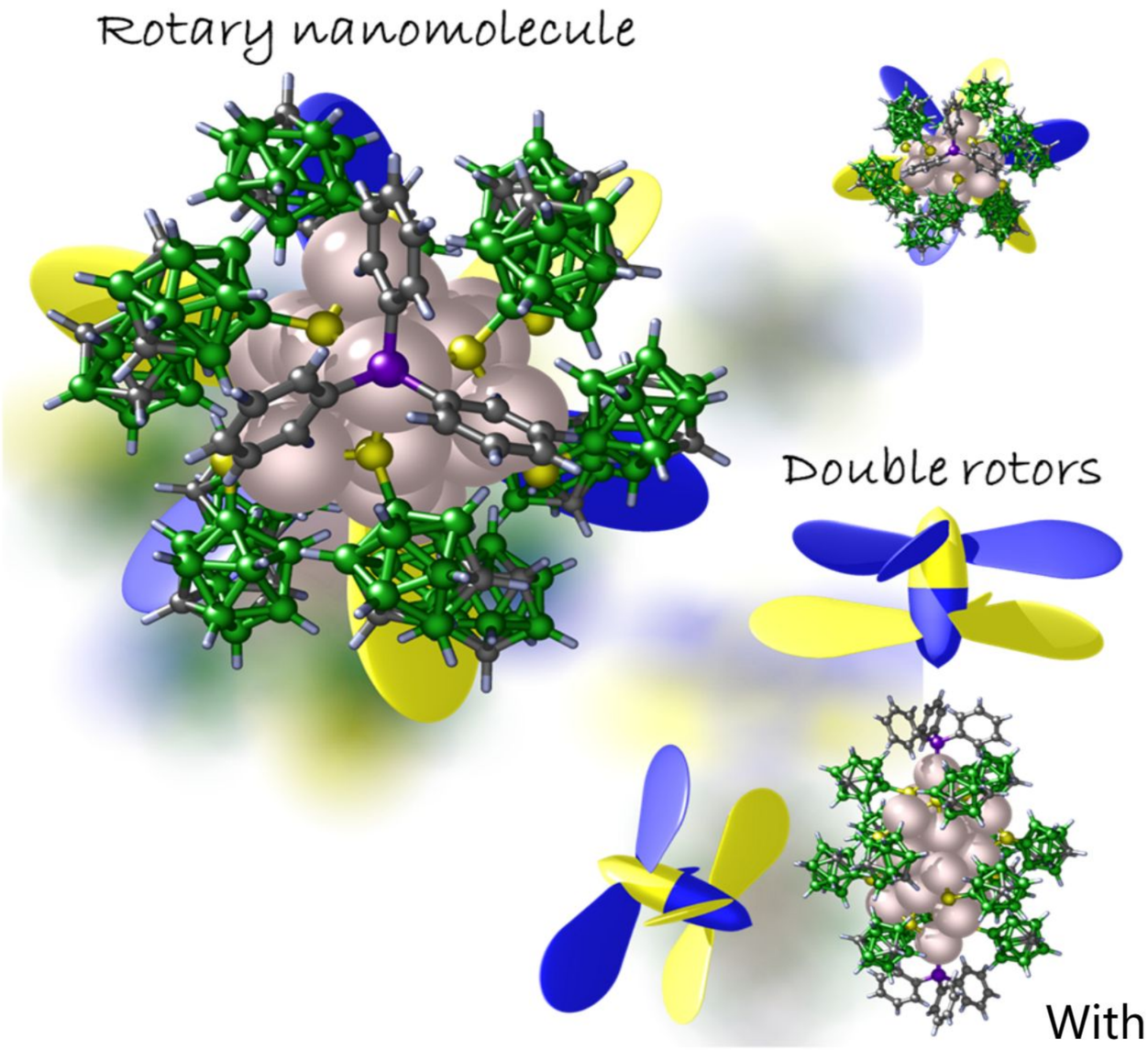
Anu George et al. *ACS Applied Materials & Interfaces*, 2012

Approaching detection limits of tens of Hg2+

Atanu Ghosh et al. Anal. Chem. 201

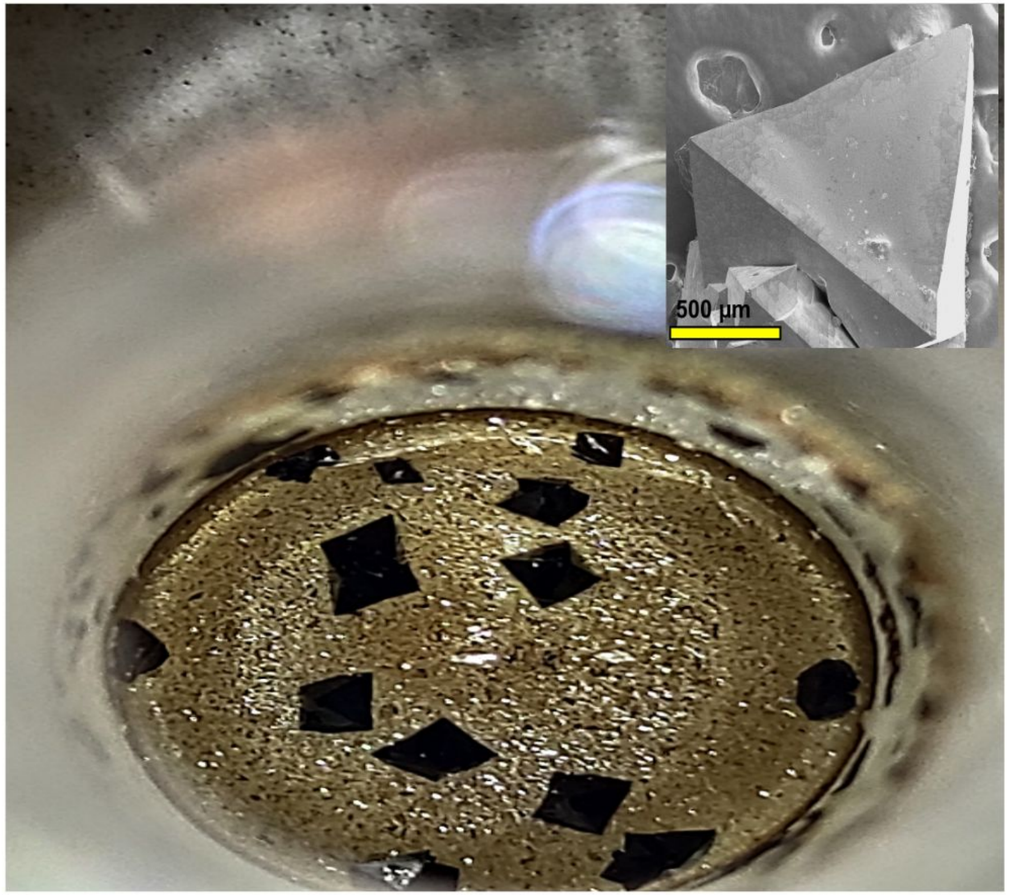
Mercury quenching experiment using nanofiber

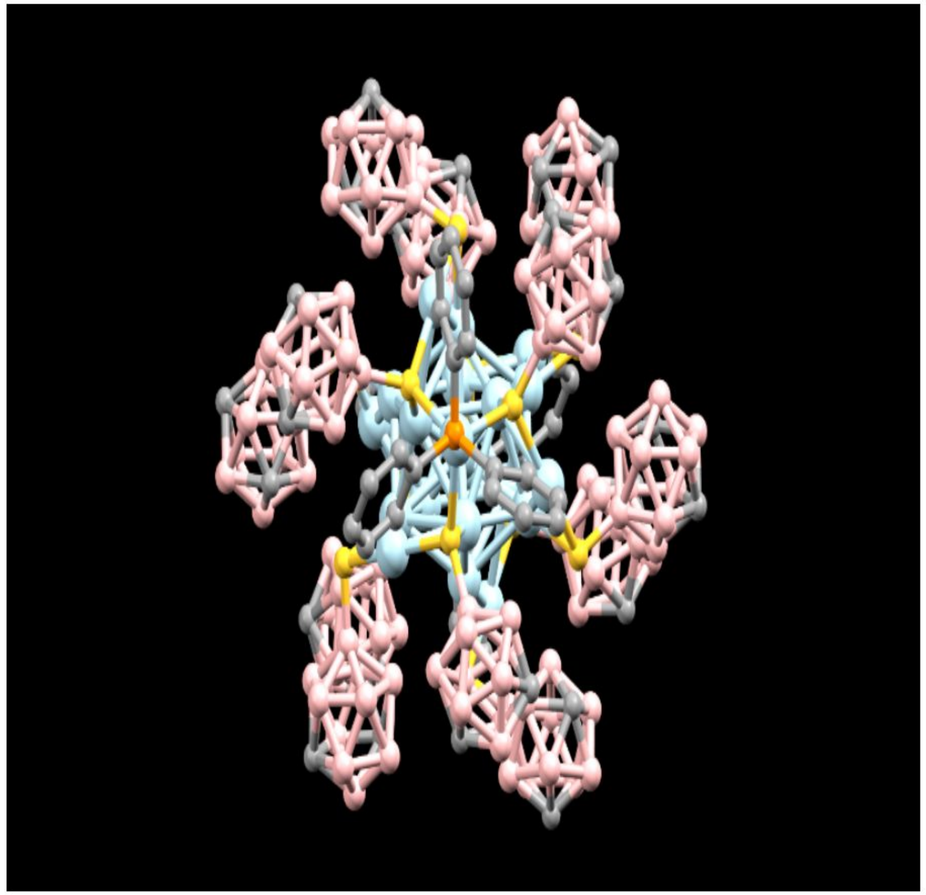
Carborane-thiol protected silver nanomolecule



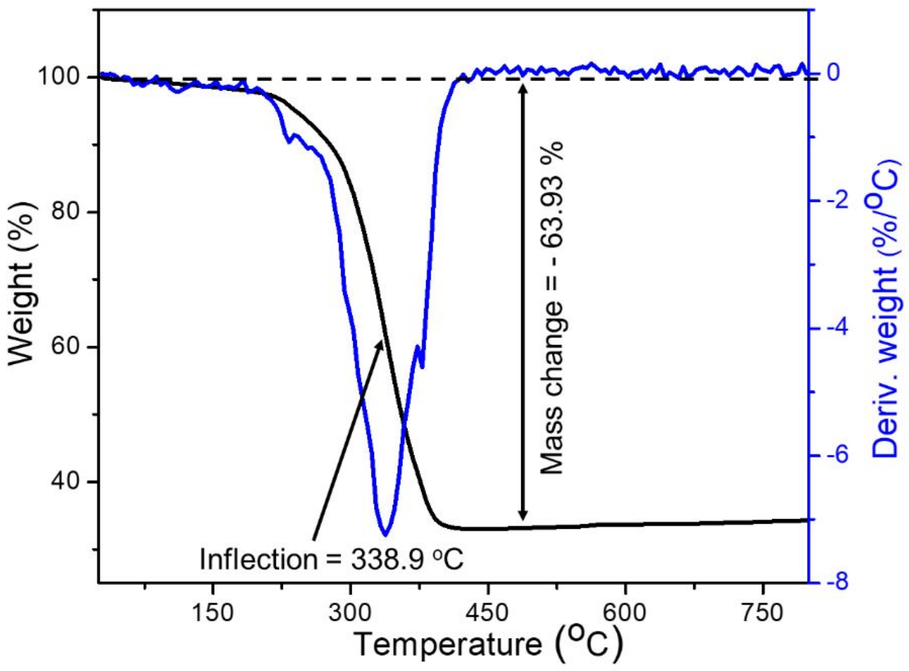
With Tomas Base

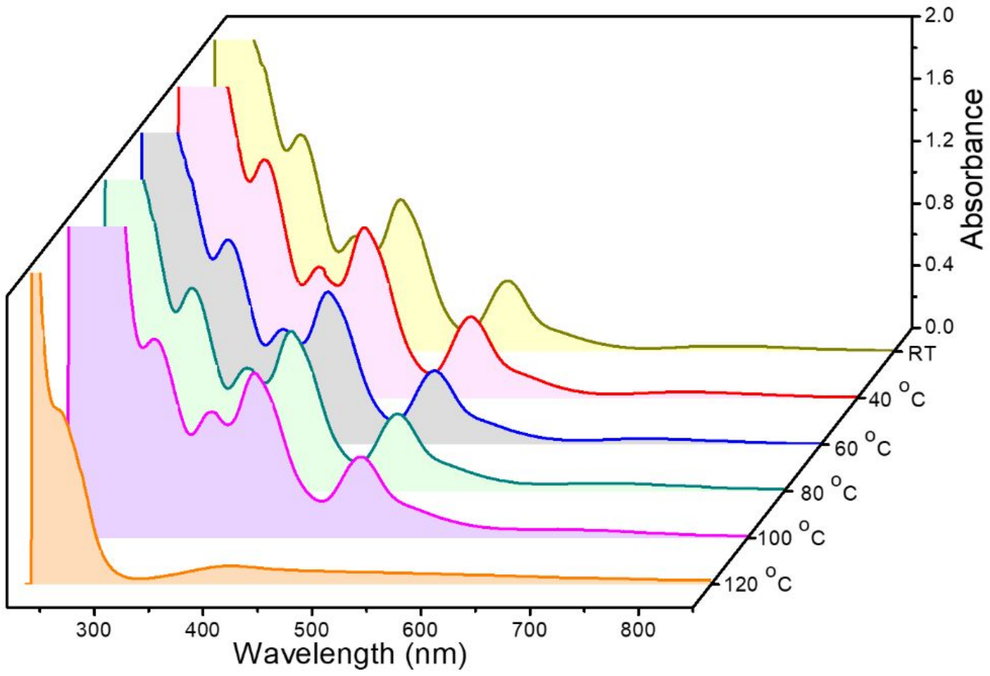
Jana *et. al*, Inorganic Chemistry (2022)


500 µm



Thermal stability

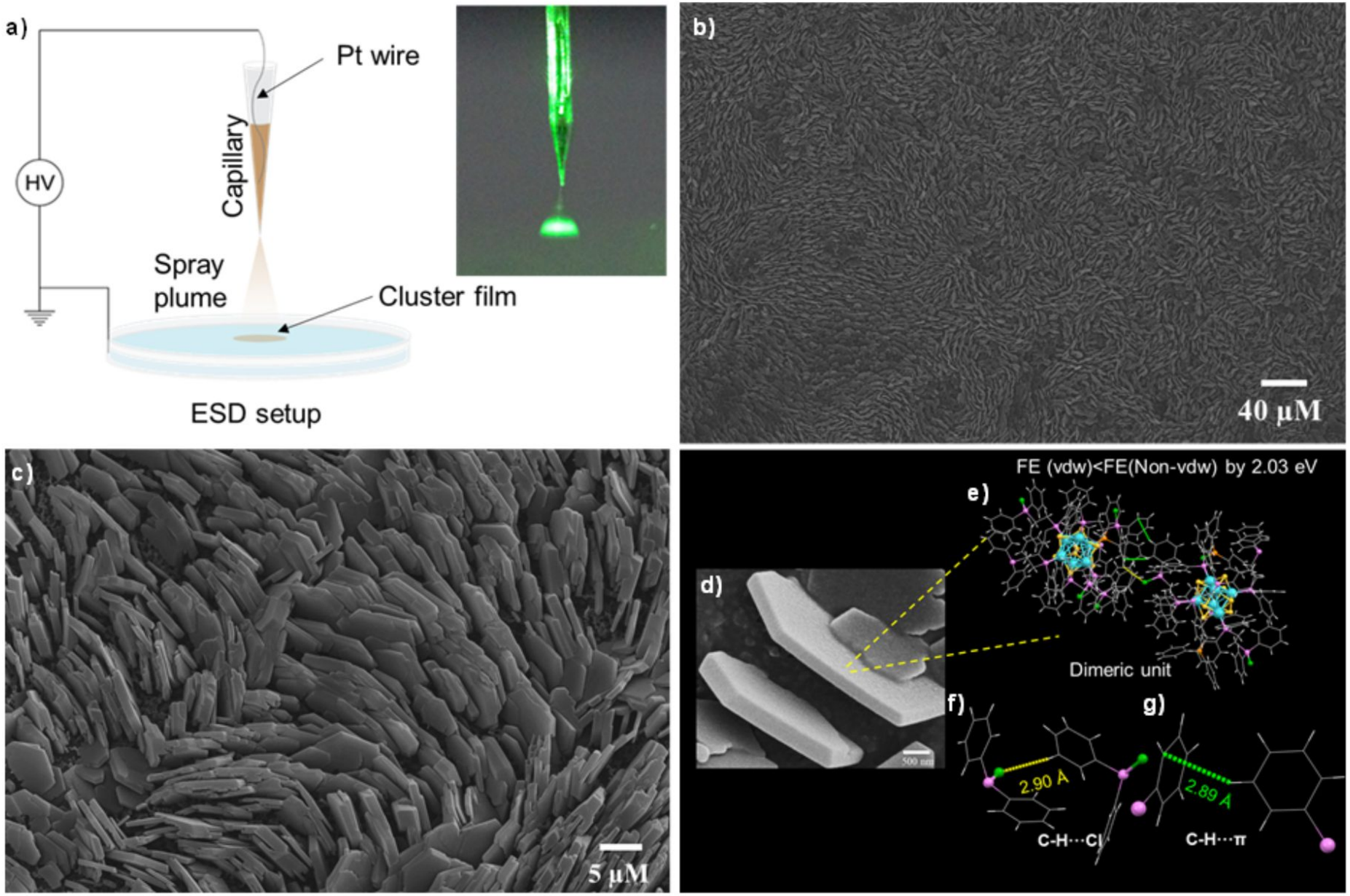




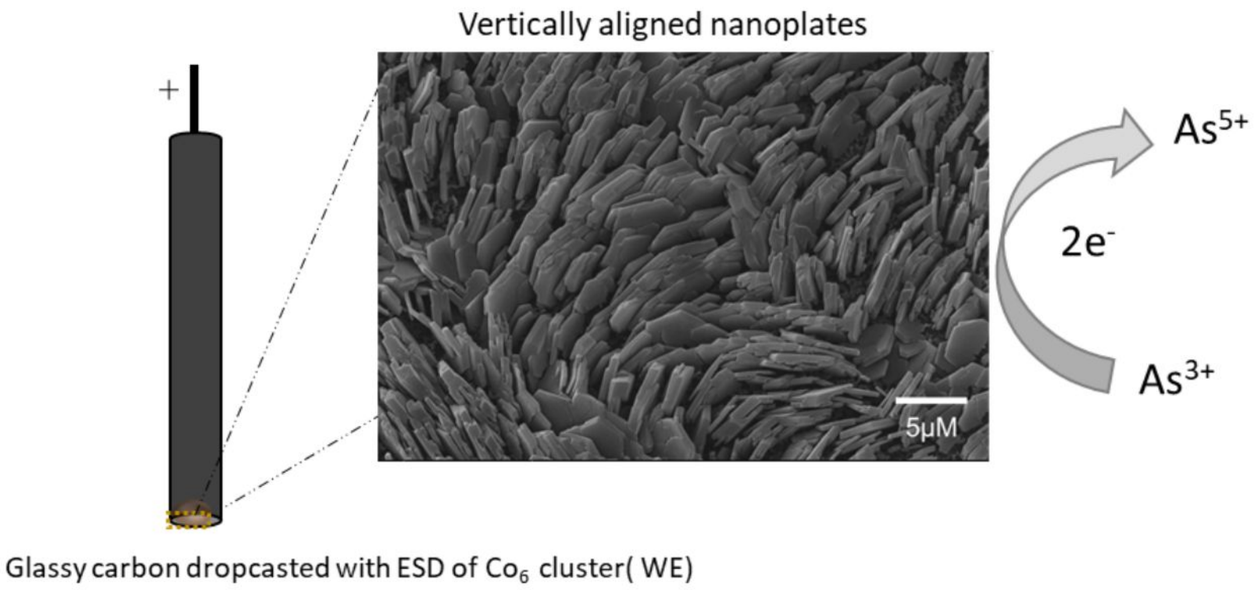
New electrodes - Aligned nanoplates of Co6S 8

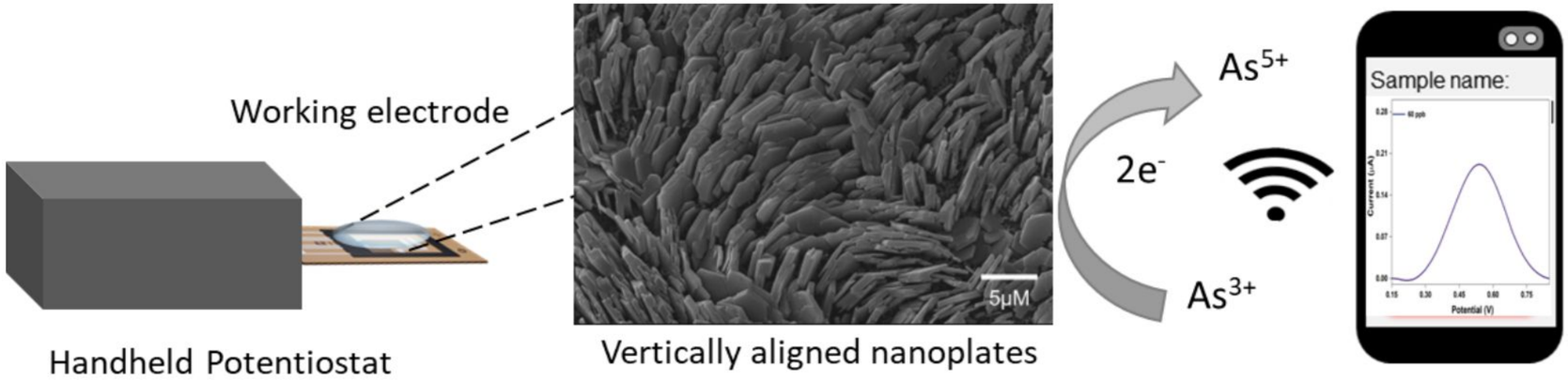
1,2-bis(diphenylphosphino)ethane (DPPE)

Electrospray deposition



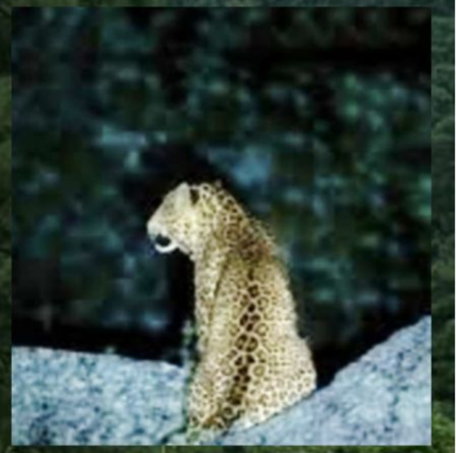
Sensing



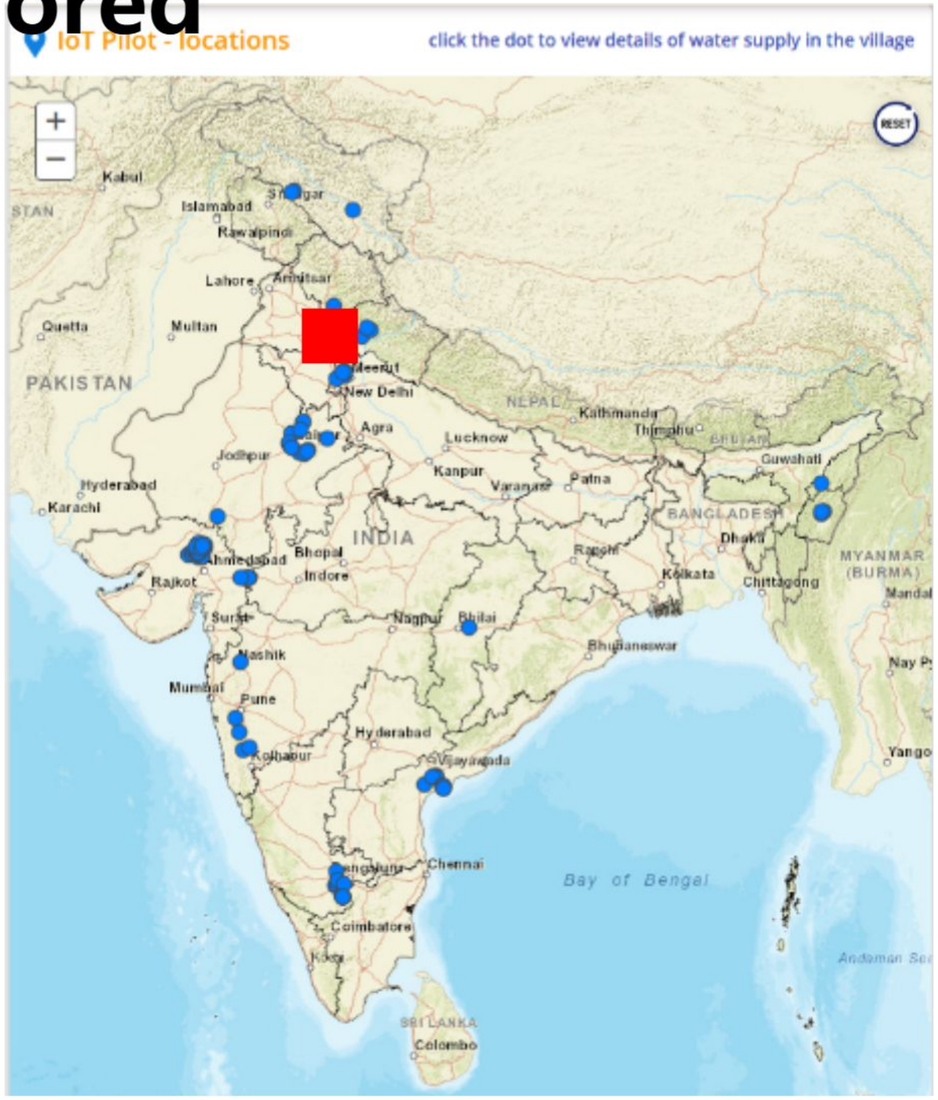


Anagha Jose et al. *ACS Materials Lett.,* 5 (2023) 893–899.


ब्रेक फास्ट

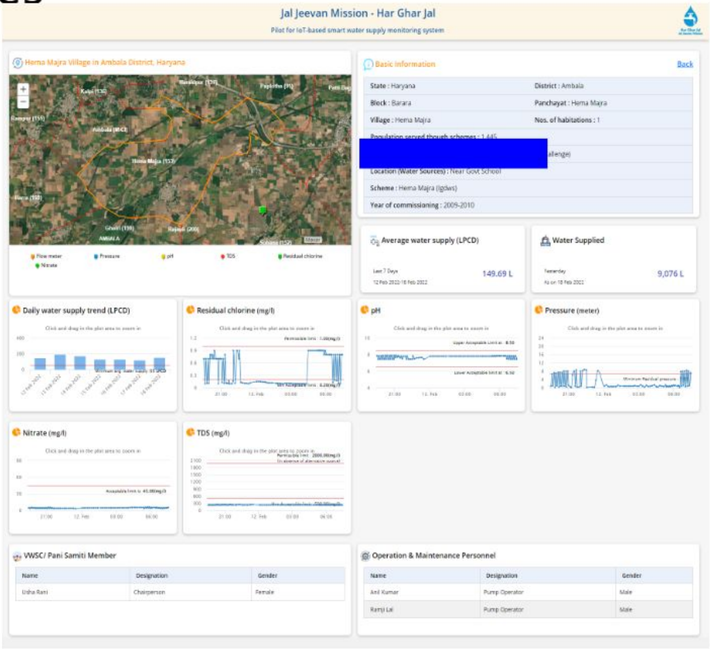


India’s water is being monitored



IITM/IISc

Installations made by four companies

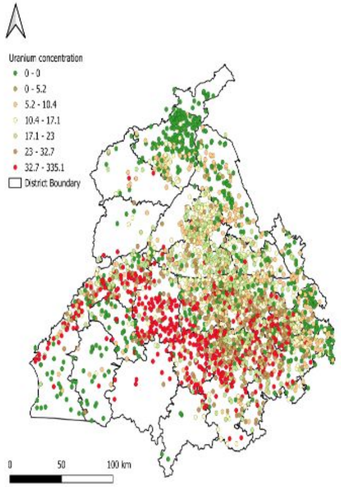


Full video at https://www.youtube.com/watch?v=fiJyptbXBtM

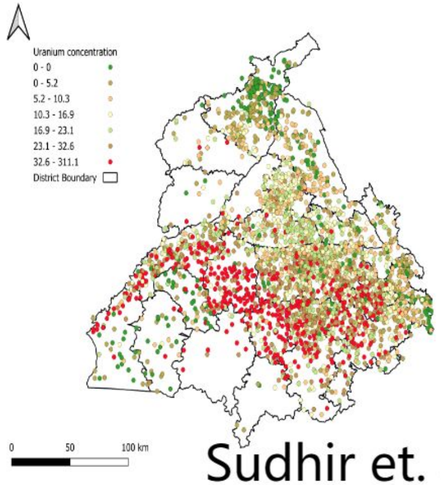
Clean water for all

https://www.peopleswaterdata.org

Arsenic poisoning across the world



[1]



Sudhir et. al. Unpublished

scale has been added like figure 1

E. Shaji, M. Santosh, K. V. Sarath, Pranav Prakash, V. Deepch and B. V. Divya, Geoscience Frontiers, 12 (2021) 101079.

Can Water Microdroplets Make Soil?

A path to sustainable nanotechnology

Science

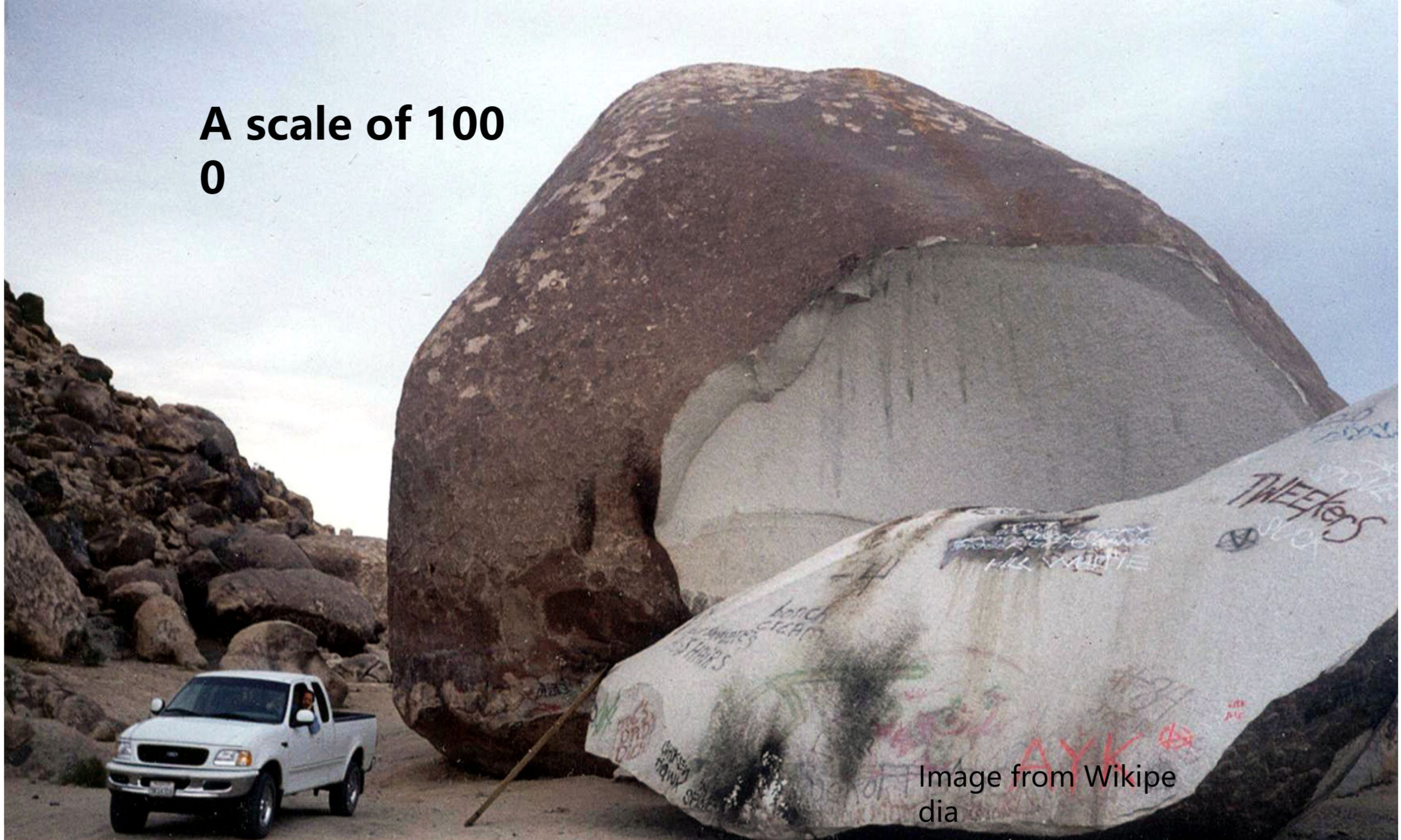


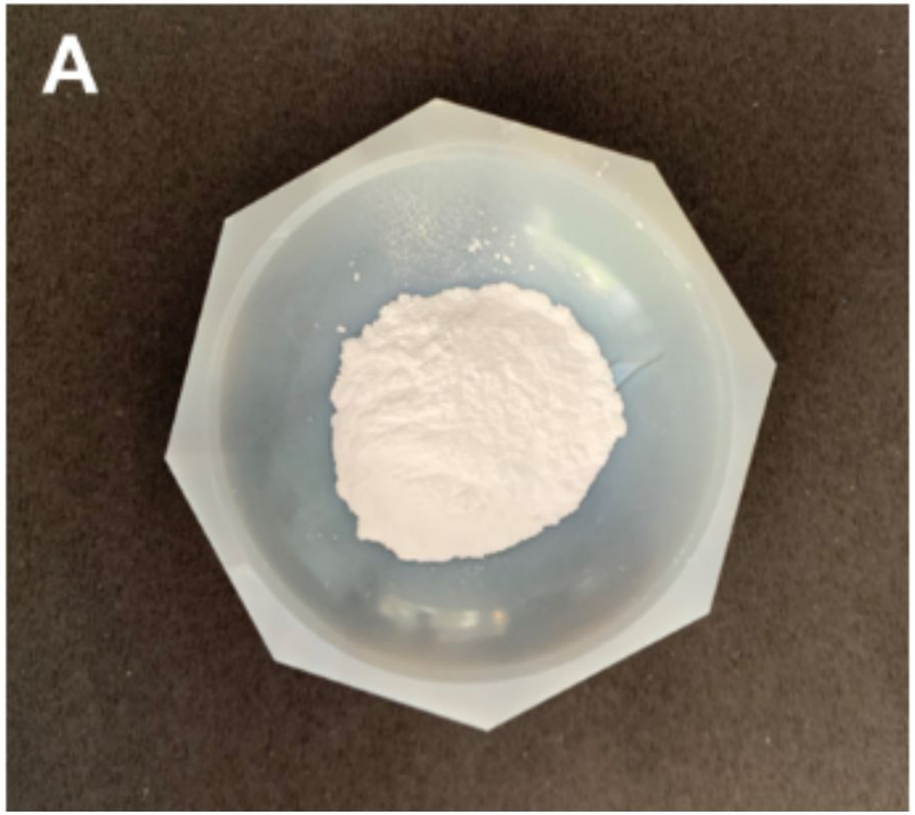
Image from Wikipe
dia

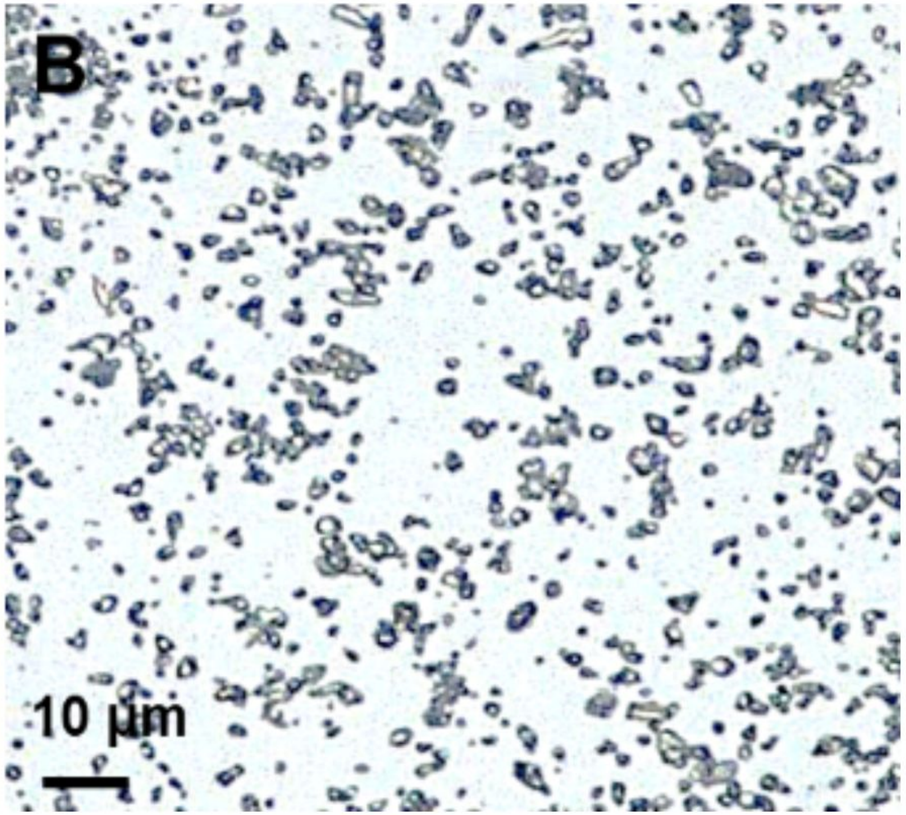
Functional Nanomaterials


Thanks to ChatGP
T

Sand, the Ubiquitous Material

Images from Wikipe
dia

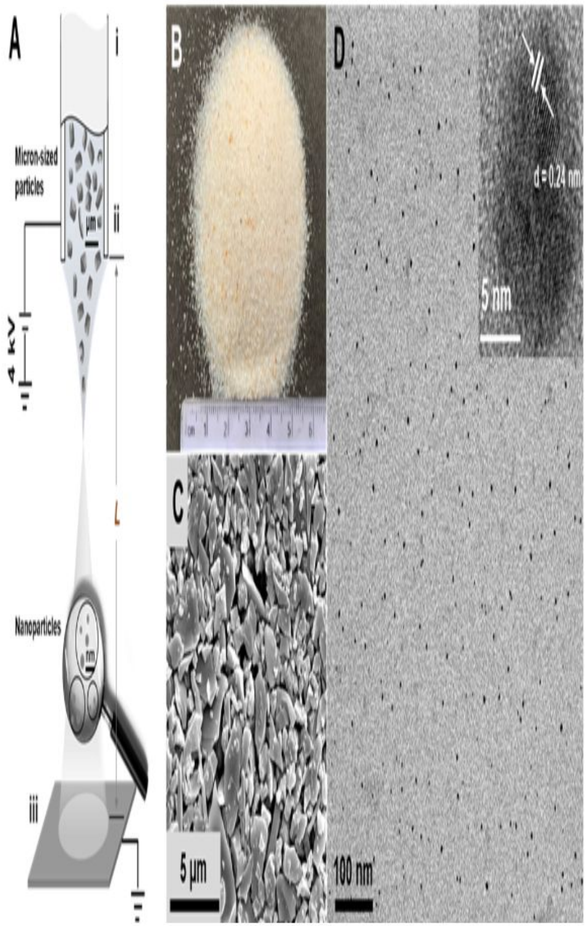


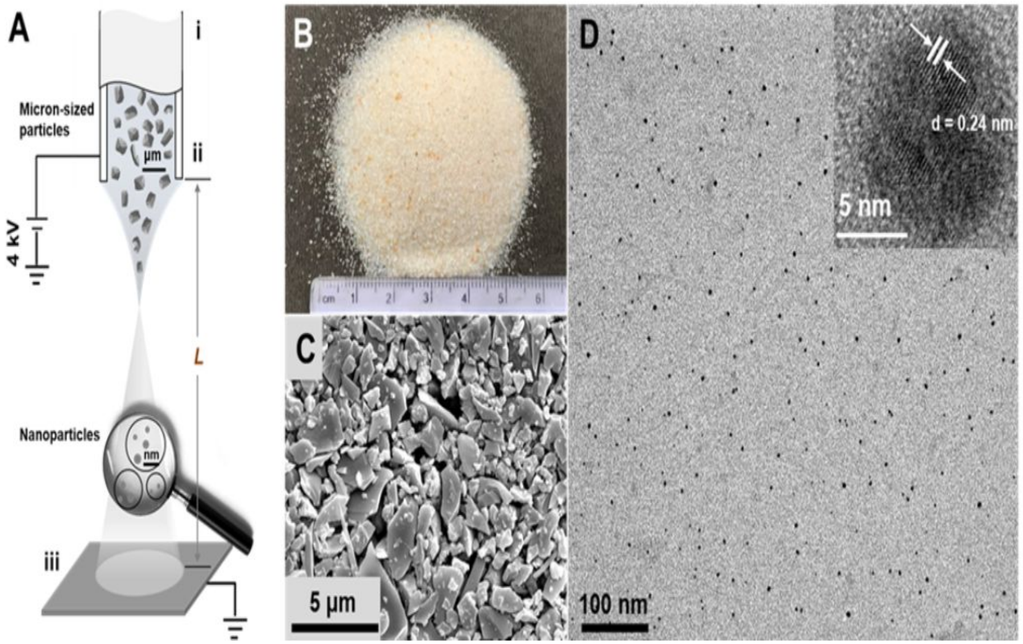


Ground silica

Optical image of silica

Weathering of Minerals in Microdroplets

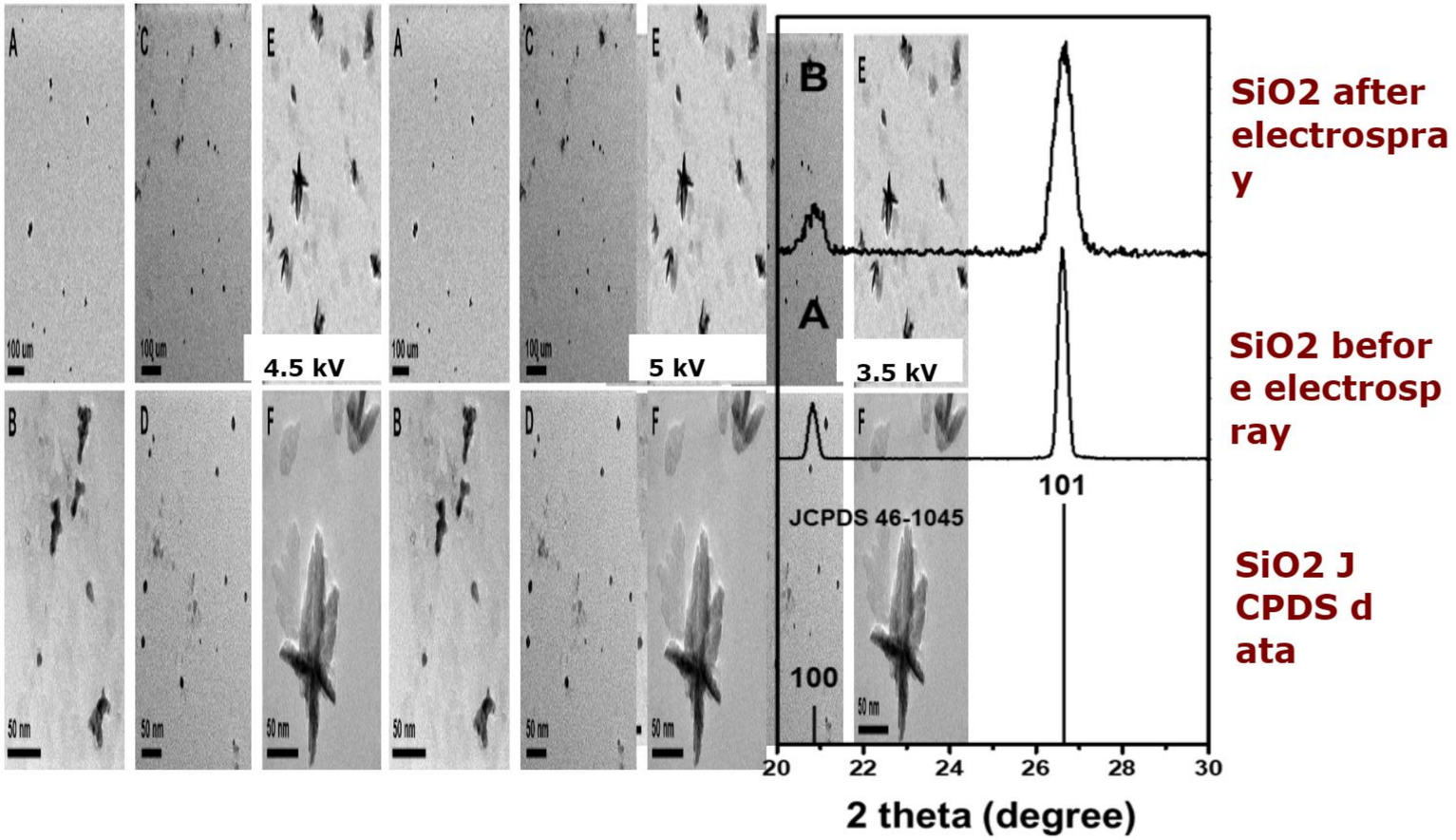




Spoorthi, et. al., *Science*, 2024

Ruby, Fused Alumin
a

Fragmentation of Silica – Varying Conditions



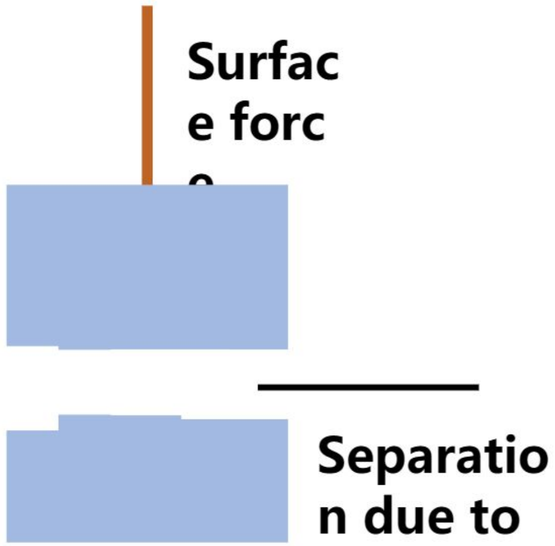
SiO2 after electrospray

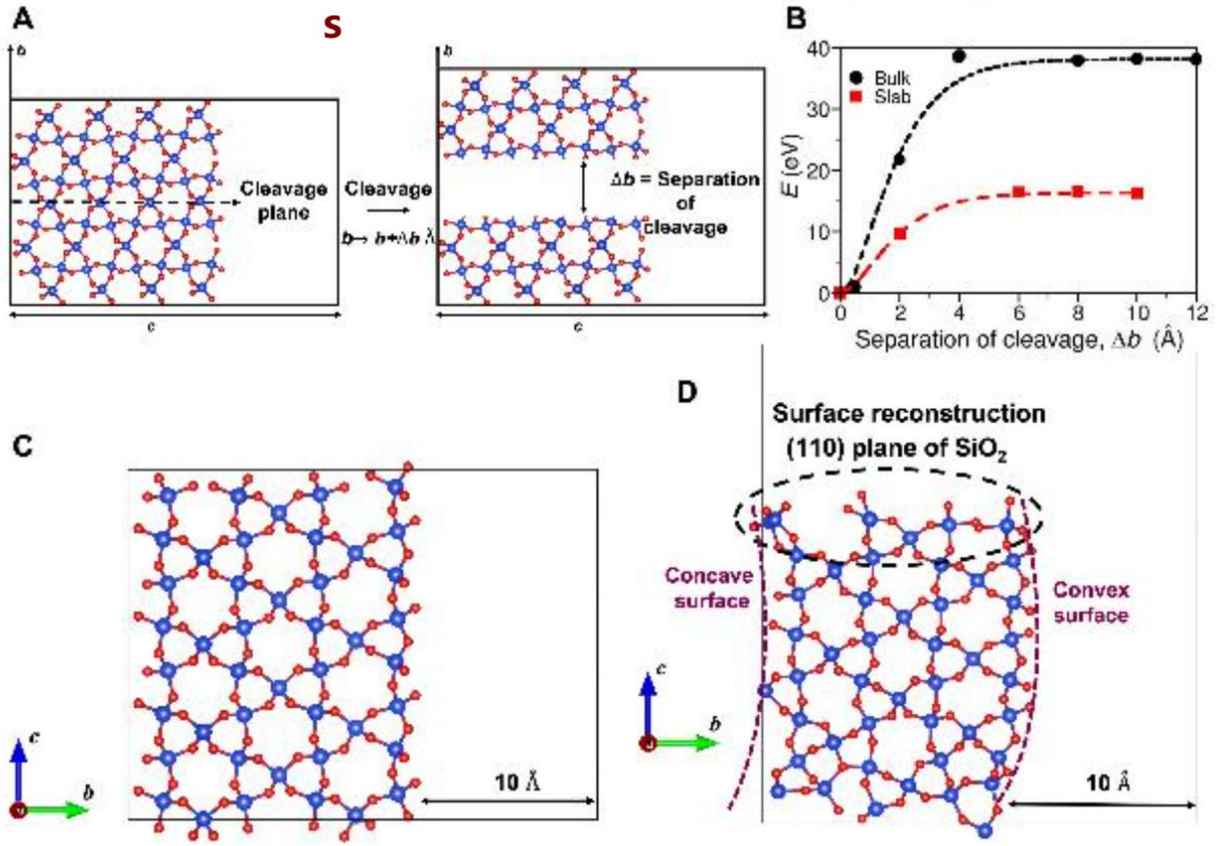
SiO2 before electrospray

SiO2 JCPDS data

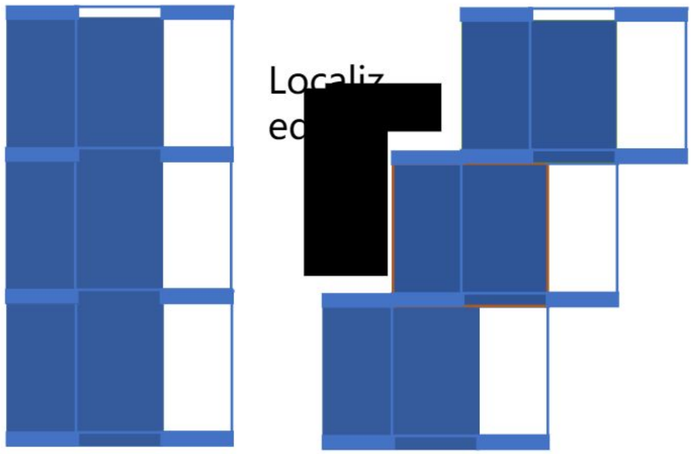
Mechanism: Cleavage

The process of cleavage and surface reconstruction visualized with first-principles simulation s





Mechanism: Slip



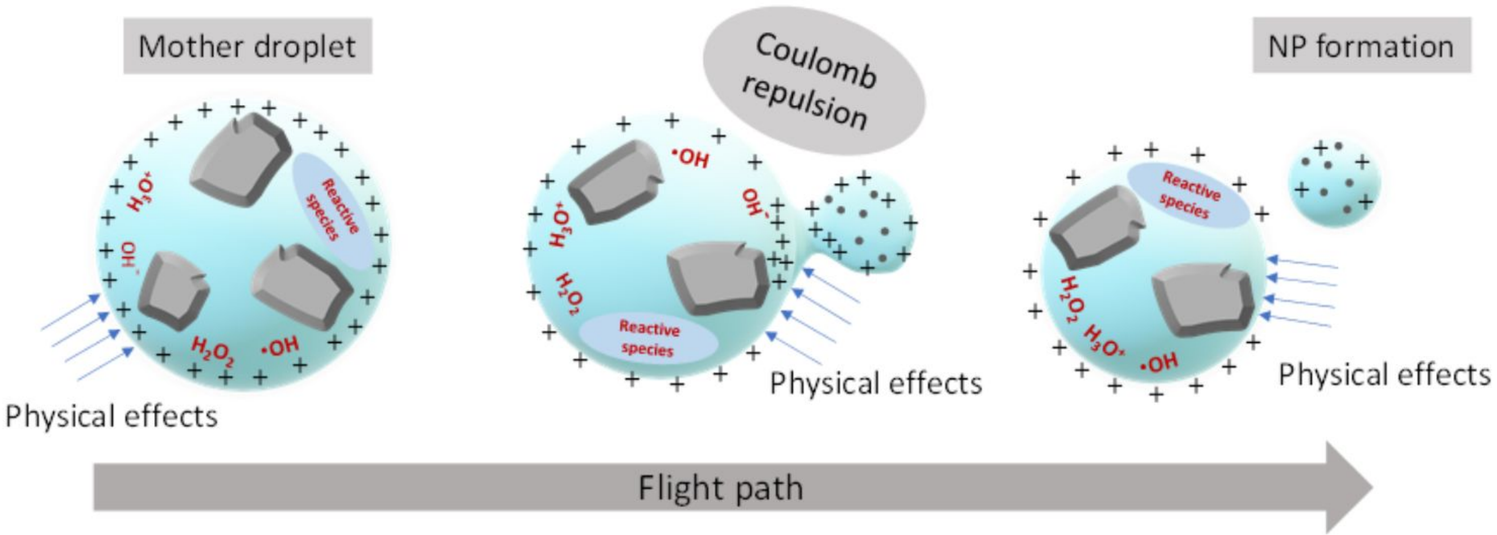
This instability leads to the formation of a sta cking fault on the (010) plane, achieved with slip localized at (010) plane

Stacking fault

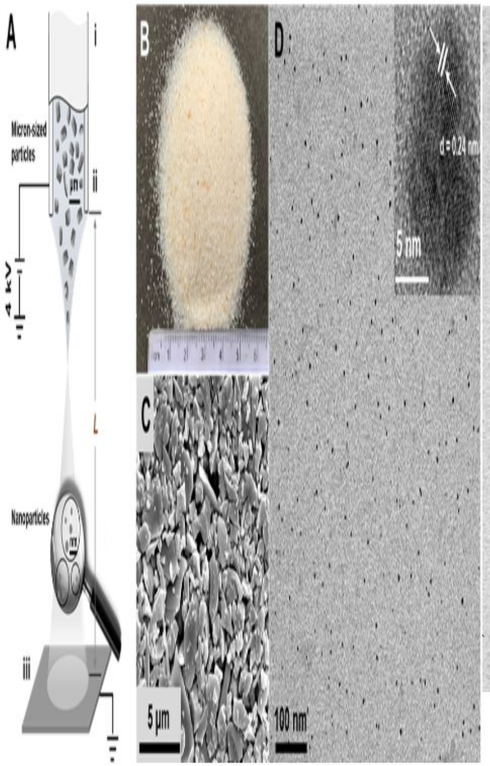
$\vec{b} \rightarrow \vec{b_0} + (x, 0, z)$,

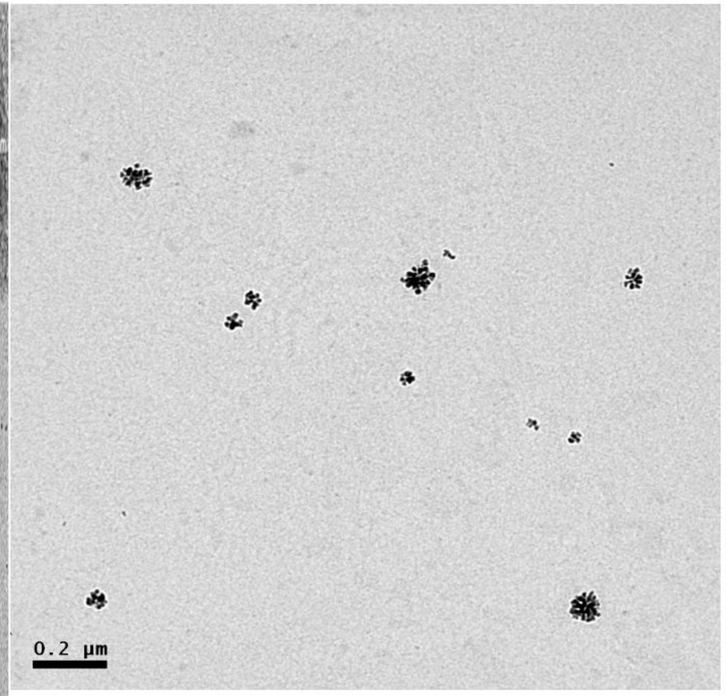
(□□, □□ ∈ [0,1]) - fractional coordinates

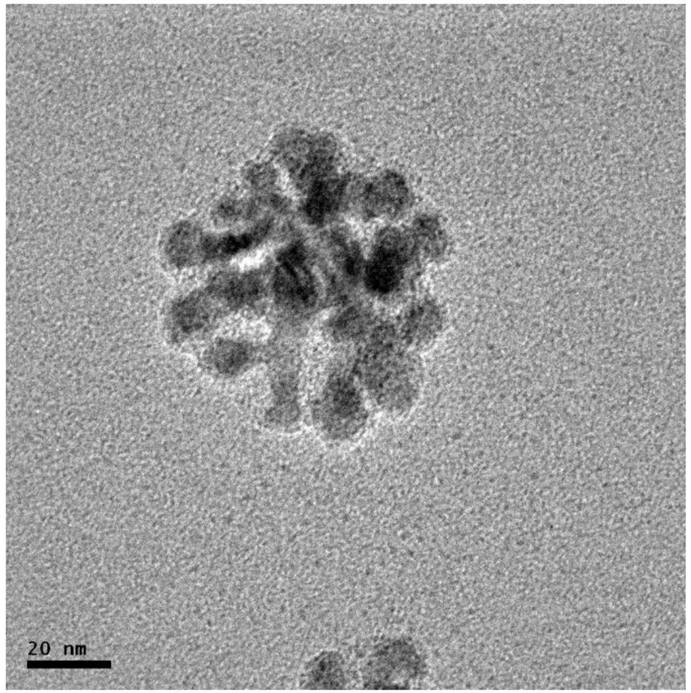
Mechanism of nanoparticle formation



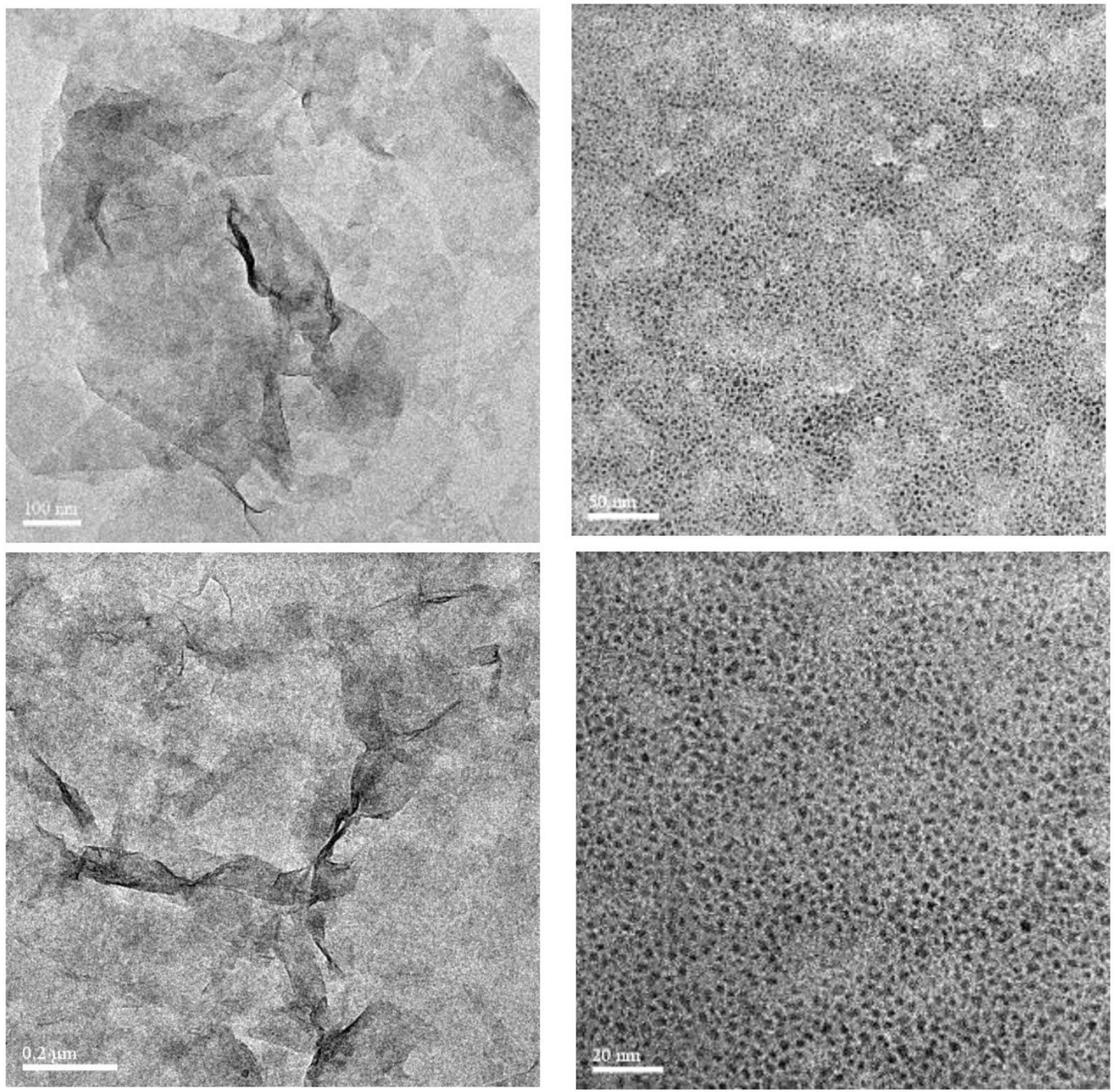
How do they form?







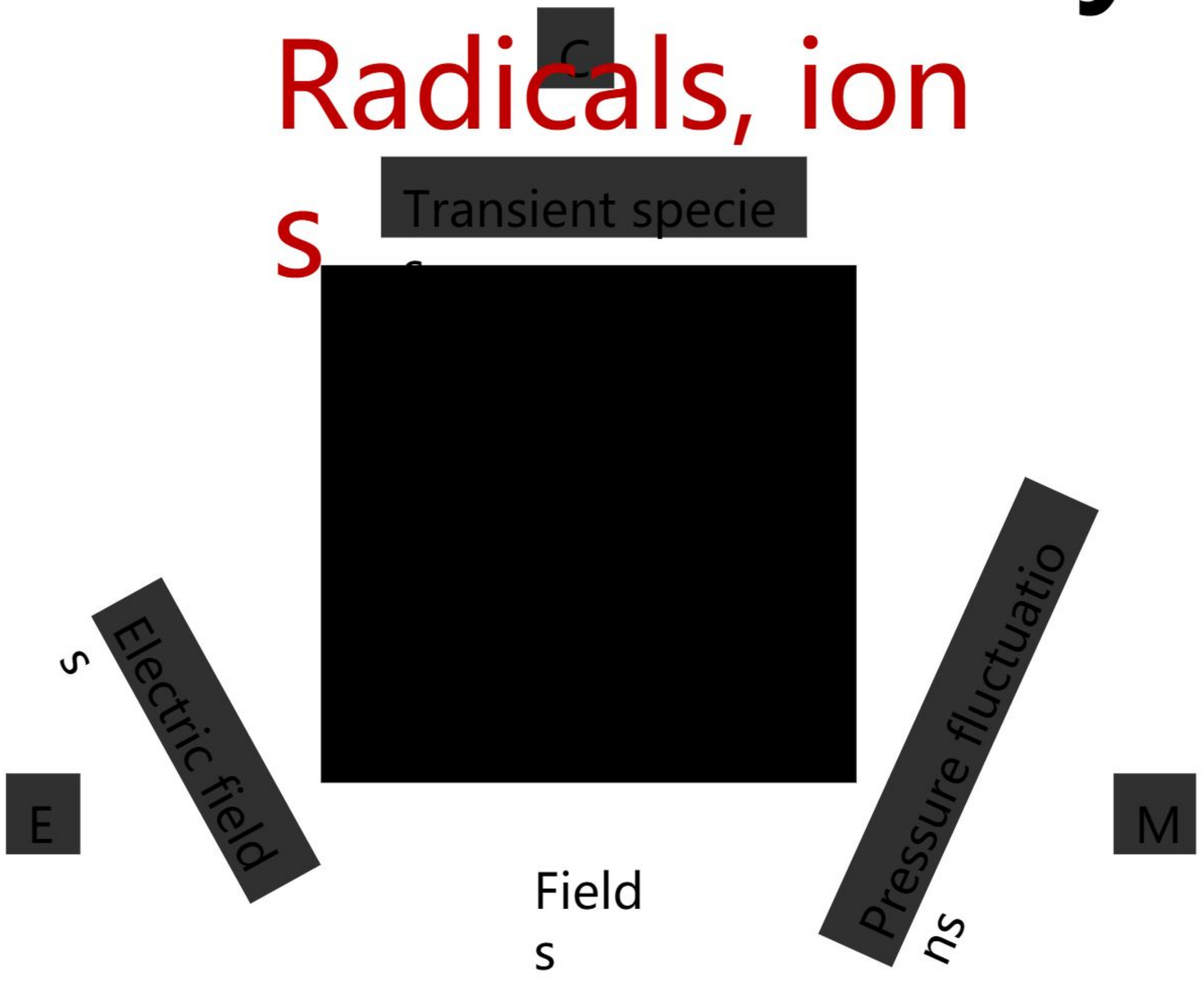
MoS2 Nanosheets



MoS2 Nanosheet

MoS2 Nanoparticles

Grand unification of synthesis



MV cm-1

MPa


C
E
M
C
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ChatGPT


Thanks to ChatGP
T

Vision

Make soil using proce
ssed wastewater and
make deserts bloom.

International Centre for Clean Wa
ter

https://iccw.world

https://iccw.world/iccw-impact-map/

An ocean of opportunities

Water presents a unique opportunity to find a purpose in life.

Conclusions

Atomically precise clusters and new molecular materials.
Affordable clean water with advanced materials is possible at scale.
Natural minerals break spontaneously in charged water microdroplets.
Clathrate hydrates exist in ultrahigh vacuum.
Implications of all these are profound for sustainability.
New research is needed in these areas.

Affordable, inclusive, sustainable and contextual excellen ce

Collaborato

Water team at IIT: A. Sreekumaran Nair, Anshup, M. Udhaya Sankar, Amrita Chaudhary, Renjis T. Tom, T. S. Sreeprasad, Udayabhaskararao Thumu, M. S. Bootharaju, K. R. Krishnadas, Kalamesh Chaudhari, Soujit Sengupta, Depanjan Sarkar, Avijit Baidya, Swathy Jakka Ravindran, Abhijit Nag, S. Vidhya, Biswajit Mondal, Krishnan Swaminathan, Azhardin Gnayee, Sudhakar Chennu, A. Suganya, Rabiul Islam, Sritama Mukherjee, Tanvi Gupte, Jenifer Shantha Kumar, A. Anil Kumar, Ankit Nagar, Ramesh Kumar Soni, Tanmayaa Nayak, Sonali Seth, Shihabudheen M. Maliyekkal, G. Velmurugan, Wakeel Ahmed Dar, Ganapati Natarajan, N. Pugazhenthiran, A. Leelavathi, Sahaja Aigal, S.Gayathri, Bibhuti Bhusan Rath, Ananthu Mahendranath, Harsh Dave, Erik Mobegi, Egor Moses, Hemanta R. Naik, Sourav Kanti Jana, Tanmayaa Nayak, Sonali Seth…

Avula Anil Kumar, Chennu Sudhakar, Sritama Mukherjee, Anshup, and Mohan Udhaya Sankar

Funding: Department of Science and Technology, Government of India

Start-ups and partners:

PhD Theses: Bindhu Varughese, M. R. Resmi, M. Venkataramanan, N. Sandhyarani, R. Selvan, A. Sreekumaran Nair, M. J. Rosemary, Renjis T. Tom, C. Subramaniam, Jobin Cyriac, V. R. Rajeev Kumar, D. M. David Jeba Singh, Akshaya Kumar Samal, E. S. Shibu, M. A. Habeeb Muhammed, P. R. Sajanlal, T. S. Sreeprasad, J. Purushothaman, T. Udayabhaskararao, M. S. Bootharaju, Soumabha Bag, Robin John, Kamalesh Chaudhari, Ammu Mathew, Indranath Chakraborty, Radha Gobinda Bhuin, Ananya Baksi, Amitava Srimony, Anirban Som, Rabin Rajan Methikkalam, K. R. Krishnadas, Soujit Sengupta, Depanjan Sarkar, Atanu Ghosh, Rahul Narayanan, Avijit Baidya, Shridevi Bhat, Papri Chakraborty, Swathy Jakka Ravindran, C. K. Manju, Abhijit Nag, S. Vidhya, Jyoti Sarita Mohanty, Debasmita Ghosh, Jyotirmoy Ghosh, Md. Bodiuzzaman, Biswajit Mondal, Tripti Ahuja, Esma Khatun, Krishnan Swaminathan, K. S. Sugi, Amrita Chakraborty, Sudhakar Chennu, Sritama Mukherjee, Madhuri Jash, Sandeep Bose, Md. Rabiul Islam, Pallab Basuri, Mohd Azhardin Ganayee, Tanvi Gupte, Ankit Nagar, Srikrishnarka Pillalamarri, Arijit Jana, Paulami Bose, Gaurav Viswakarma, Vishal Kumar, Jayoti Roy, A. Anil Kumar, Jenifer Shantha Kumar

MS Theses: Ananthu Mahedranath, Ramesh Kumar Soni

>25 Post-doctoral fellows, >130 masters students and visitors

Indian Institute of Technology Madras

ıamurthi/V. Kamakoti

Associate Editor
ACS Sustainable Resource Management

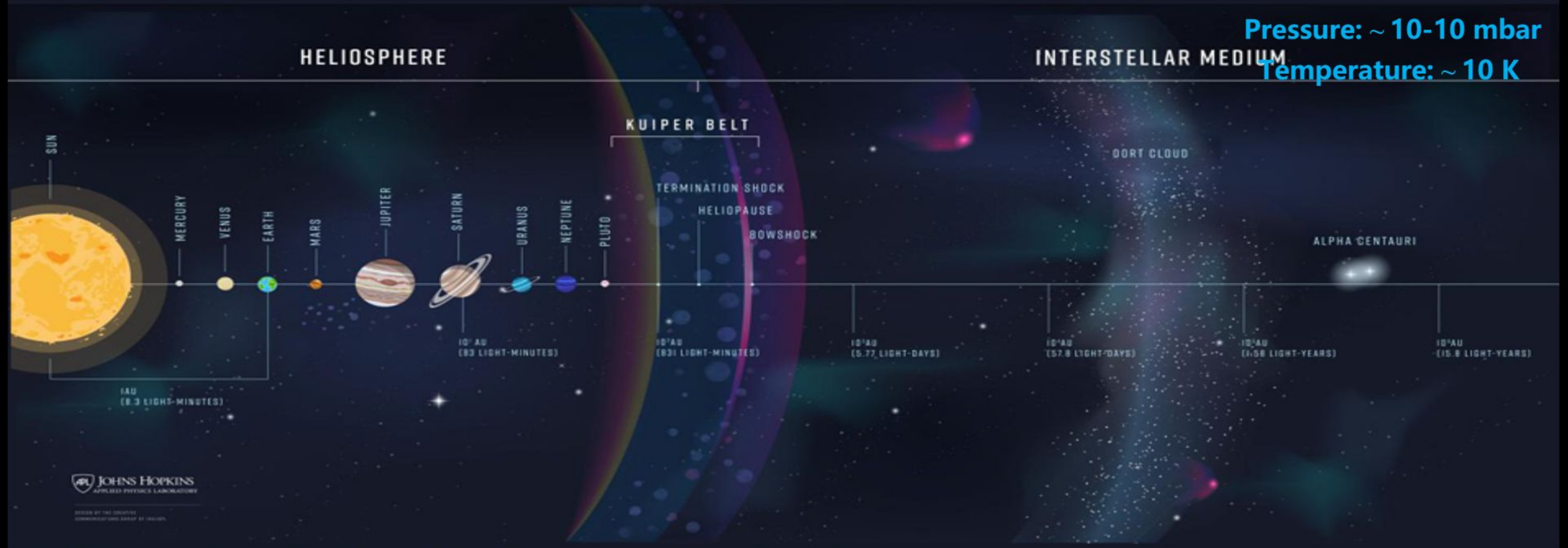
RESEARCH GROUP

THEMATIC UNIT OF EXCELLENCE

Can Clathrate Hydrates Exist in Space?

Exploring astrobiology

Interstellar medium

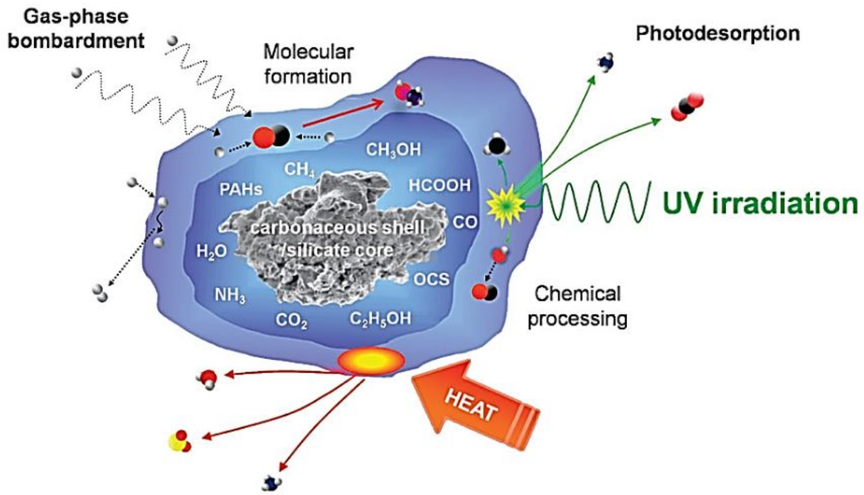


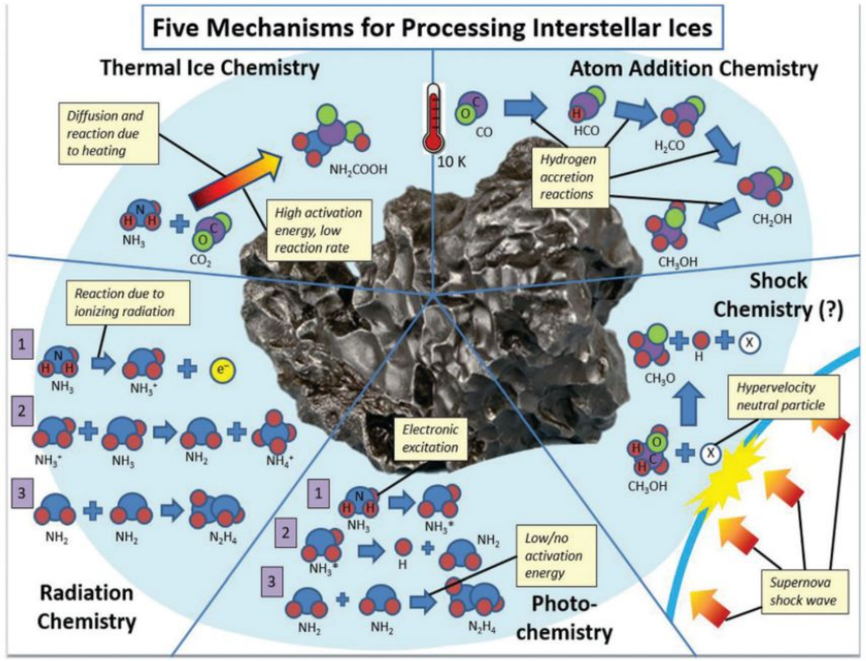
Pressure: ~ 10-10 mbar
Temperature: ~ 10 K

Diffuse clouds: T ~ 100 K, n ~ 100 molecules per cm3
Dense clouds: T ~ 10-100 K, n ~ 104-108 molecules per cm3
On Earth sea level: T ~ 300 K, n ~ 3×1019 molecules per cm3

https://spaceref.com/science

Interstellar ices





Silicates and carbonaceous material – 0.01-0.5 μm

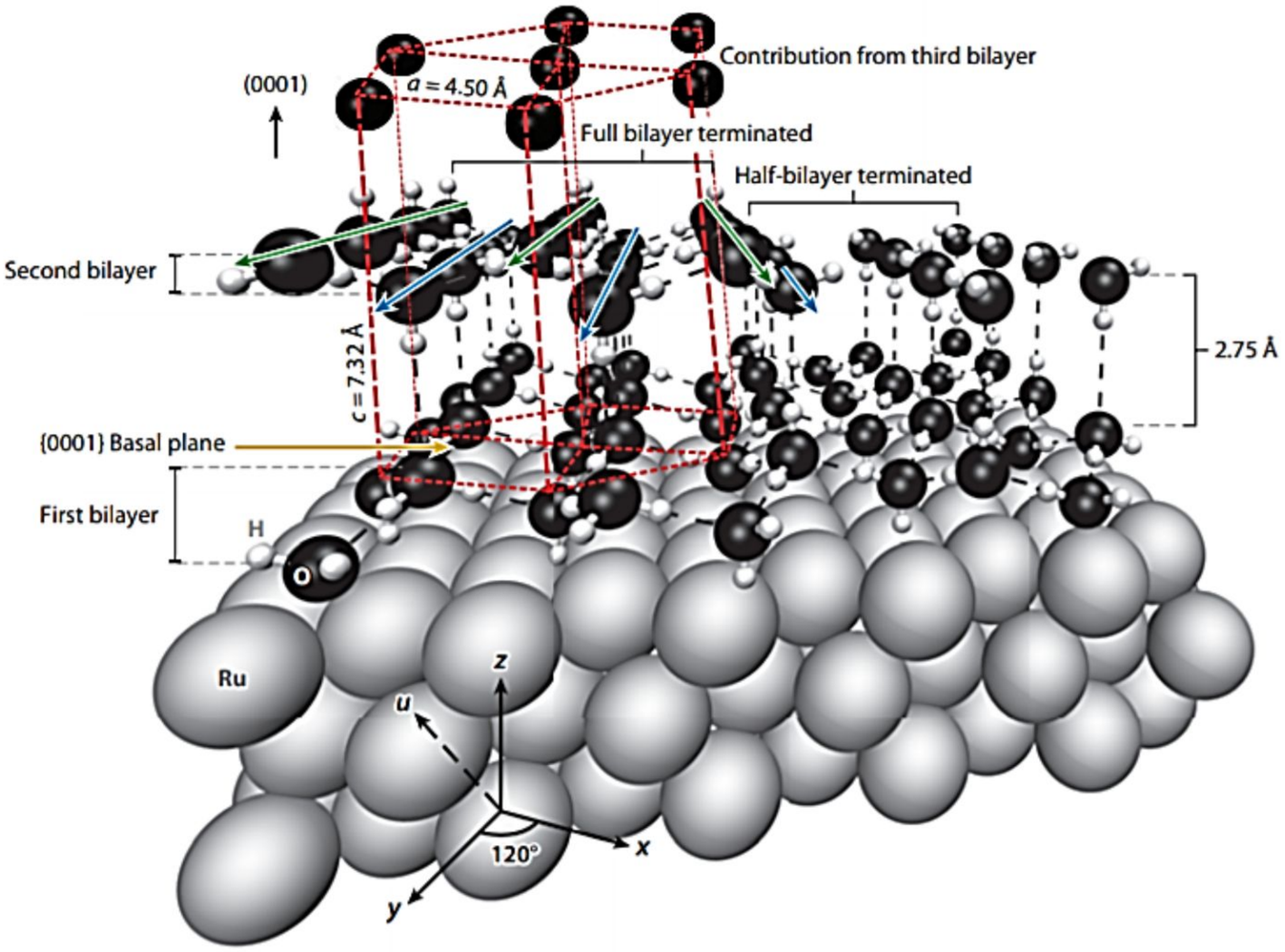
Arumainayagam, C. R. *et al.*, *Chem. Soc. Rev.*, **2019**, *48*, 2293–2314

Instrumentation

115-400 nm

Bag, S. *et al.*, *Rev. Sci. Instrum.* **2014**, *85*, 014103/1-014103/7

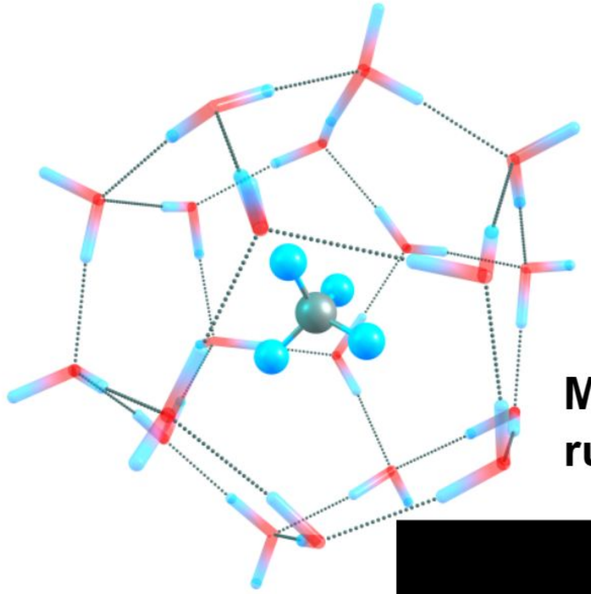
Viswakarma, *G. et al., J. Phys. Chem. Lett.*, **2023**, *14*, 2823–2829



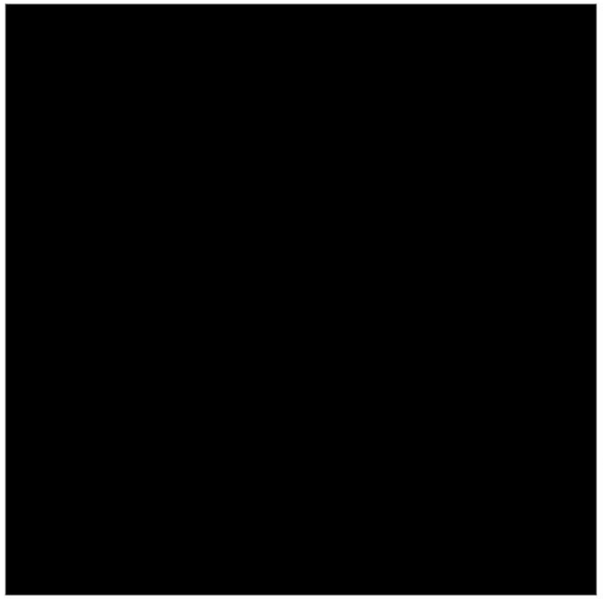
Bag, S. *et al.*, *Annu. Rev. Anal. Chem.* **2013**, *6*, 97–118

Clathrate hydrates in interstellar environment

Sample inlet tubes



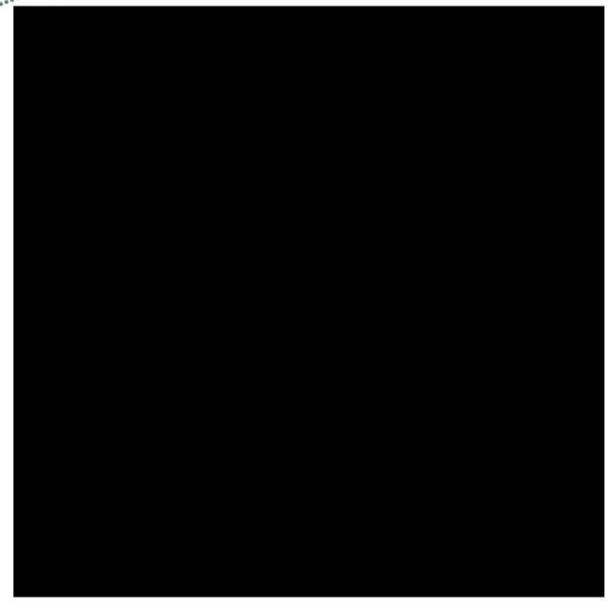
Methane hydrate st
ructure; 512 cage



Co-deposition at 10 K

Annealing

Varying T, dependin
g on the gas



Clathrate hydrate (CH)

Clathrate hydrates in interstellar environment

A

3017 cm-1

3009 cm-1

Δω = 8 cm-1

0.005 arb. units

B

3009 cm-1

3017 cm-1

0.0025 arb. units

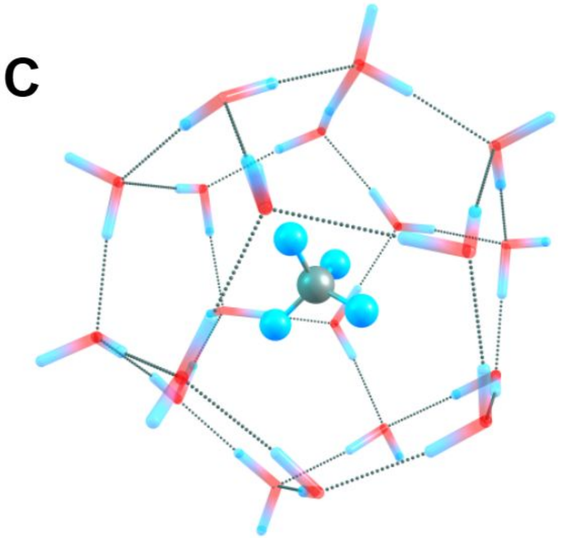
30 K

20 K

10 K

12.71% of the total CH4 is trapped

C



512 cage of CH4 hydrate

Ghosh, J. *et al., Proc. Natl. Acad. Sci. U.S.A.* **2019**, *116*, 1526-1531

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Article

Formation and Transformation of Clathrate Hydrates under Interstellar Conditions

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

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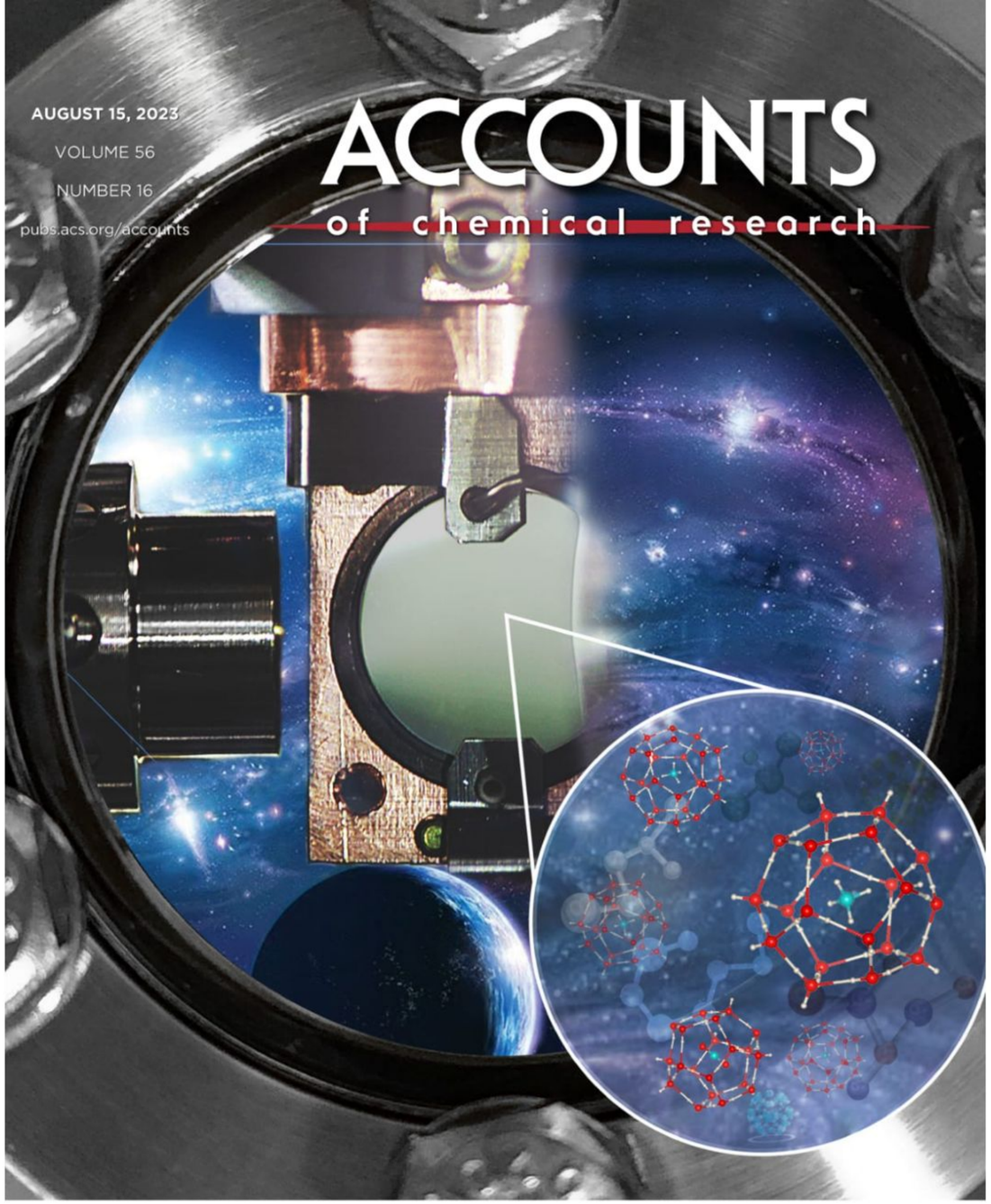

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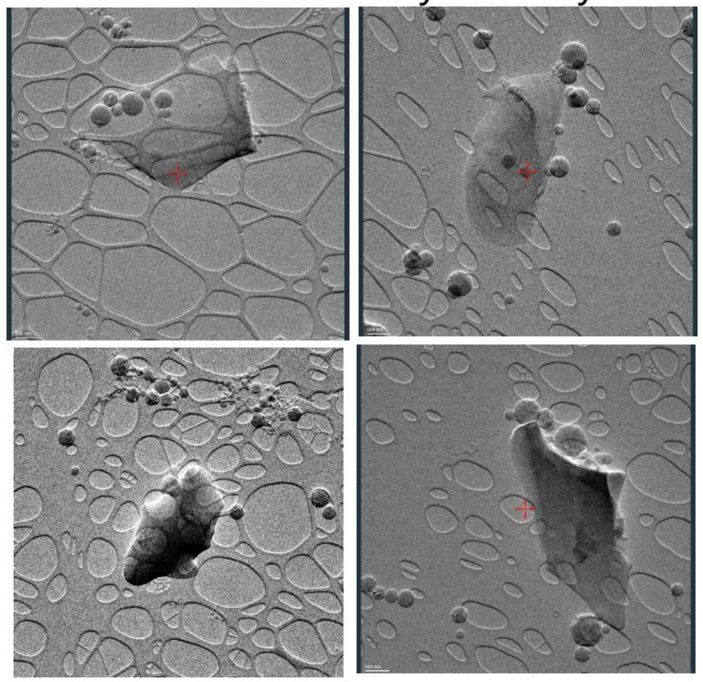
Electron diffraction of nanometer-scale crystals of clathrate hydrate

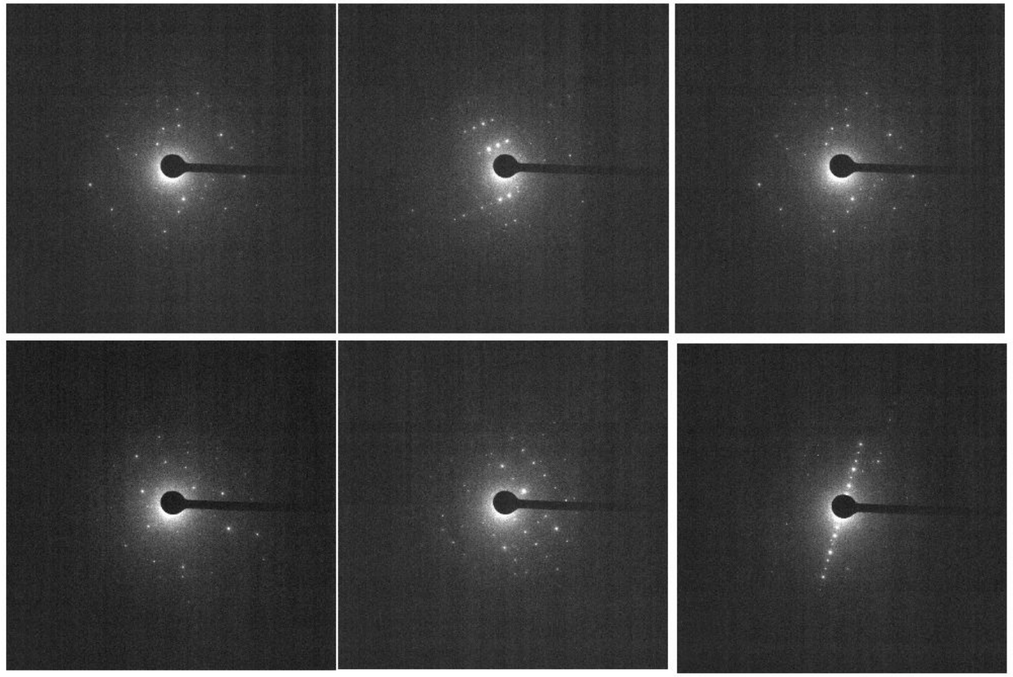
(a)

THF-CH4 Clathrate hydrate crystal

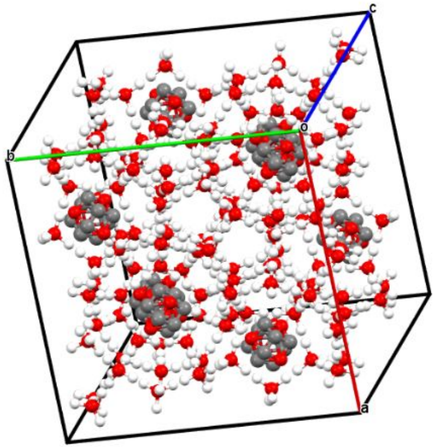


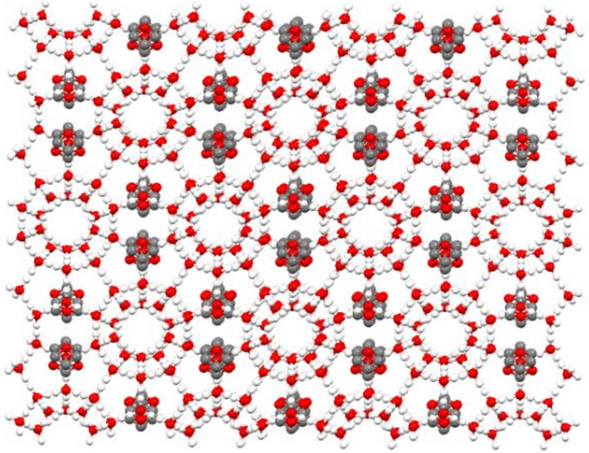
(b)

3 D electron diffraction



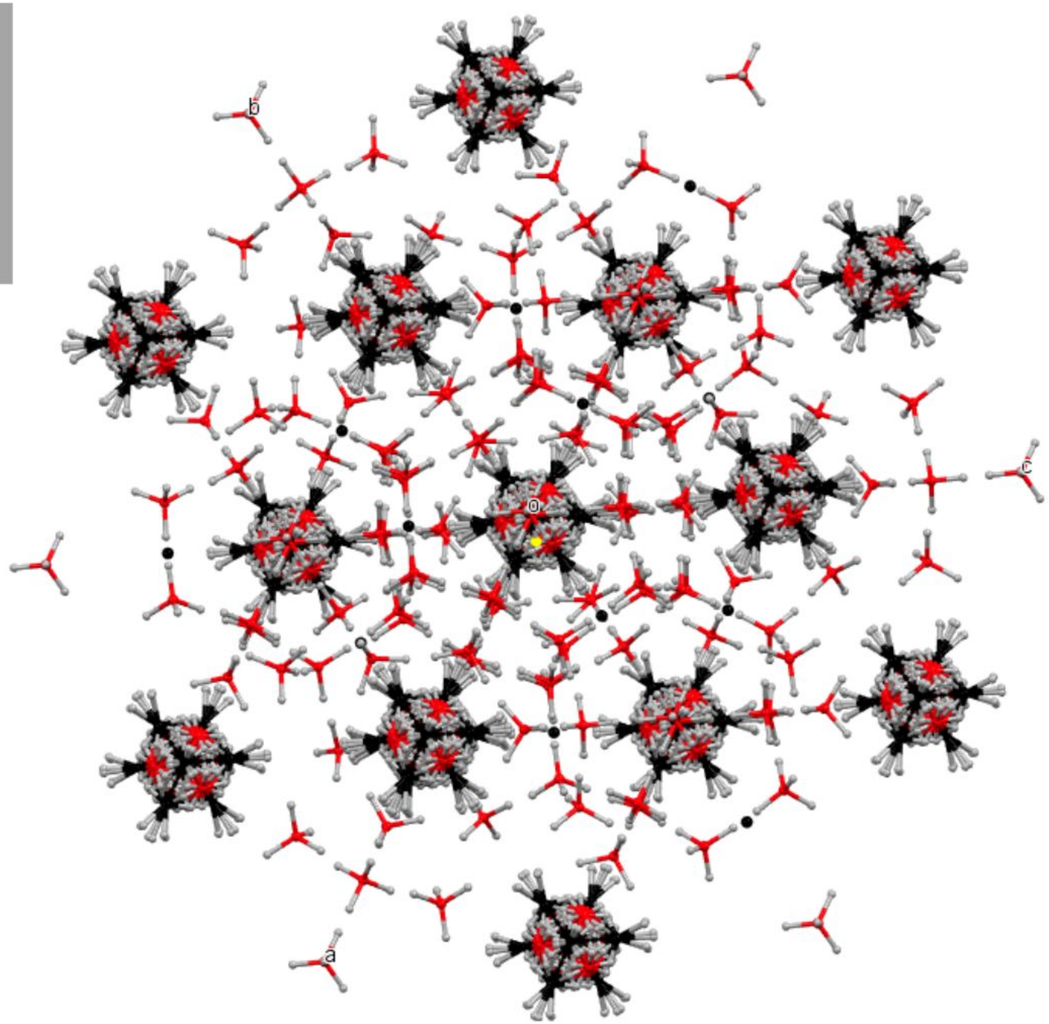
(c)

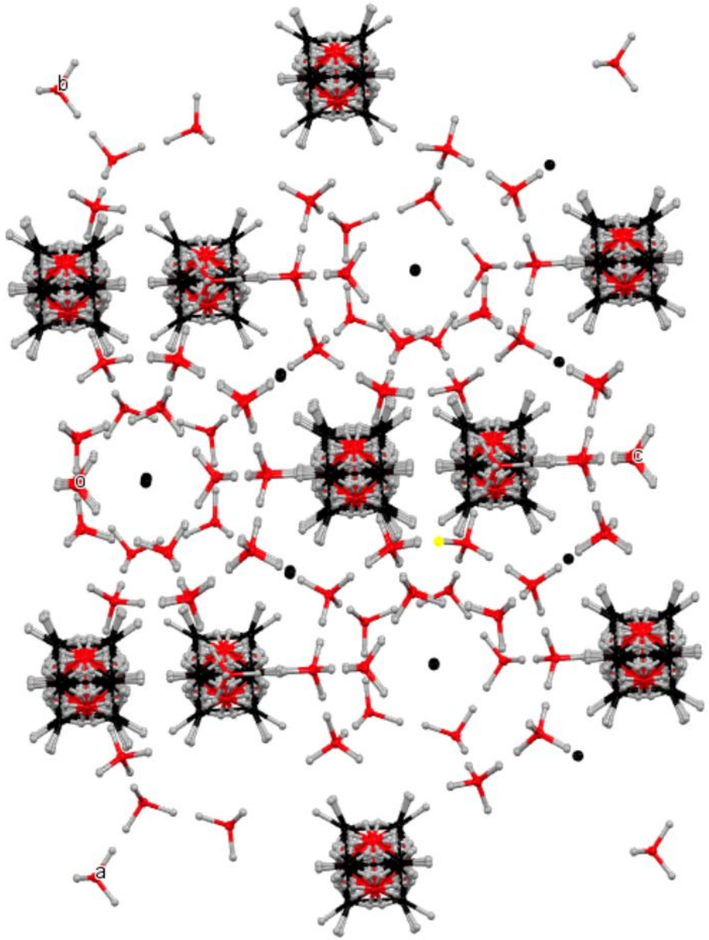




Crystal structure

MicroED – THF CH4 clathrate hydrate



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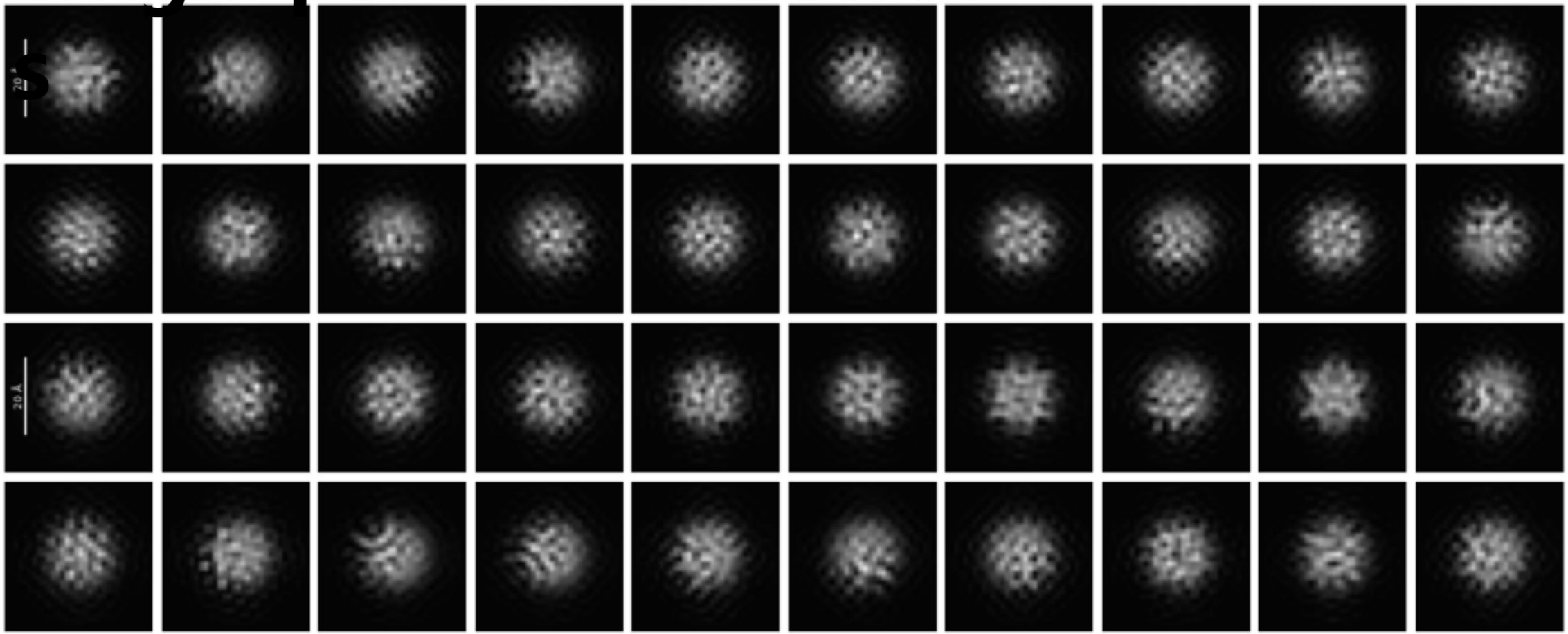
Single particles

Single particle structure



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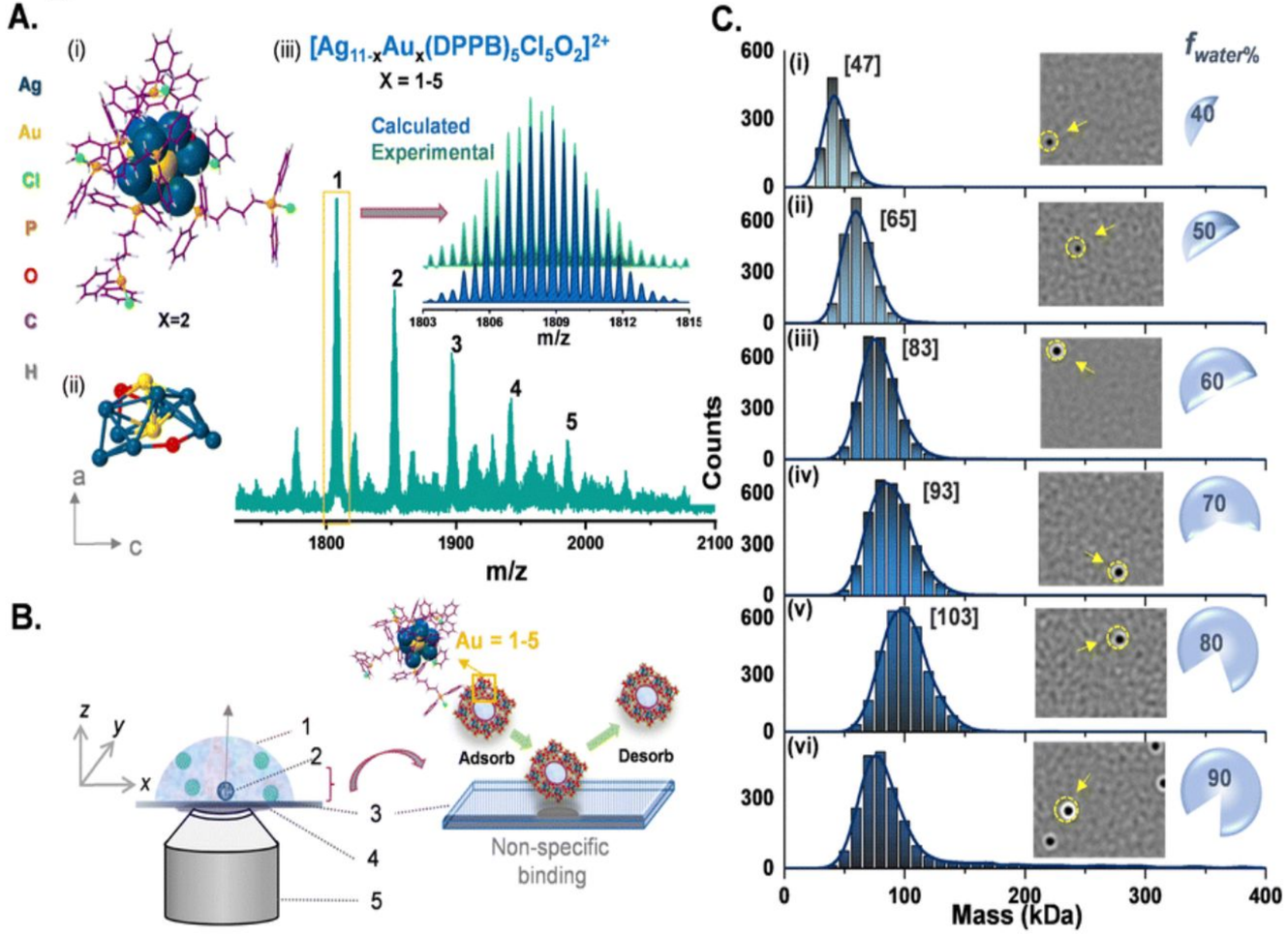
Structural Transitions and Micro-ED

Harshita Nagar, Anirban Som,... Chem. Comm. 2025

Atomic precision does not end

Mass Photometry



Key features :

Mass Range: 30 kDa to 5 MDa

J. Roy, et. al., *Chem. Commun.*, 2024,60, 6655-6658

[redacted]

es

Lopamudra et. al. Unpublish