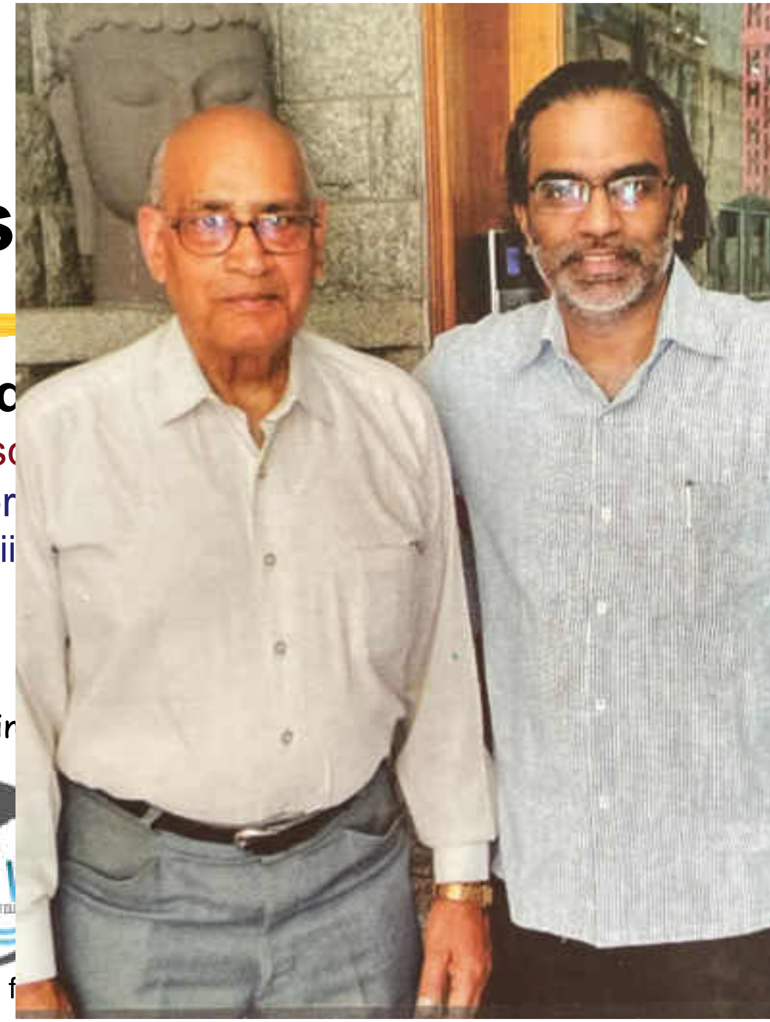
Since 1959

Atomically precis



T. Prad

Institute Professo

https://pradeepr

pradeep@ii

Co-founder

InnoNano Research Pvt. Ltd.
InnoDI Water Technologies Pvt. Ltd.
VayuJAL Technologies Pvt. Ltd.
Aqueasy Innovations Pvt. Ltd.
Hydromaterials Pvt. Ltd.
EyeNetAqua Pvt. Ltd.
Deepspectrum Analytics Pvt. Ltd.

Professor-ir

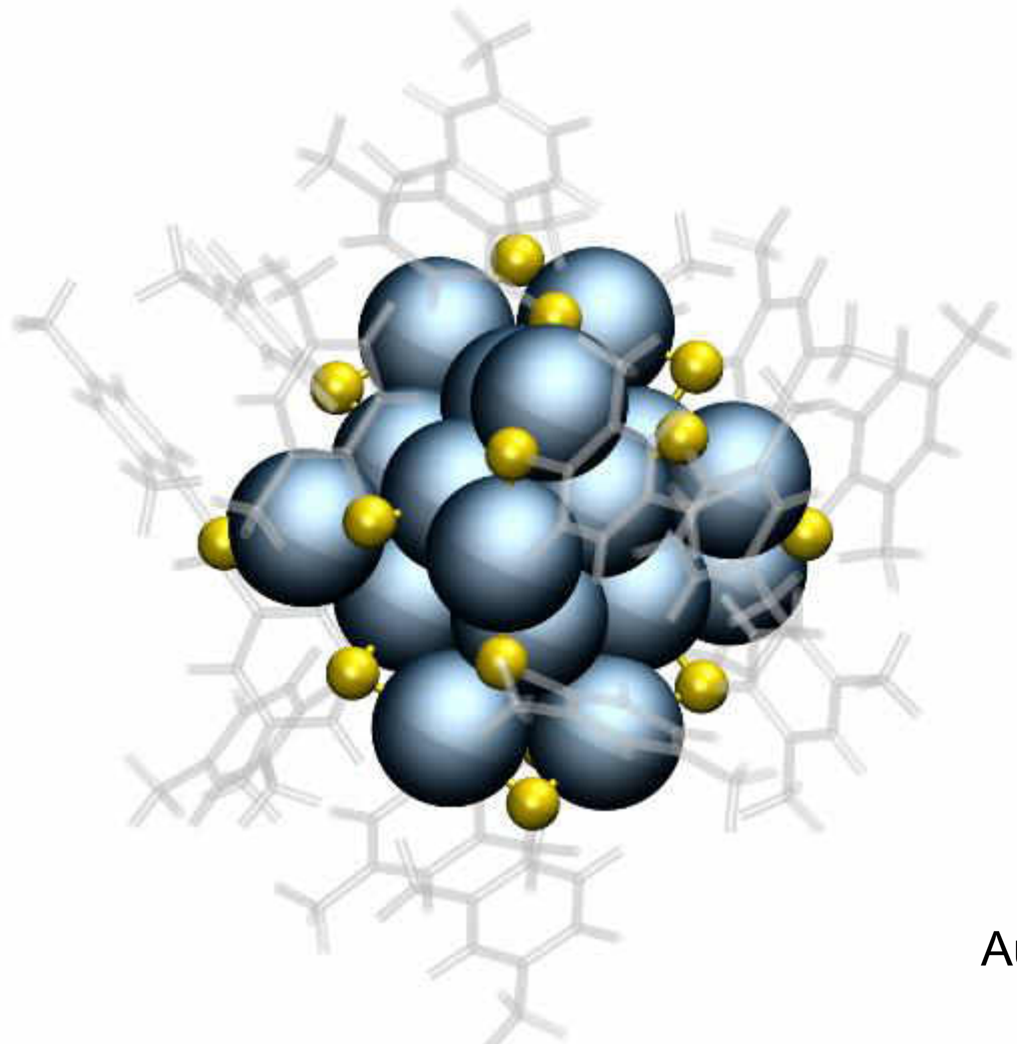
Associate Editor

ACS Sustainable Chemistry & Engineering

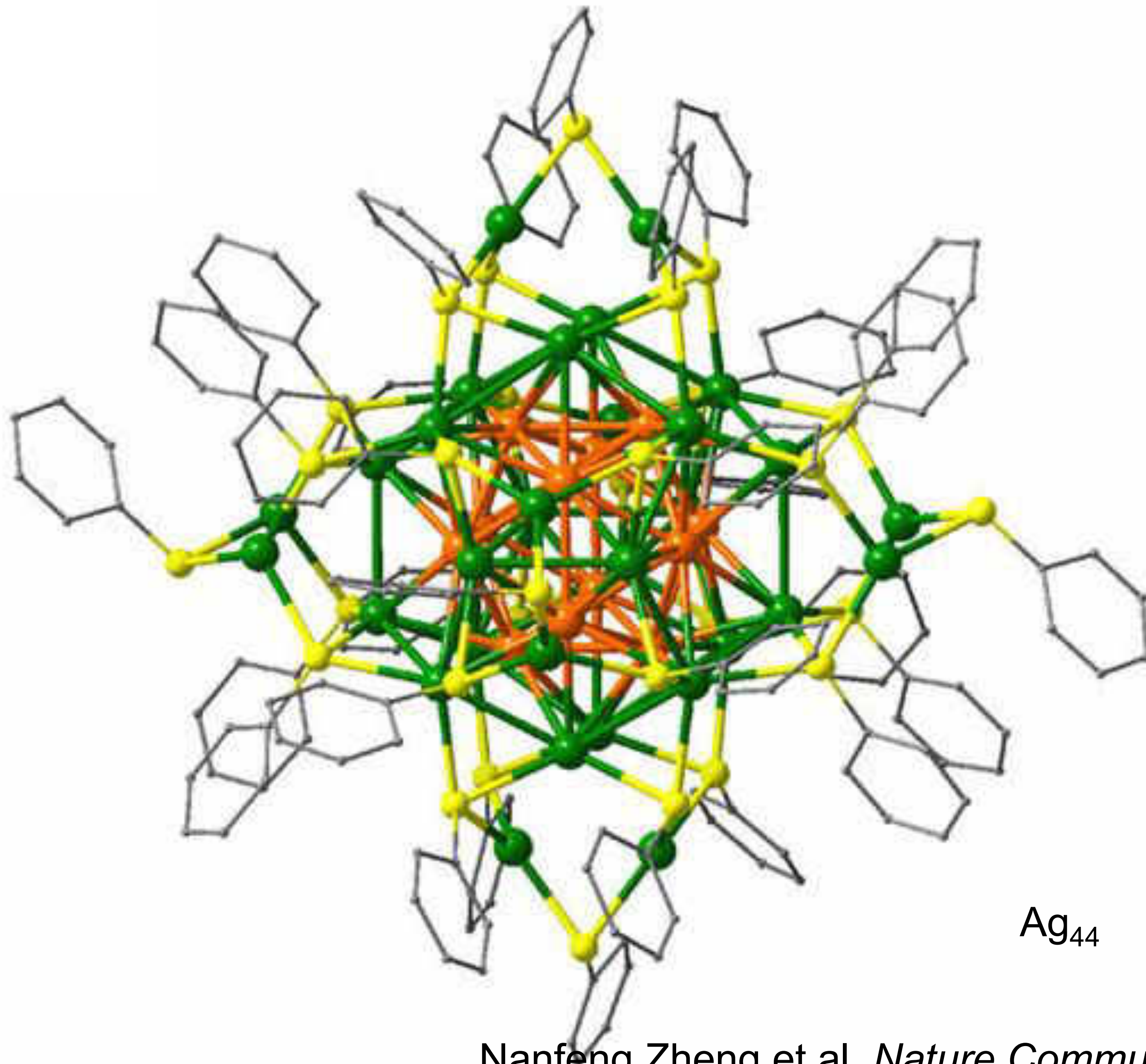
International Centre f

International Conference on Thin Films & Nanotechnology: Knowledge, Leadership, & Commercialization, ICTN-KLC 2023, IIT Madras, July 6-9, 2023

New molecules



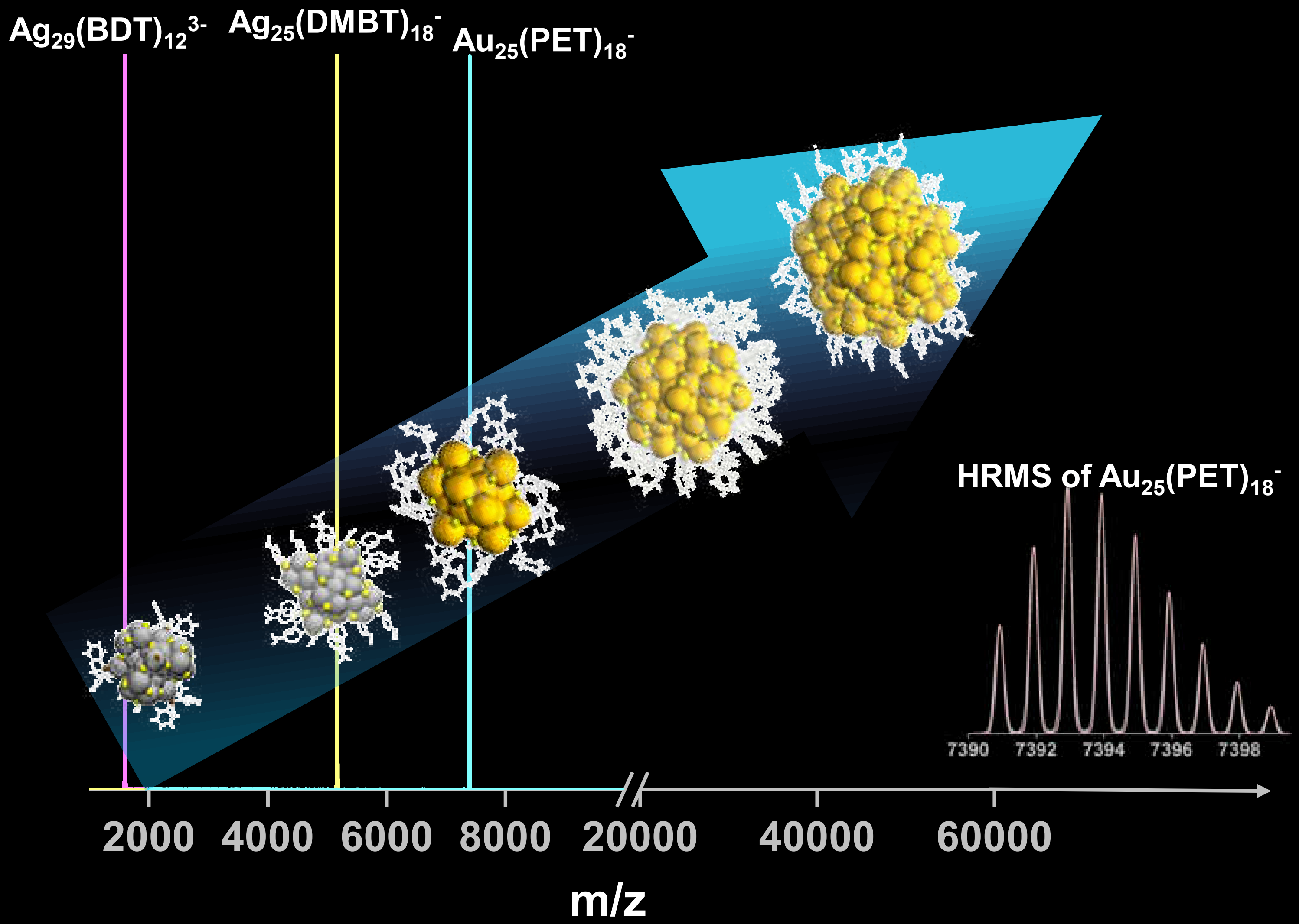
$Au_{25}, Ag_{25}, Ag_{29}$



Ag_{44}

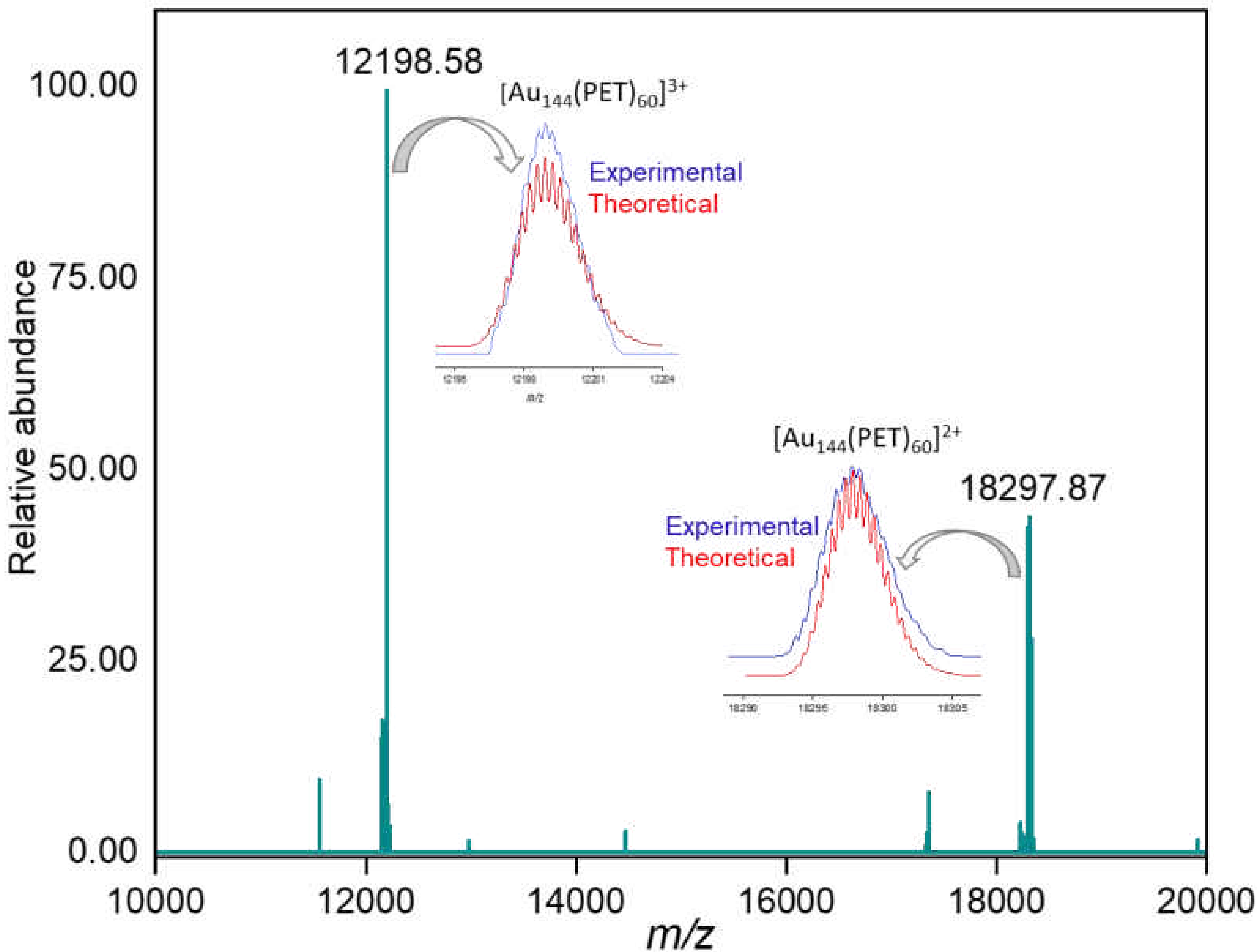
Nanfeng Zheng et al. *Nature Communications*, 2013

Terry Bigioni et al. *Nature* 2013



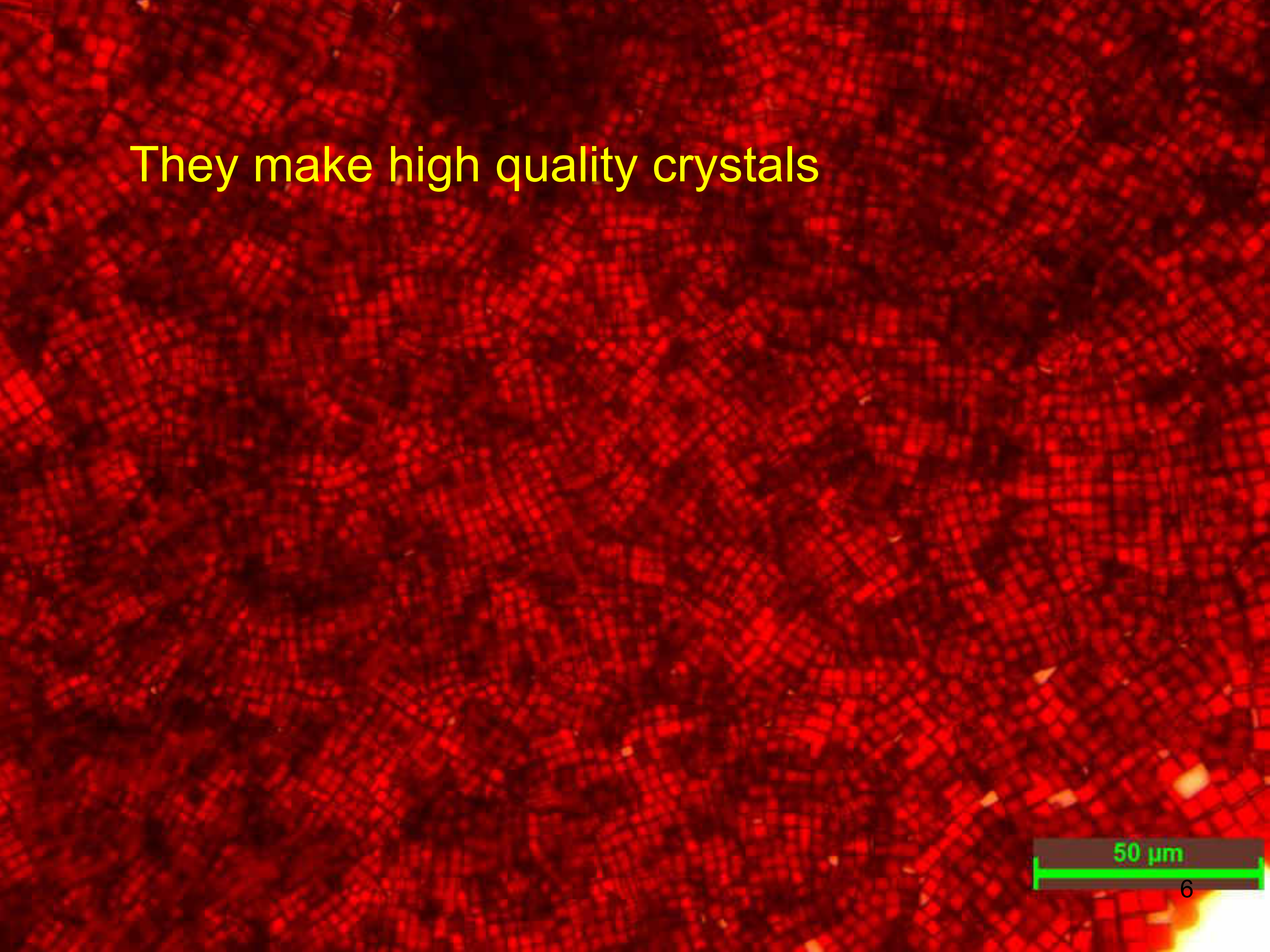
$Ag_{29}(BDT)_{12}^{3-}$
$Ag_{25}(DMBT)_{18}^{-}$
$Au_{25}(PET)_{18}^{-}$
HRMS of $Au_{25}(PET)_{18}^{-}$
7390 7392 7394 7396 7398
2000 4000 6000 8000 20000 40000 60000
m/z

$Au_{144}(PET)_{60}$

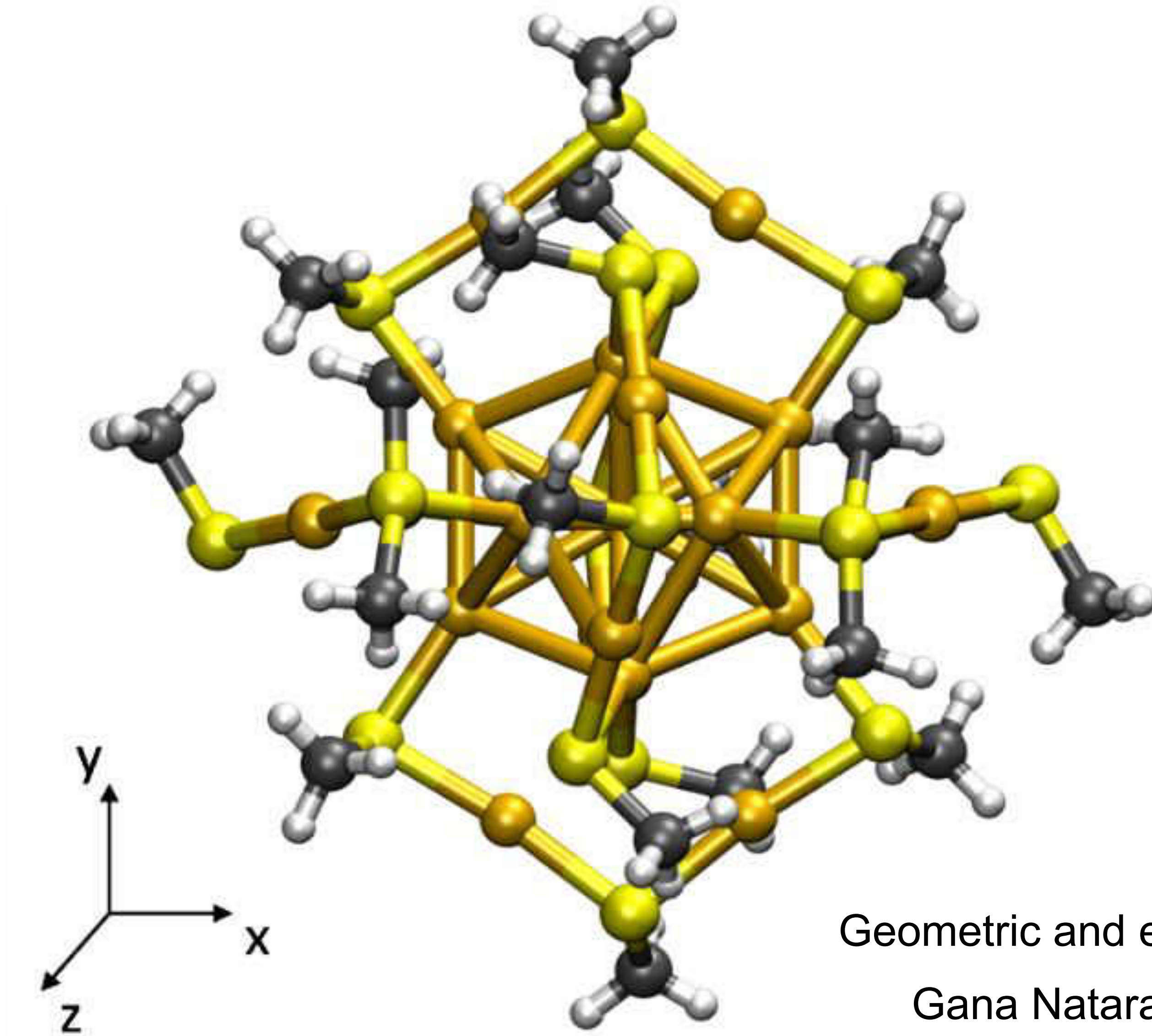


12198.58
[Au144(PET)60]3+
Experimental
Theoretical
[Au144(PET)60]2+
18297.87
Experimental
Theoretical
Relative abundance
100.00
75.00
50.00
25.00
0.00
10000
12000
14000
16000
18000
20000
m/z

They make high quality crystals



Molecular structure



Molecular materials

ACCOUNTS of chemical research

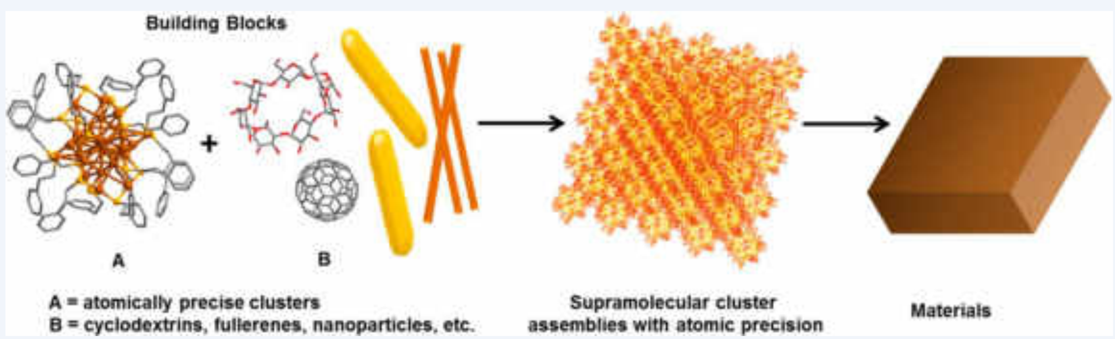
Article

pubs.acs.org/accounts

Approaching Materials with Atomic Precision Using Supramolecular Cluster Assemblies

Papri Chakraborty, Abhijit Nag, Amrita Chakraborty, and Thalappil Pradeep*

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



Molecules and their properties

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. $\times 10^{-12}$m^2/N
Coefficient of thermal expansion, 25°C	256.32 $\times 10^{-6}$ K^{-1}
Thermal Conductivity, 25°C	0.608 W/m.K

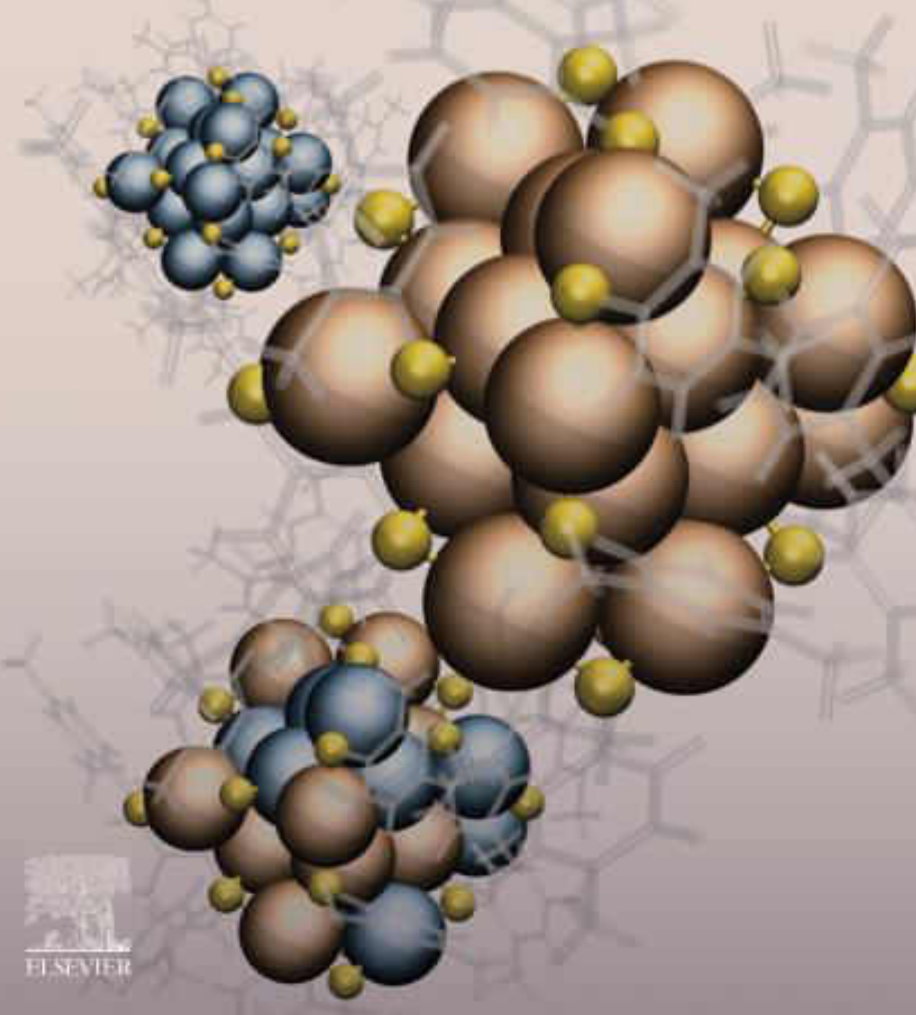
Molecular formula
Molecular weight
Molecular structure
Molecular absorption and emission
Molecular reactions
Molecular assembly
Molecular co-crystals
Ionization potential
Electron affinity

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

Future?

Edited by
Thalappil Pradeep

ATOMICALLY PRECISE METAL NANOCLUSTERS



ELSEVIER

Molecular reactions

Reactions on clusters

Reactions <u>between</u> clusters

Inter-cluster reactions

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

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

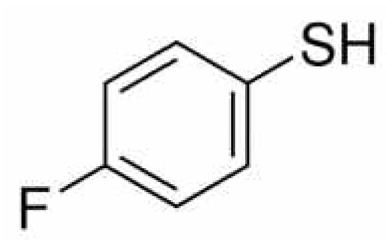
K. R. Krishnadas, Atanu Ghosh, Ananya Baksi, Indranath Chakraborty,[†] Ganapati Natarajan, and Thalappil Pradeep*

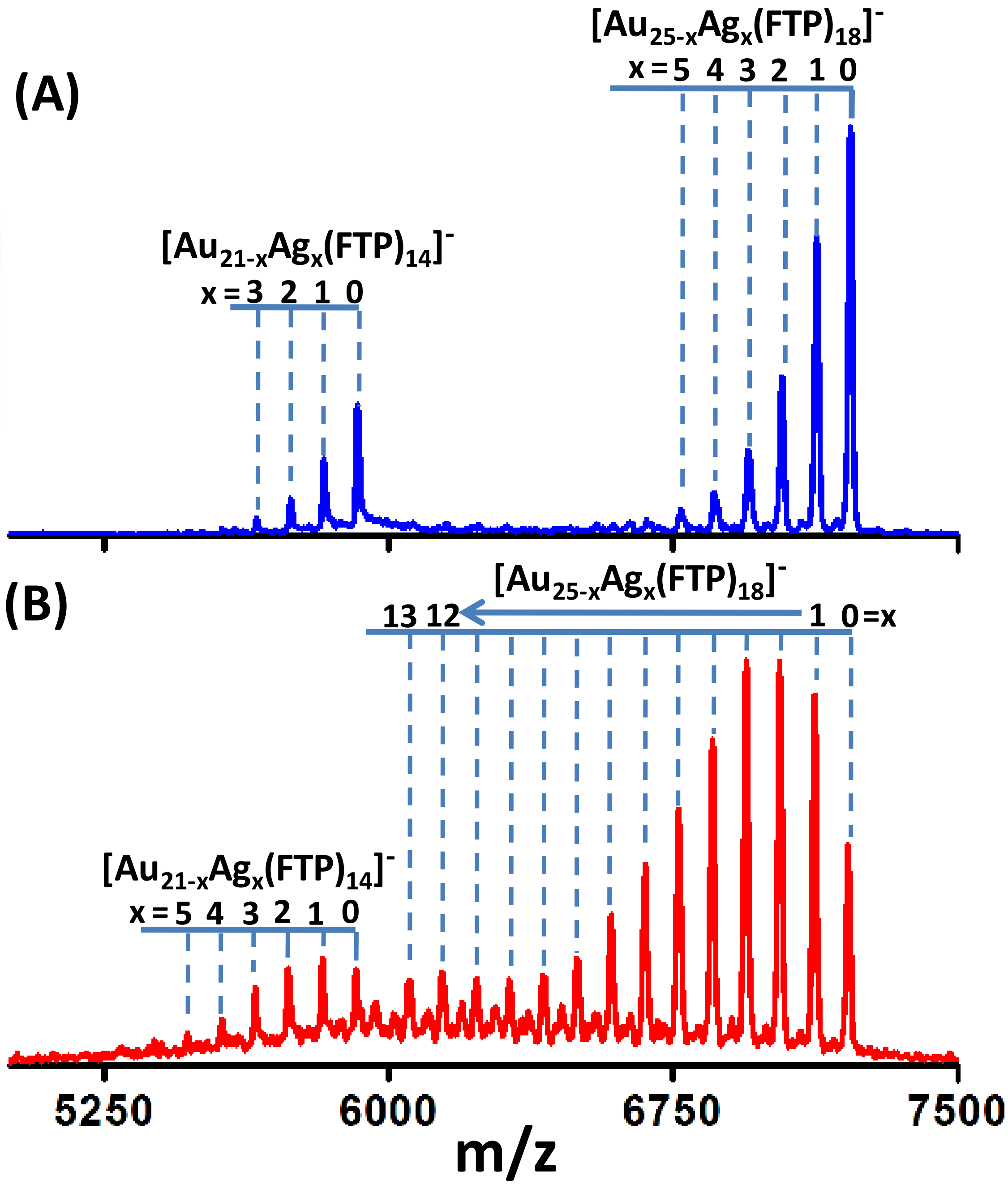
DST Unit of Nanoscience (DST UNS) and Thematic Unit of Excellence, Department of Chemistry, Indian Institute of Technology Madras, Chennai, 600 036, India

Supporting Information

$$A + B \rightarrow C + D$$

$Au_{25}(FTP)_{18} + Ag_{44}(FTP)_{30} \rightarrow Au_{25-x}Ag_x(FTP)_{18}$



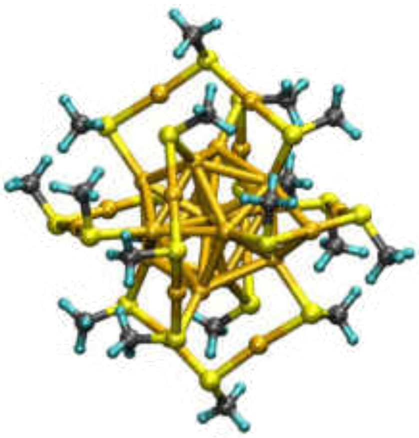


Ag_{25}-Au_{25} experiments

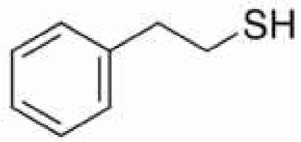
K. R. Krishnadas et al. *Nature Commun.* 2016

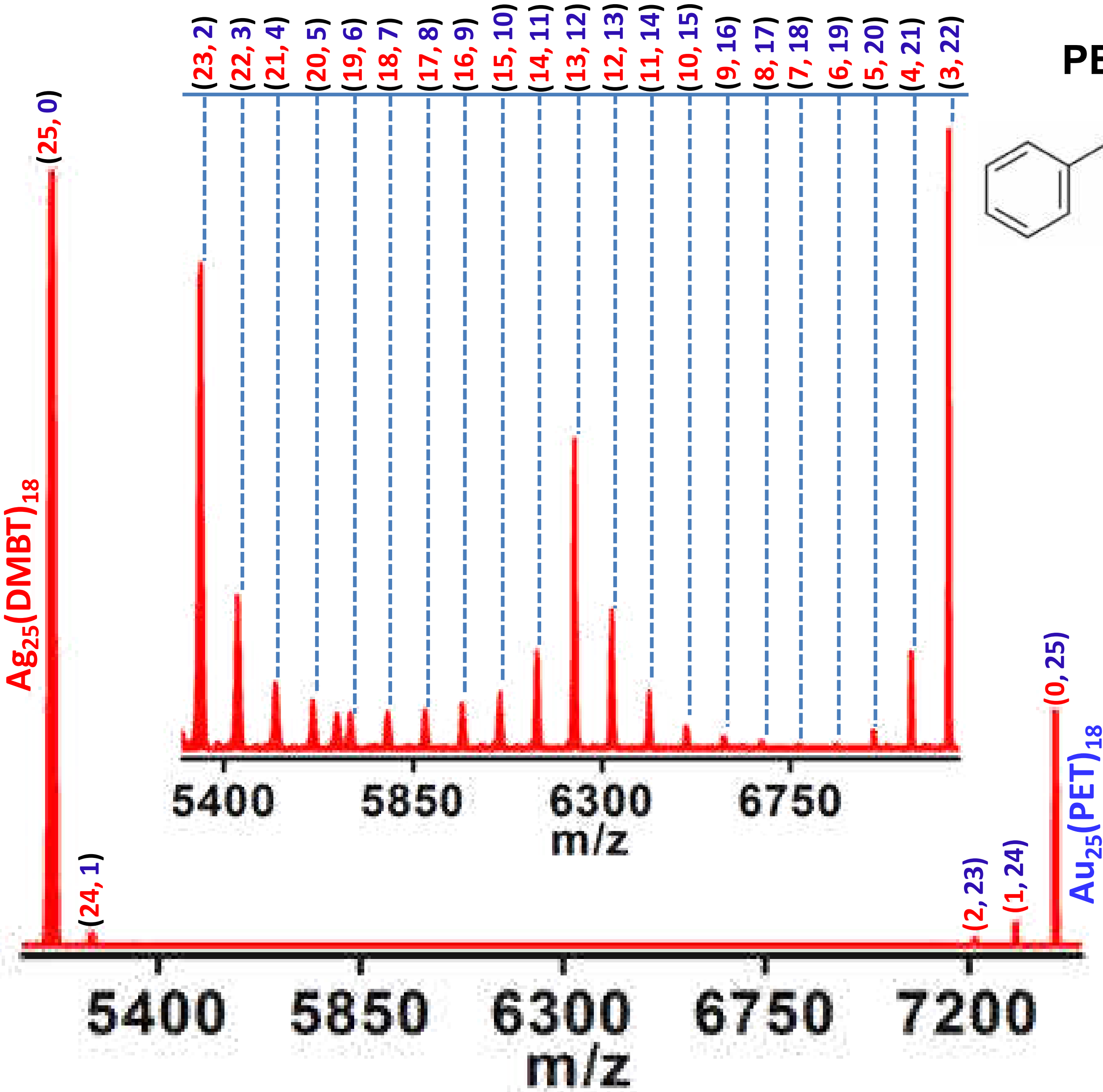
Reaction between $Au_{25}(PET)_{18}$ and $Ag_{25}(DMBT)_{18}$

DMBT

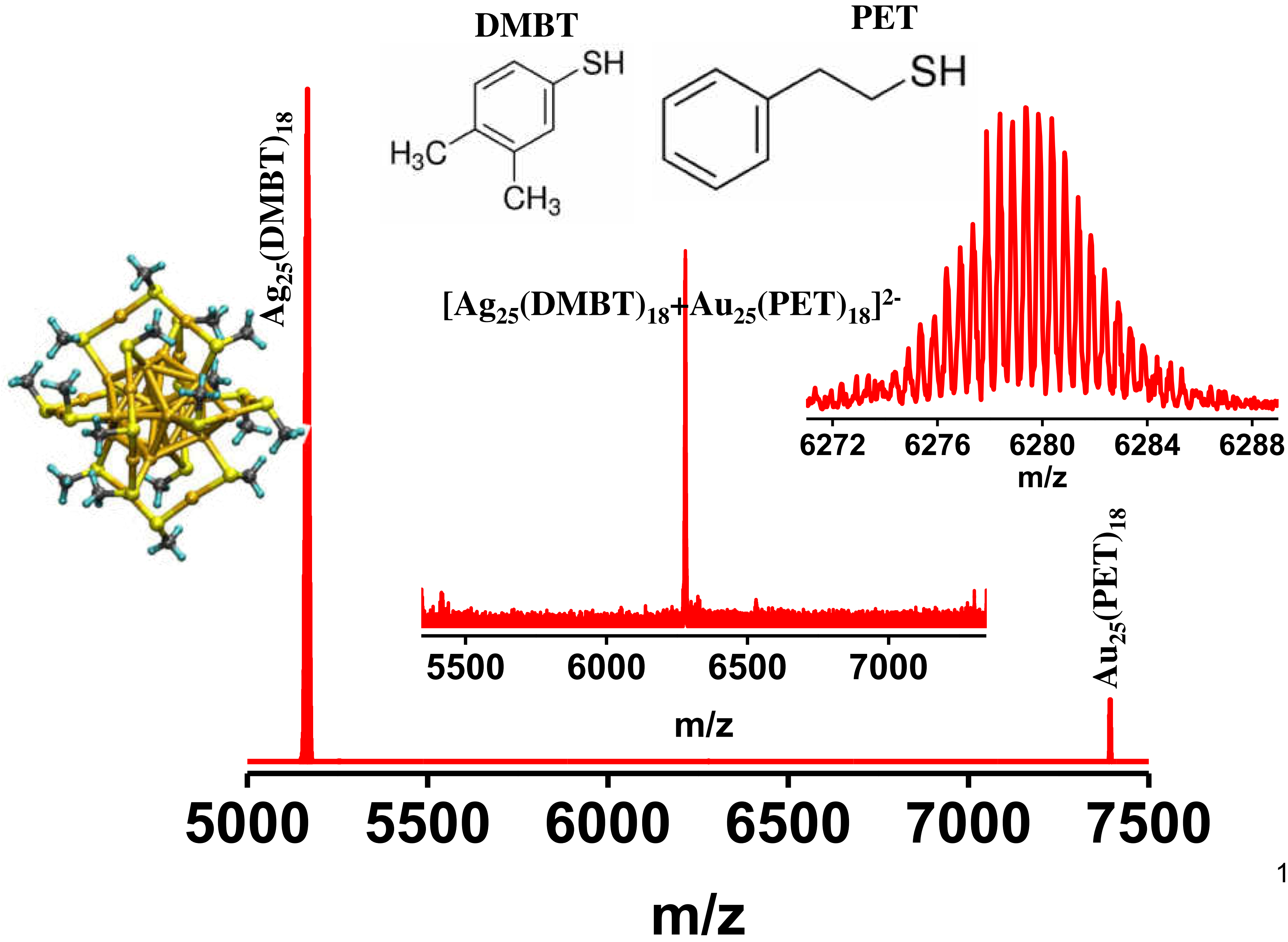


PET





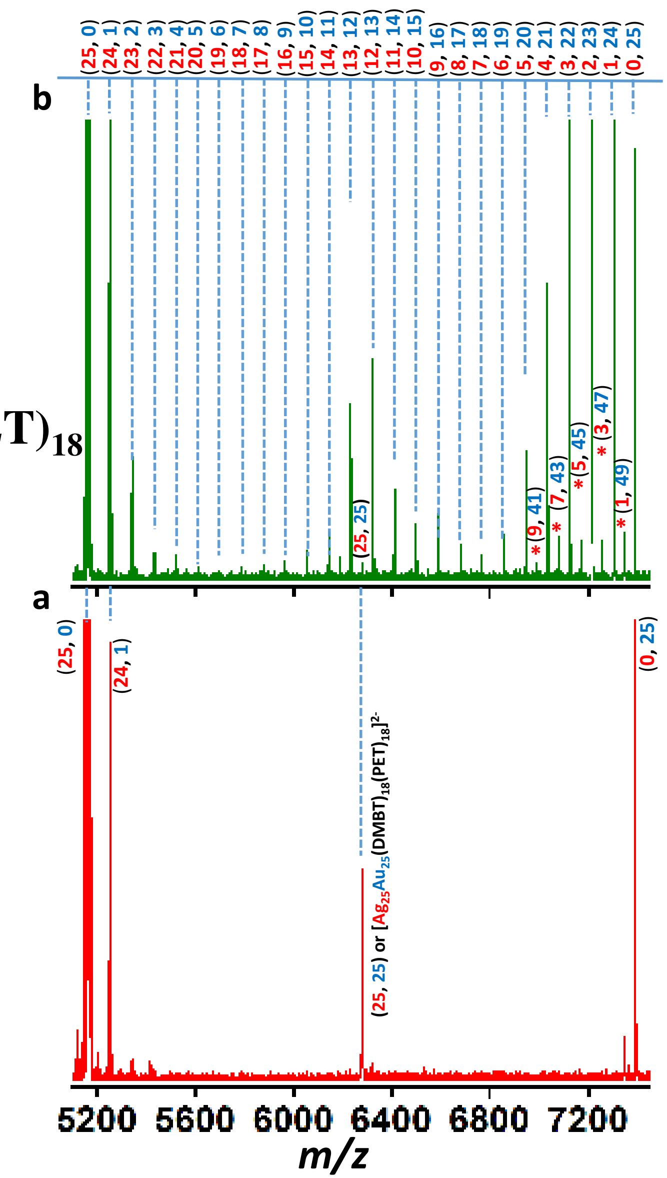
$[Ag_{25}(DMBT)_{18}+Au_{25}(PET)_{18}]^{2-}$



Evolution of alloy clusters from the dianionic adduct, $[Ag_{25}Au_{25}(DMBT)_{18}(PET)_{18}]^{2-}$

$Ag_{25}(DMBT)_{18}$:$Au_{25}(PET)_{18}$

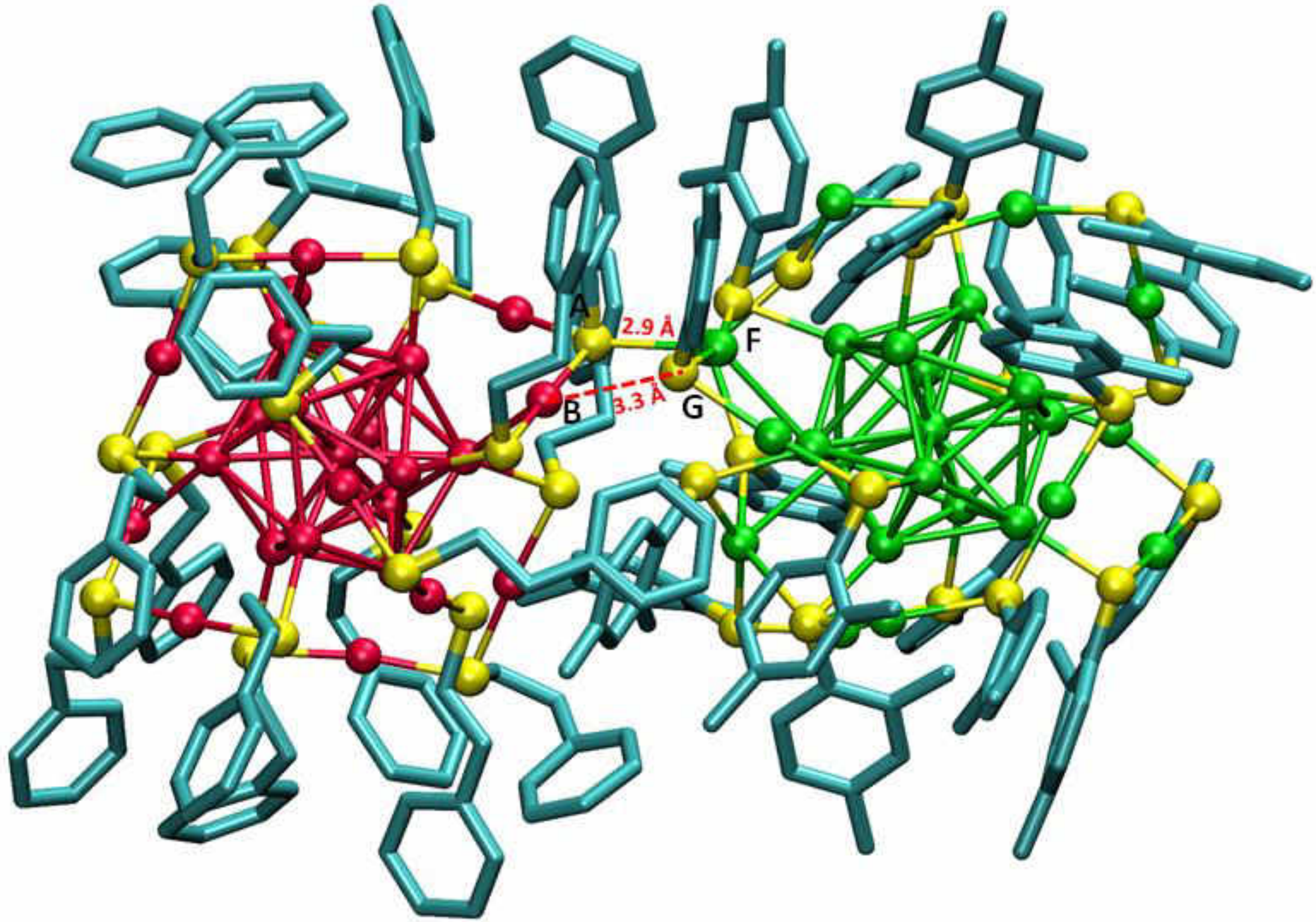
0.3:1.0

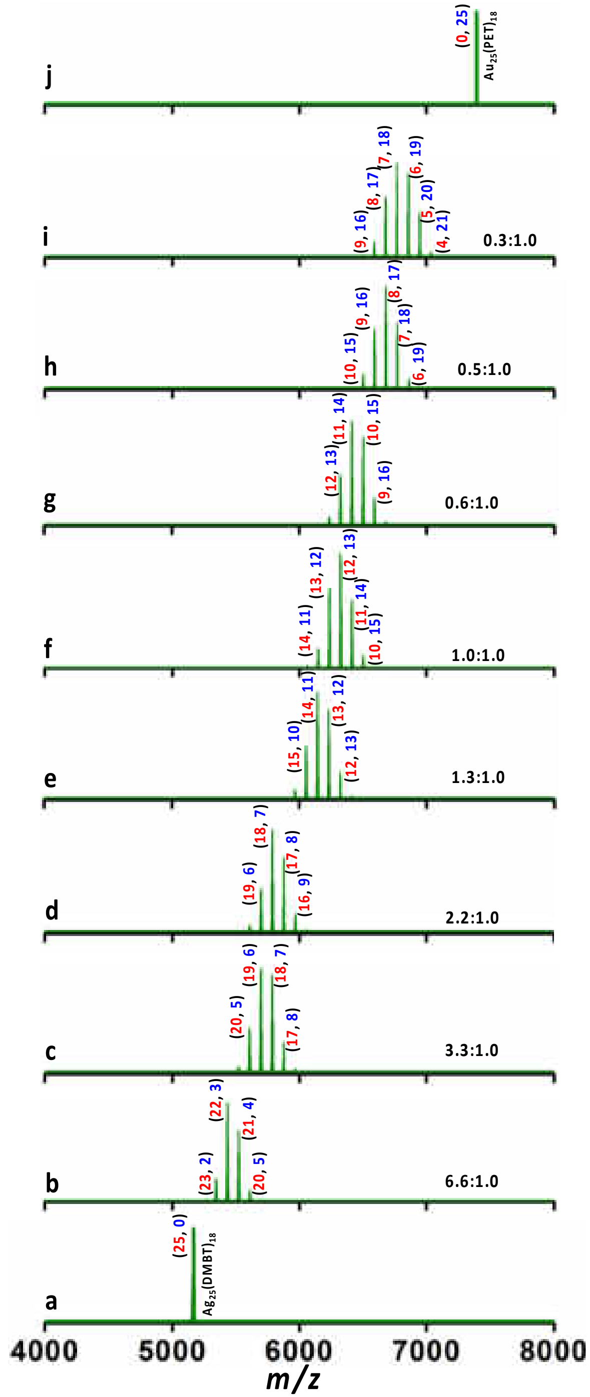


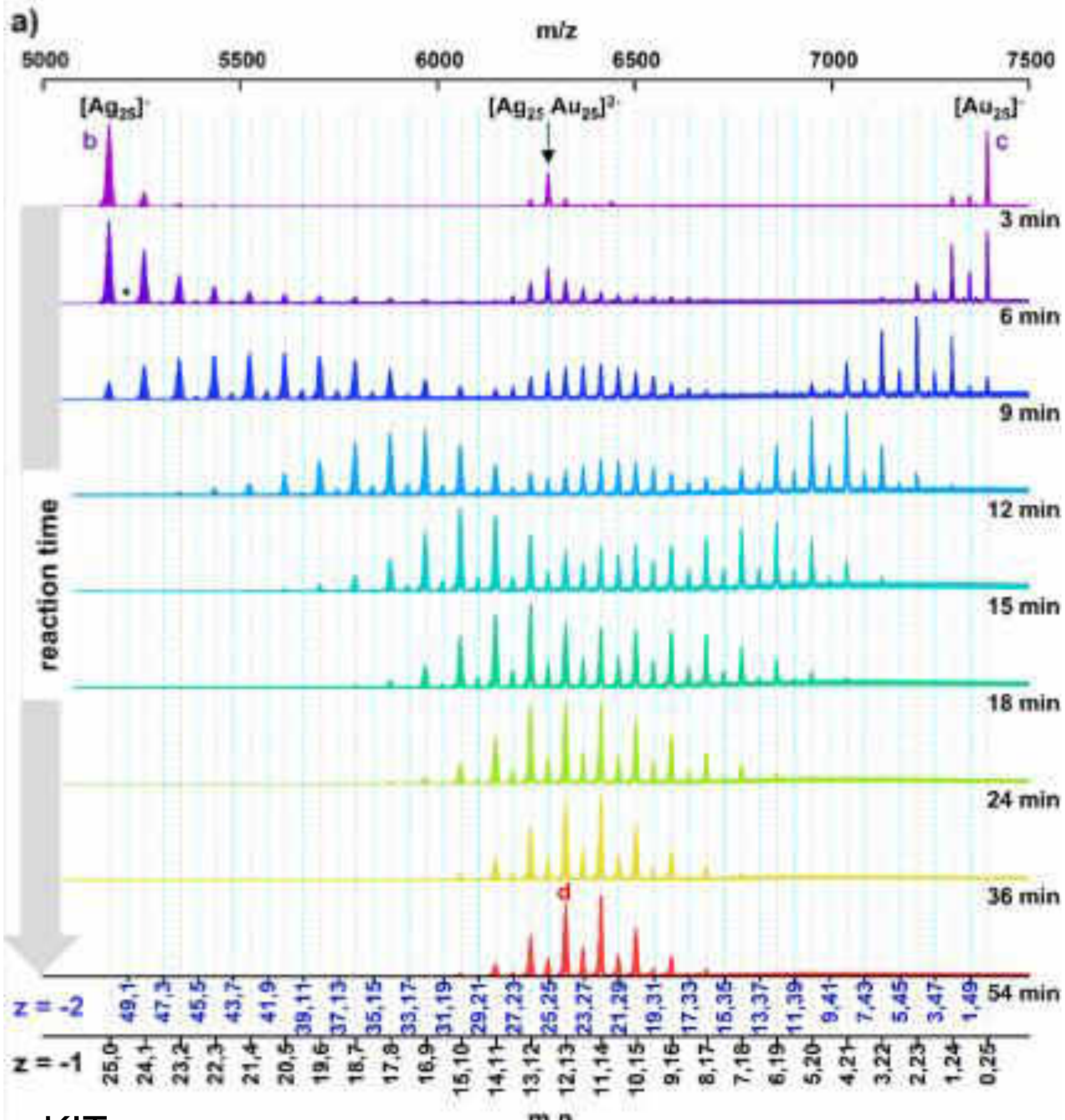
within 5 min

within 2 min

Optimized structure of $[Ag_{25}Au_{25}(DMBT)_{18}(PET)_{18}]^{2-}$



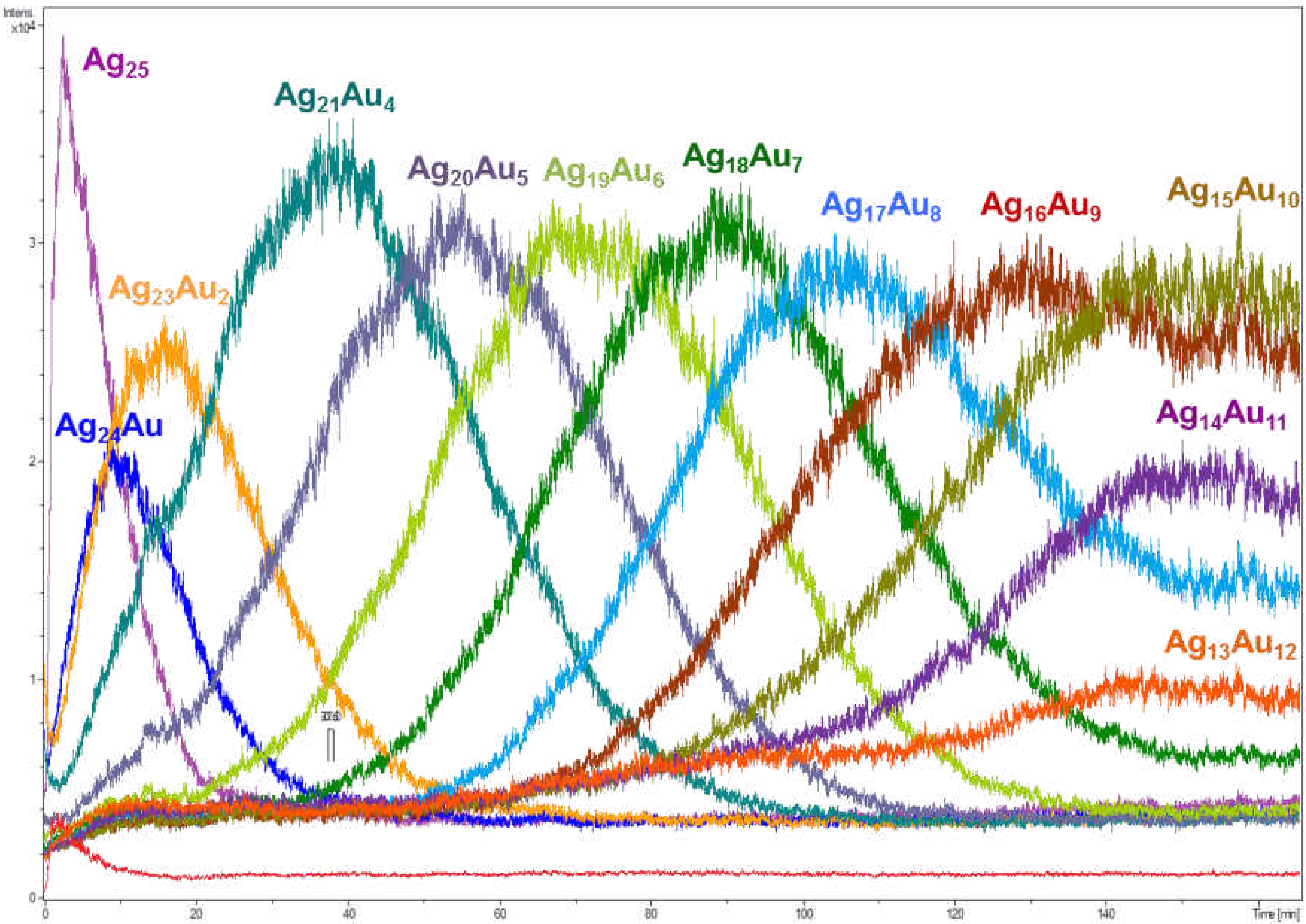

j
(0, 25)
$Au_{25}(PET)_{18}$
i
(9, 16)
(8, 17)
(7, 18)
(6, 19)
(5, 20)
(4, 21)
0.3:1.0
h
(10, 15)
(9, 16)
(8, 17)
(7, 18)
(6, 19)
0.5:1.0
g
(12, 13)
(11, 14)
(10, 15)
(9, 16)
0.6:1.0
f
(14, 11)
(13, 12)
(12, 13)
(11, 14)
(10, 15)
1.0:1.0
e
(15, 10)
(14, 11)
(13, 12)
(12, 13)
1.3:1.0
d
(19, 6)
(18, 7)
(17, 8)
(16, 9)
2.2:1.0
c
(20, 5)
(19, 6)
(18, 7)
(17, 8)
3.3:1.0
b
(23, 2)
(22, 3)
(21, 4)
(20, 5)
6.6:1.0
a
(25, 0)
$Ag_{25}(DMBT)_{18}$
4000
5000
6000
7000
8000
m/z



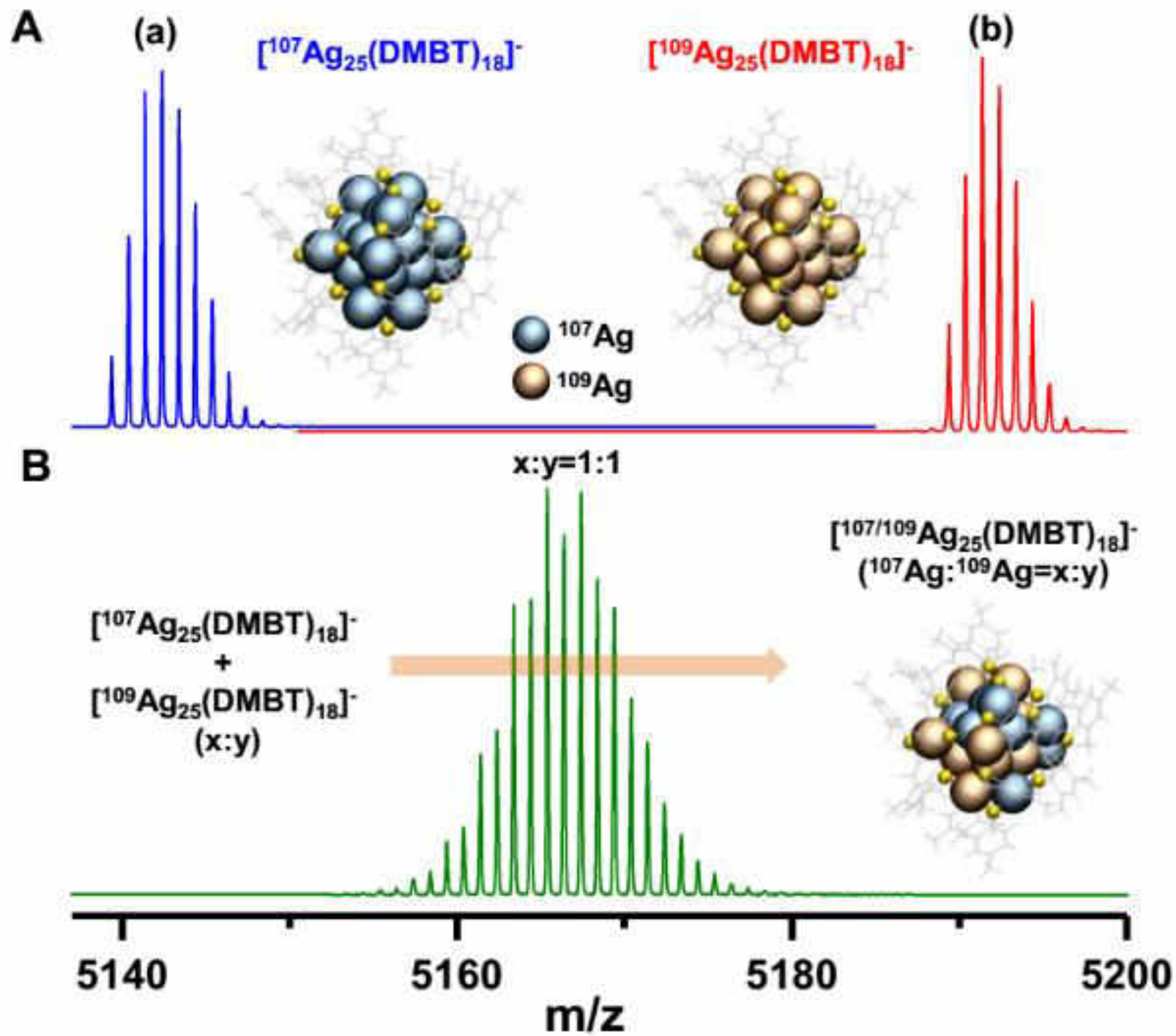
Manfred Kappes, KIT

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

Kinetics of the exchange (monitored on the Ag_{25} side)

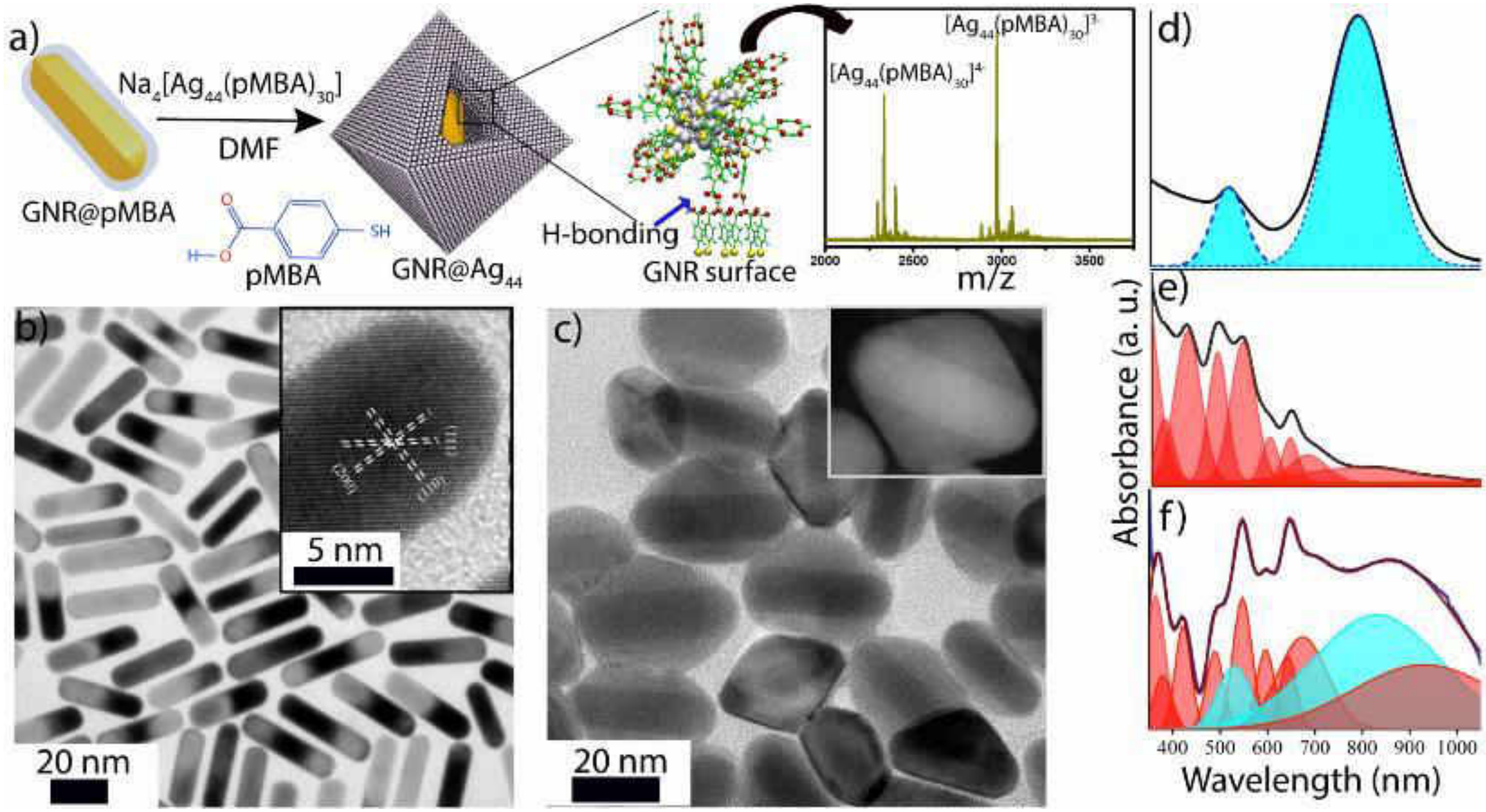


Isotopic exchange

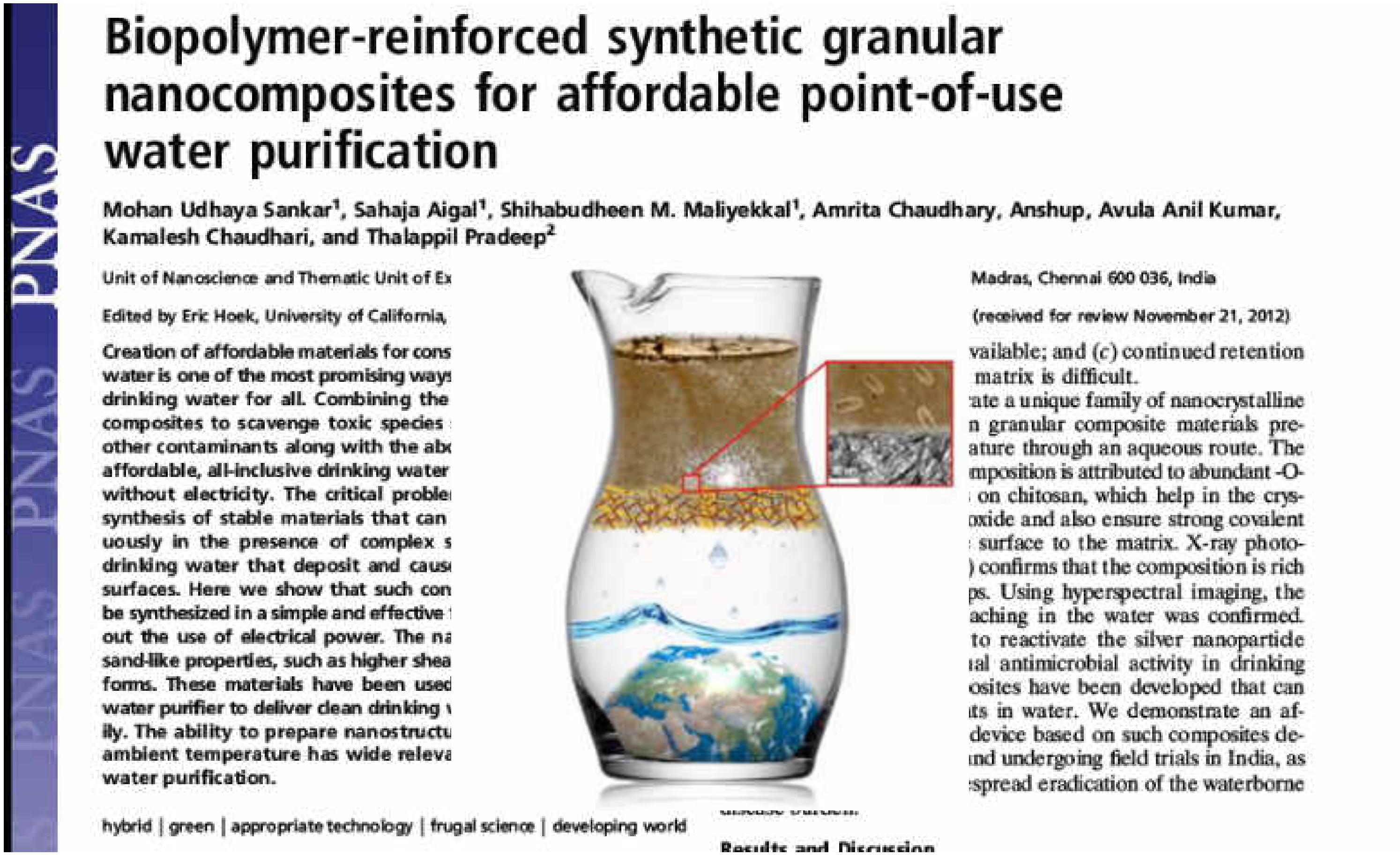


Papri Chakraborti, et. al. Science Advances, 2019.

Atomically precise nanocluster assemblies encapsulating plasmonic gold nanorods



Chakraborty, A. et al., Angew. Chem. Int. Ed. **2018,** 57, 6522–6526.


PNAS PNAS PNAS PNAS

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

Mohan Udhaya Sankar[1], Sahaja Aigal[1], Shihabudheen M. Maliyekkal[1], Amrita Chaudhary, Anshup, Avula Anil Kumar, Kamalesh Chaudhari, and Thalappil Pradeep[2]

Unit of Nanoscience and Thematic Unit of Ex … Madras, Chennai 600 036, India

Edited by Eric Hoek, University of California, … (received for review November 21, 2012)

Creation of affordable materials for cons water is one of the most promising ways drinking water for all. Combining the composites to scavenge toxic species other contaminants along with the ab affordable, all-inclusive drinking water without electricity. The critical proble synthesis of stable materials that can uously in the presence of complex s drinking water that deposit and caus surfaces. Here we show that such con be synthesized in a simple and effective out the use of electrical power. The na sand-like properties, such as higher shea forms. These materials have been used water purifier to deliver clean drinking ily. The ability to prepare nanostructu ambient temperature has wide releva water purification.

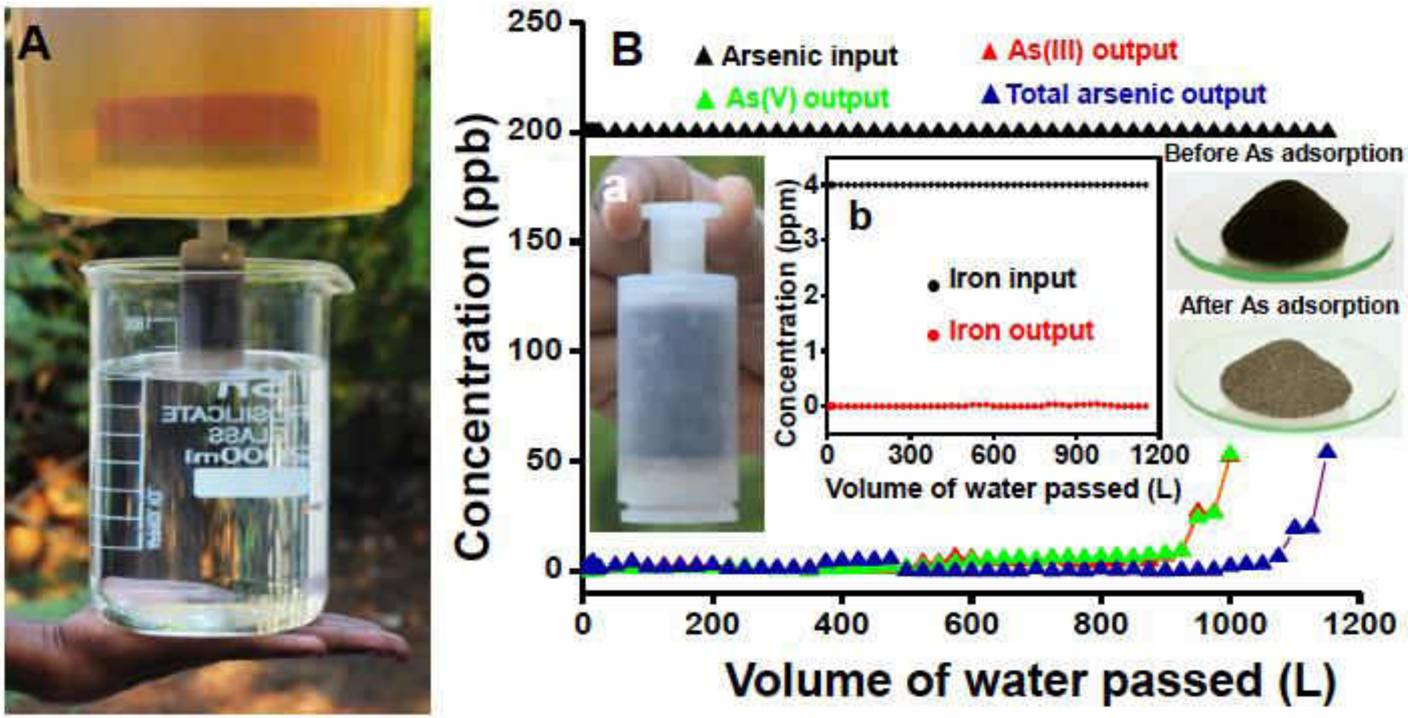
hybrid | green | appropriate technology | frugal science | developing world

vailable; and (*c*) continued retention matrix is difficult. ate a unique family of nanocrystalline n granular composite materials pre- ature through an aqueous route. The mposition is attributed to abundant -O- on chitosan, which help in the crys- oxide and also ensure strong covalent surface to the matrix. X-ray photo-) confirms that the composition is rich ps. Using hyperspectral imaging, the aching in the water was confirmed. to reactivate the silver nanoparticle ial antimicrobial activity in drinking osites have been developed that can its in water. We demonstrate an af- device based on such composites de- and undergoing field trials in India, as spread eradication of the waterborne

Results and Discussion

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

Range of materials, their affordability and safety



Safety of spent media, TCLP

A. Anil Kumar, et. al. *Adv. Mater.*, 29 (2016) 1604260.

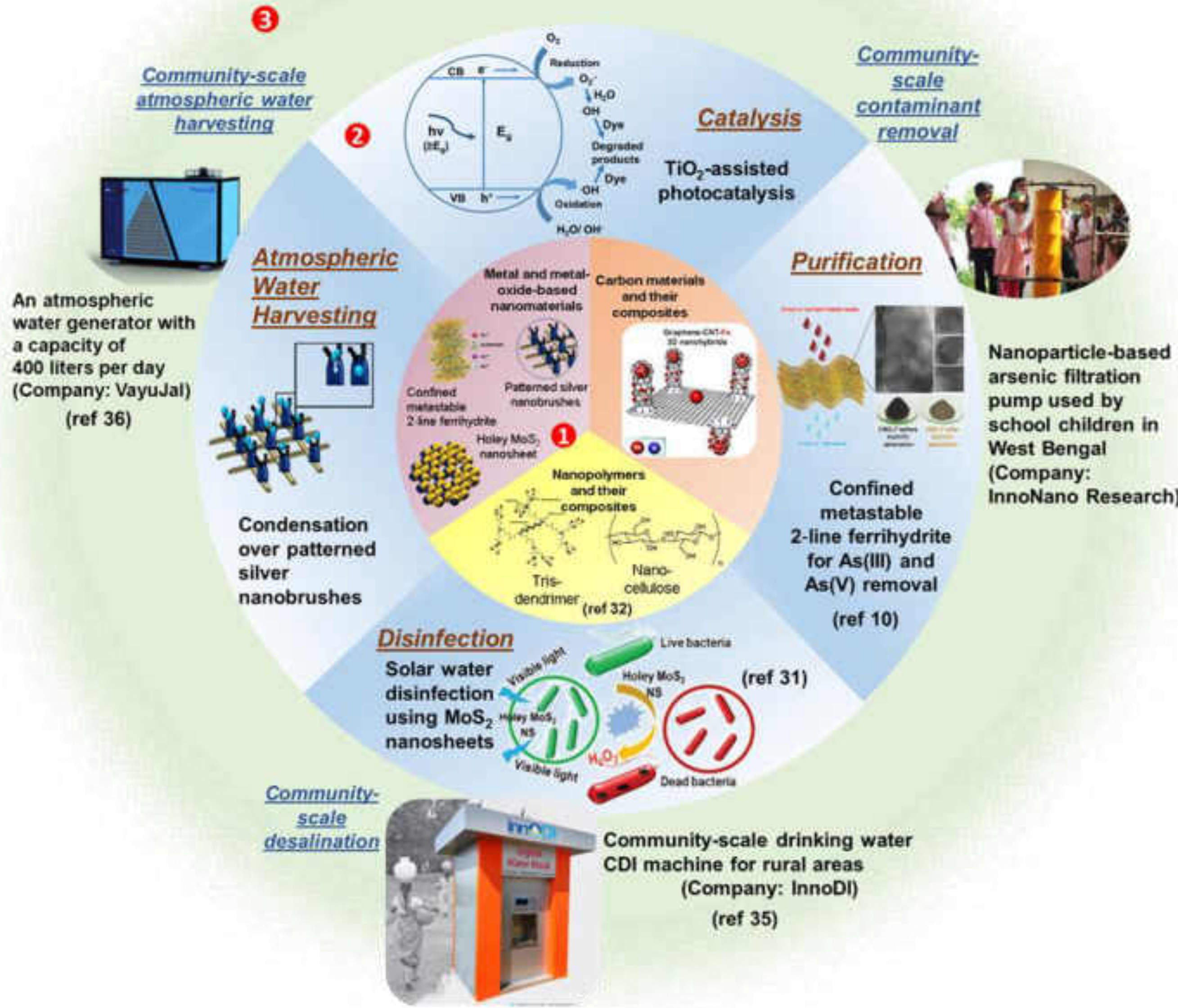
Clean water for everyone

ACS Sustainable Chemistry & Engineering Editorial, December 2016

We developed environmentally friendly water positive nanoscale materials for affordable, sustainable and rapid removal of arsenic from drinking water.

There are over 1700 community installations across the country, serving 1.3 million people with arsenic and iron-free water every day.

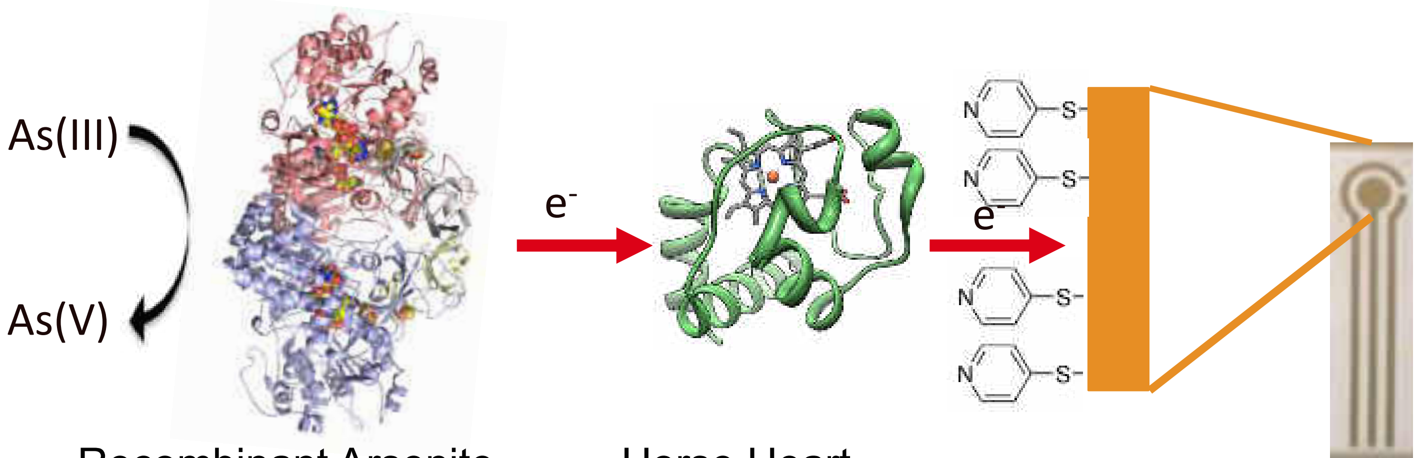
Evolution of materials to products



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

Biosensor Design

1st Generation Design (Mediated Electrochemistry)



Buffer: pH 7-8

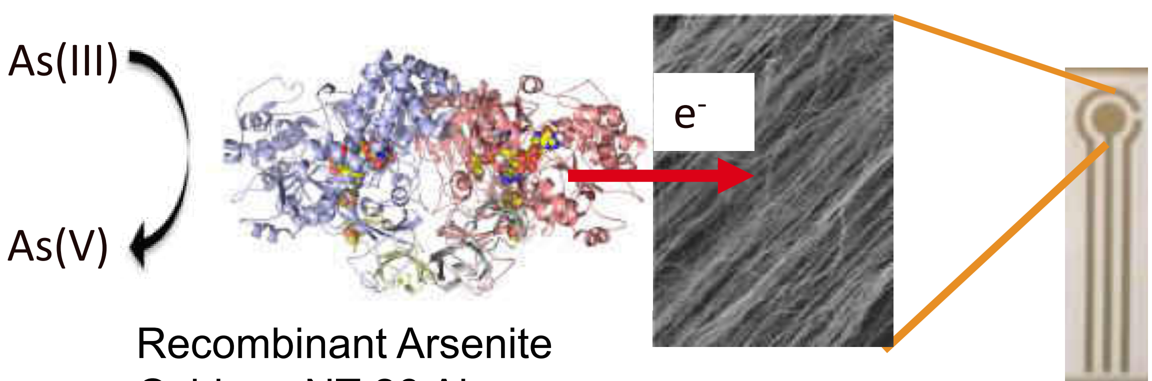
Recombinant Arsenite Oxidase NT-26 Aio

Horse Heart Cytochrome C

Aldrithiol

Low-cost Gold sputtered thin film on PET substrate

2nd Generation Design (Direct Electron Transfer)

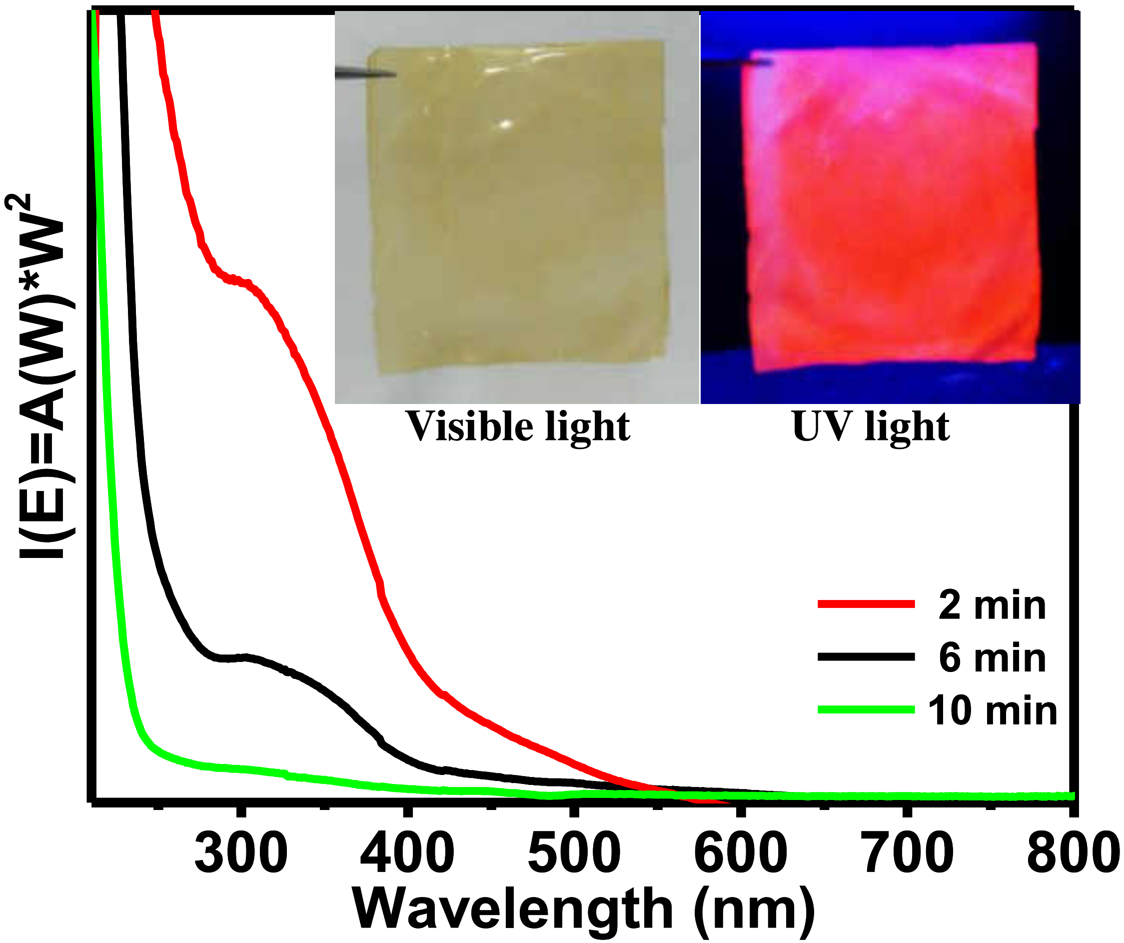


Recombinant Arsenite Oxidase NT-26 Aio

low-cost nanostructured electrodes which interact directly with enzyme (e.g. graphene or CNT).

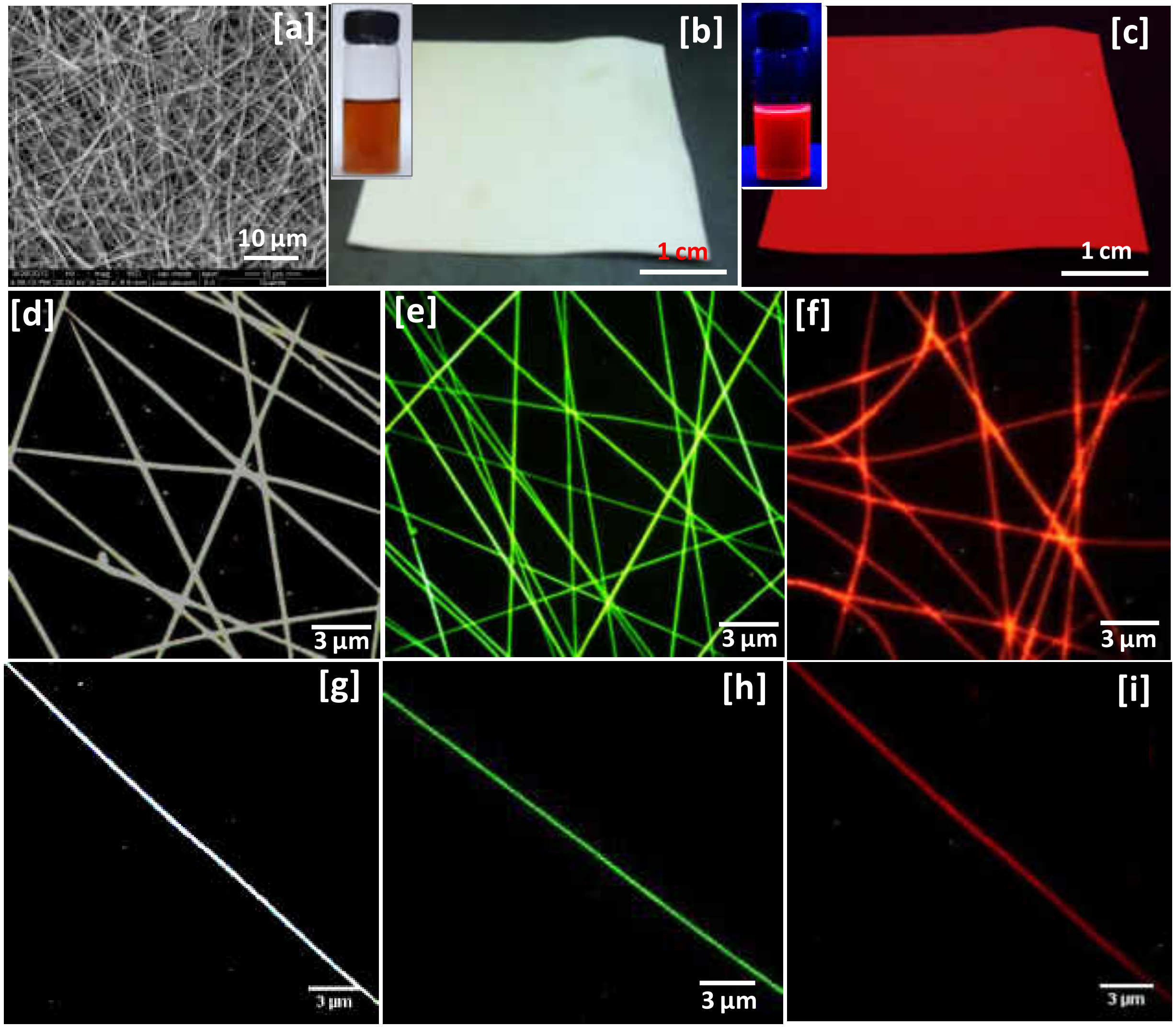
Bio-nano Consulting & Imperial College, London

Cluster-based metal ion sensing



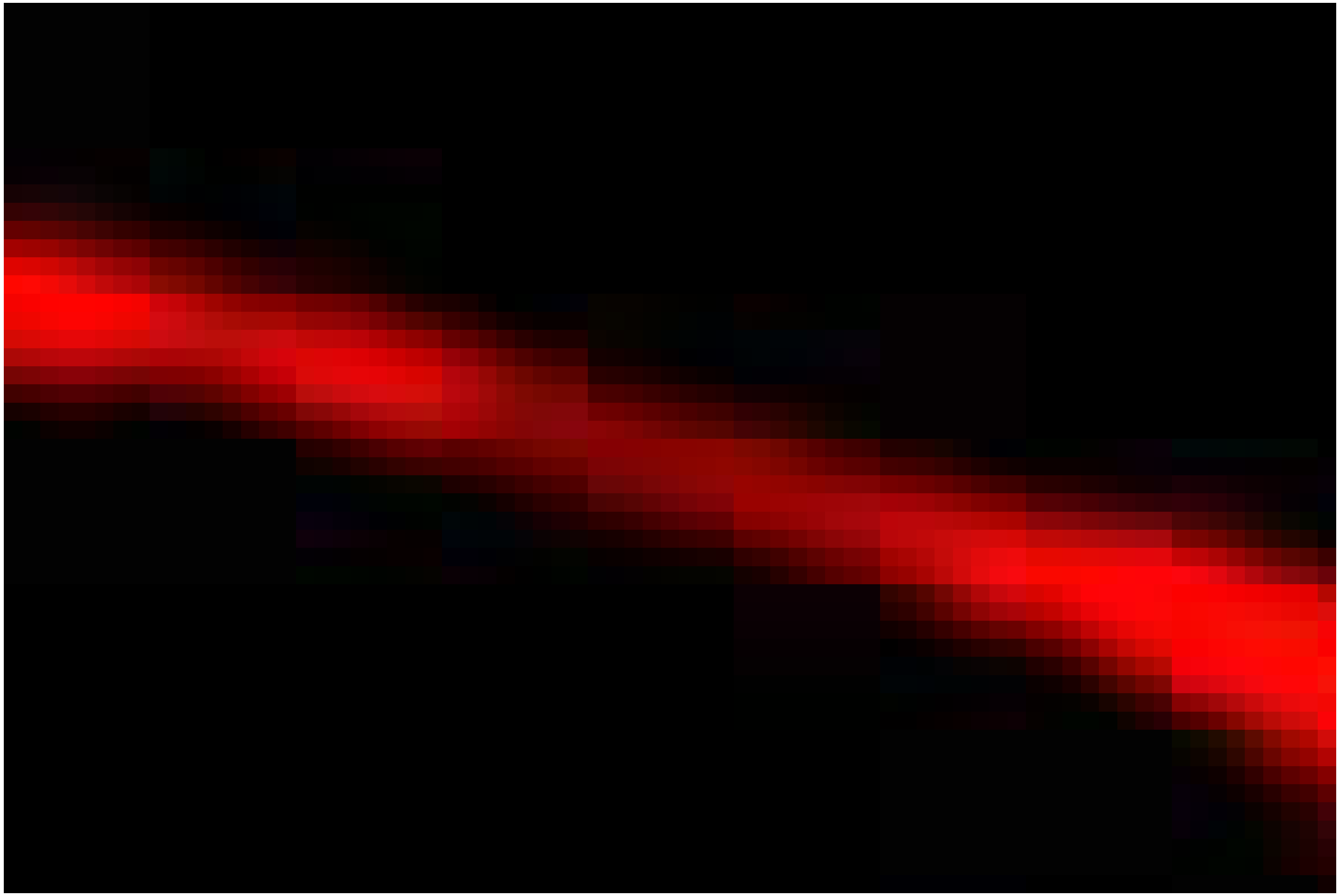
Decrease in the absorption of Au_{15} as a biofilm is dipped into the cluster solution. Inset: Free standing quantum cluster loaded film in visible light and UV light.

Approaching detection limits of tens of Hg^{2+}

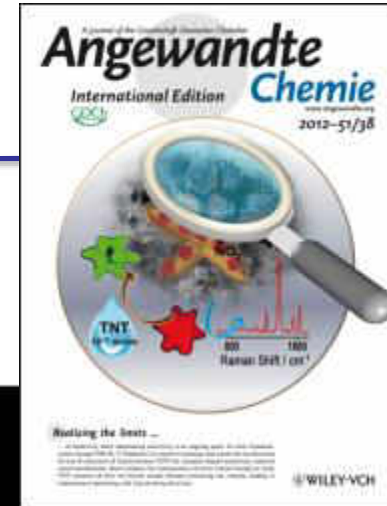


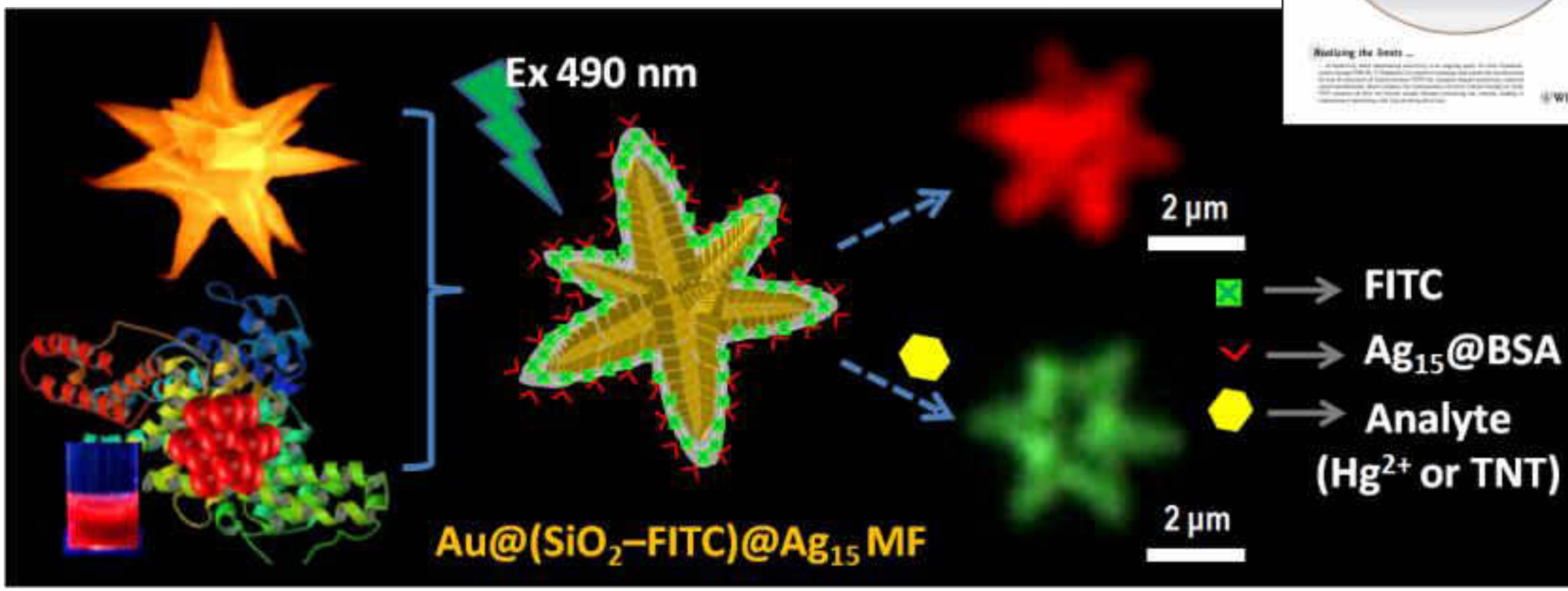
Atanu Ghosh et al. Anal. Chem. 2014.

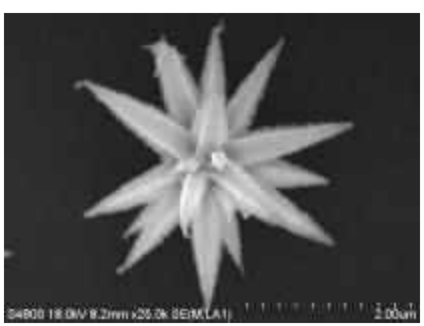
Mercury quenching experiment using nanofiber



Sub-zeptomolar detection



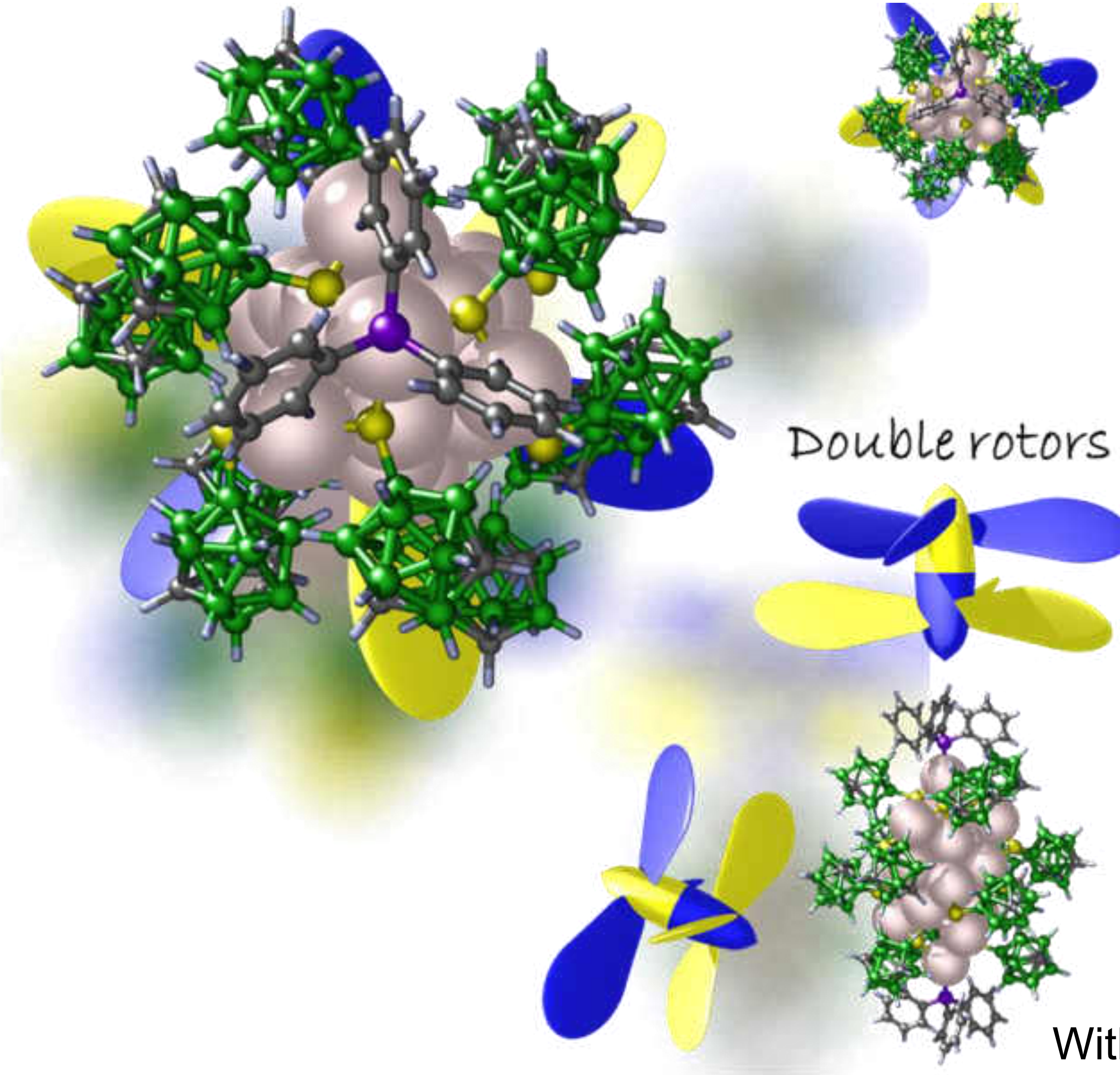




Featured in:
The Hindu, Telegraph, Times of India, etc.
C&E News
and many others

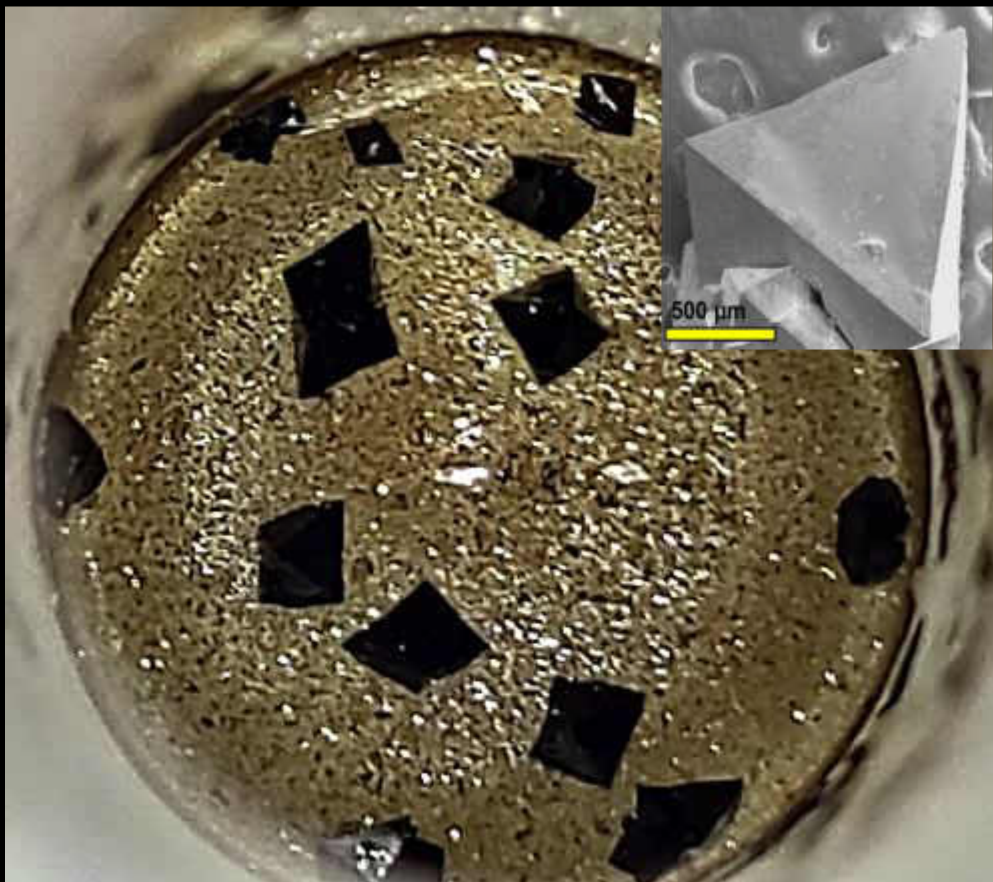
Ammu Mathew, et al. Angew. Chem. Int. Ed. 2012

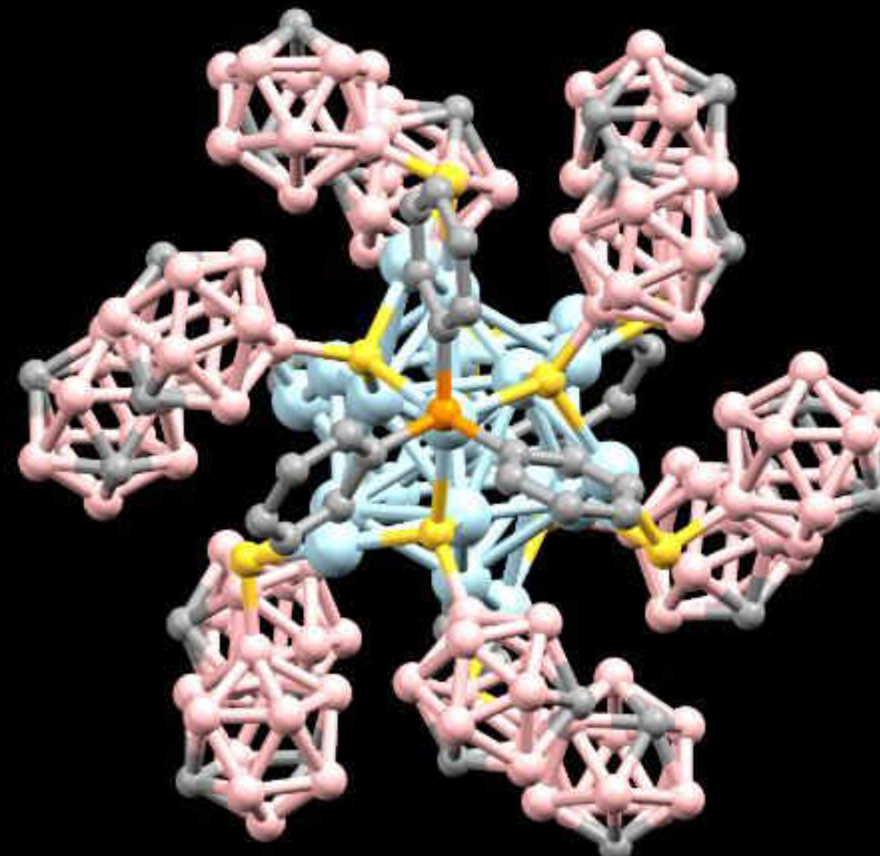
Carborane-thiol protected silver nanomolecule



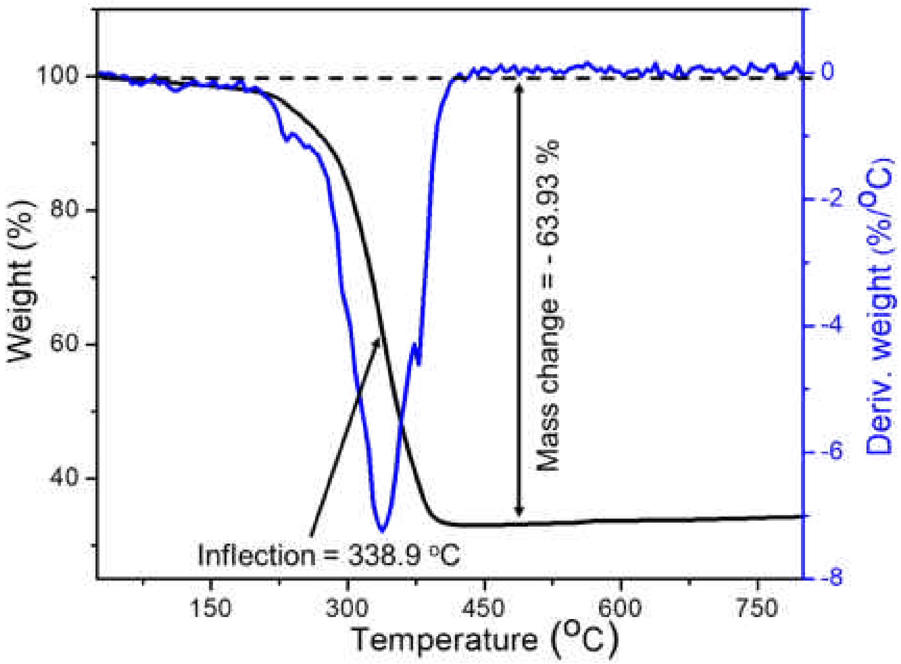
With Tomas Base

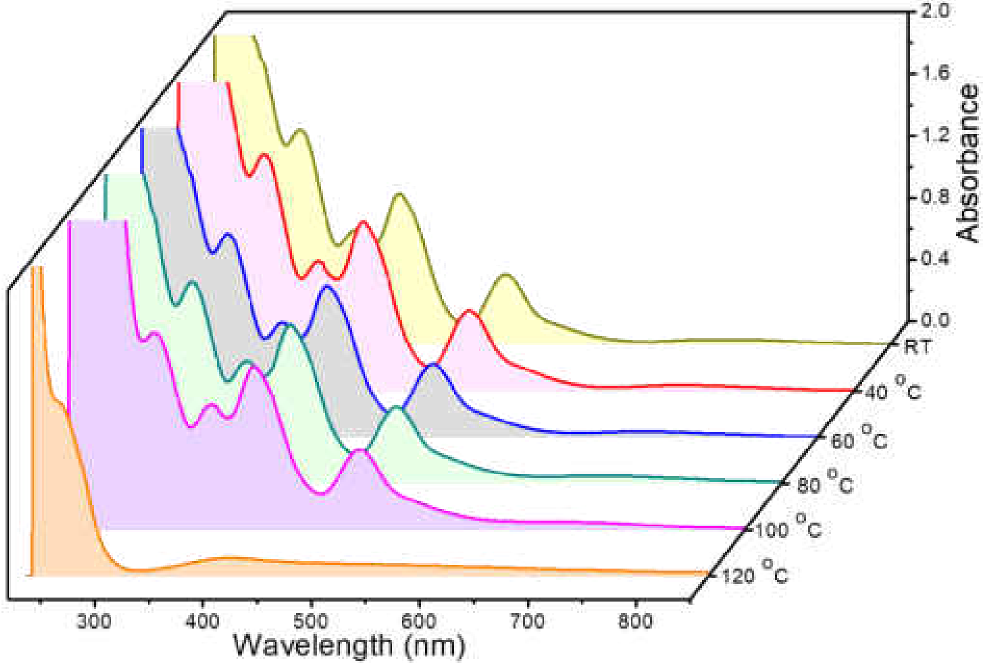
Jana *et. al*, Inorganic Chemistry (2022)


500 µm

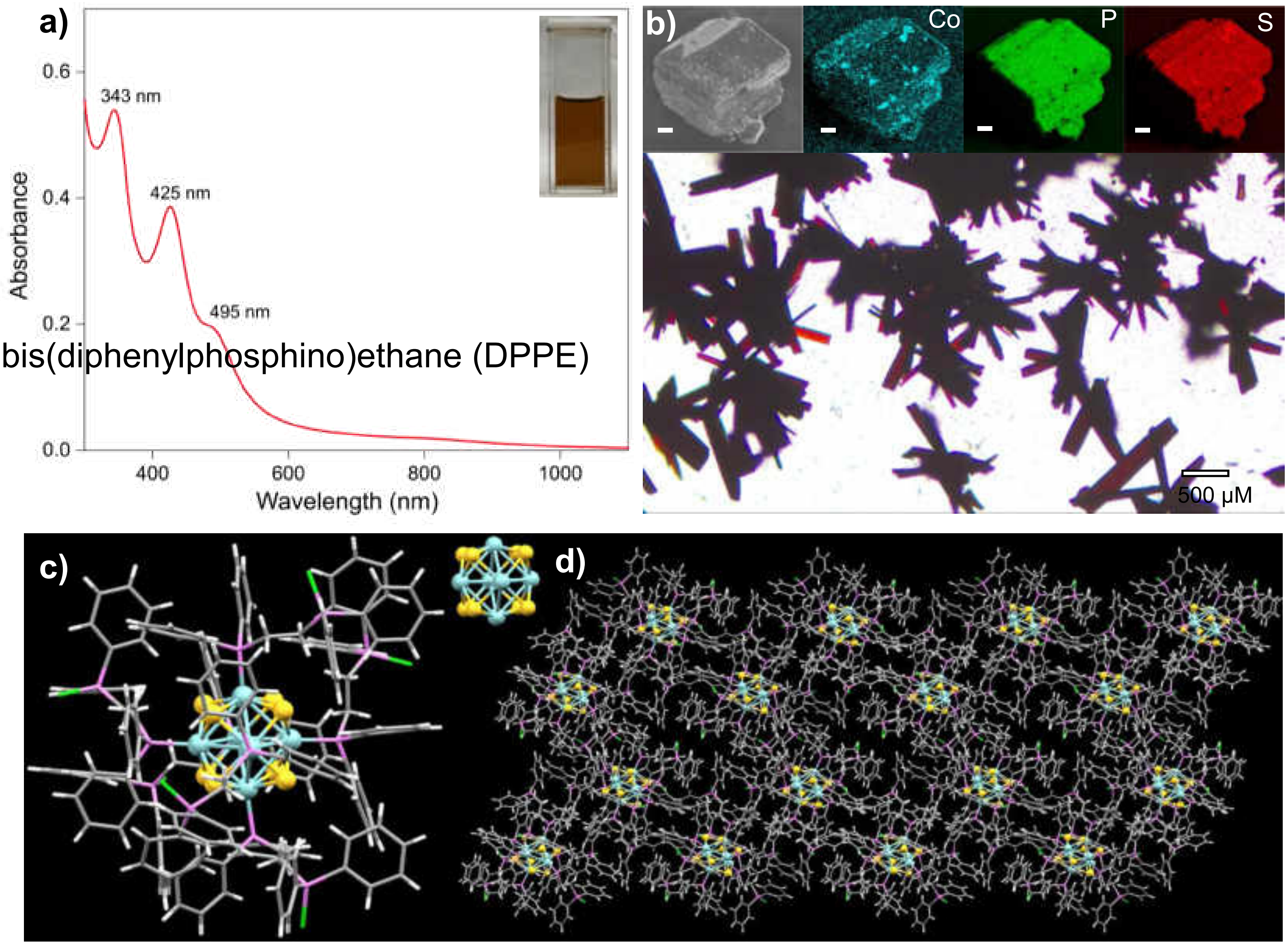


Thermal stability

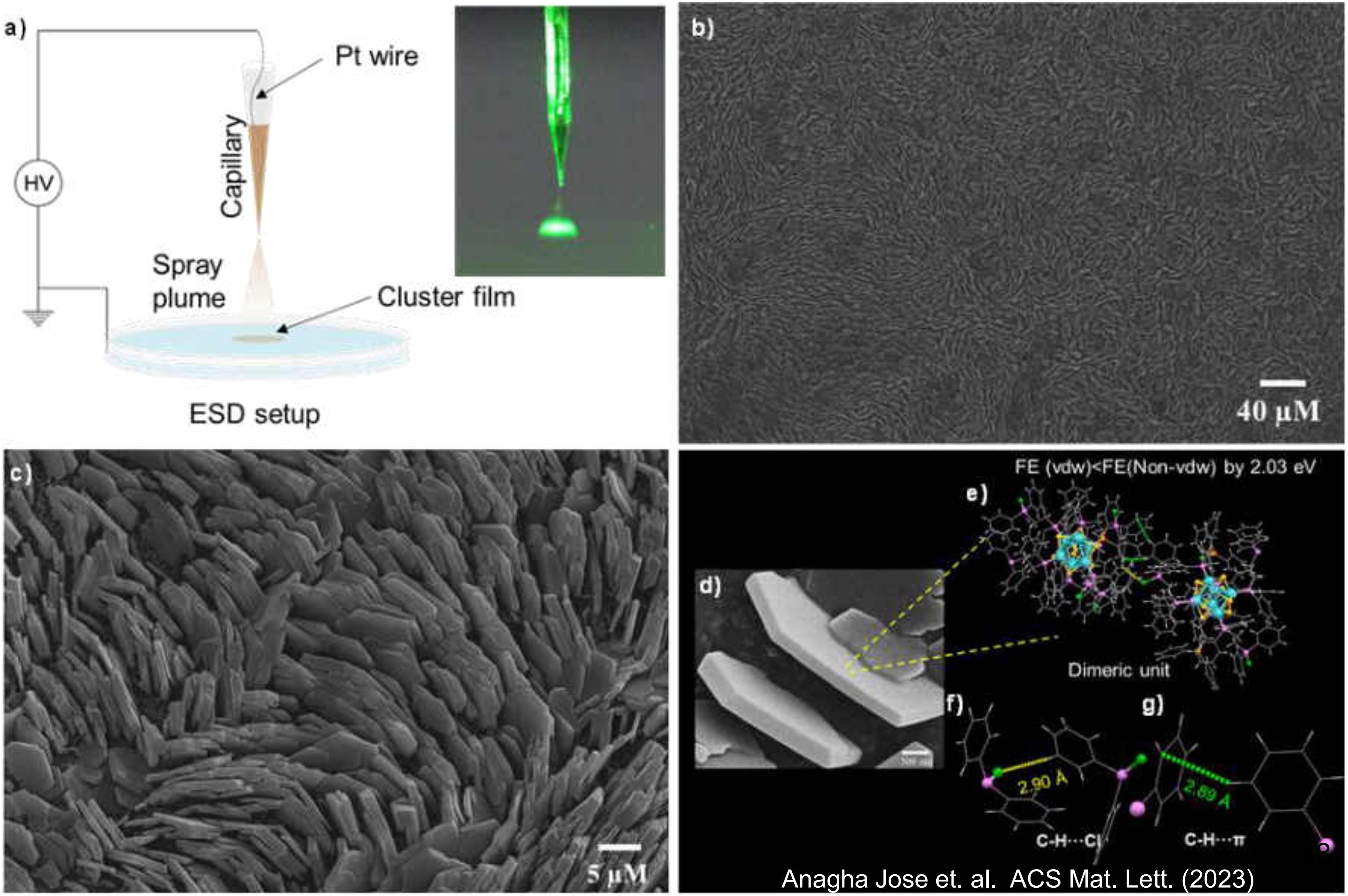




New electrodes - Aligned nanoplates of Co_6S_8

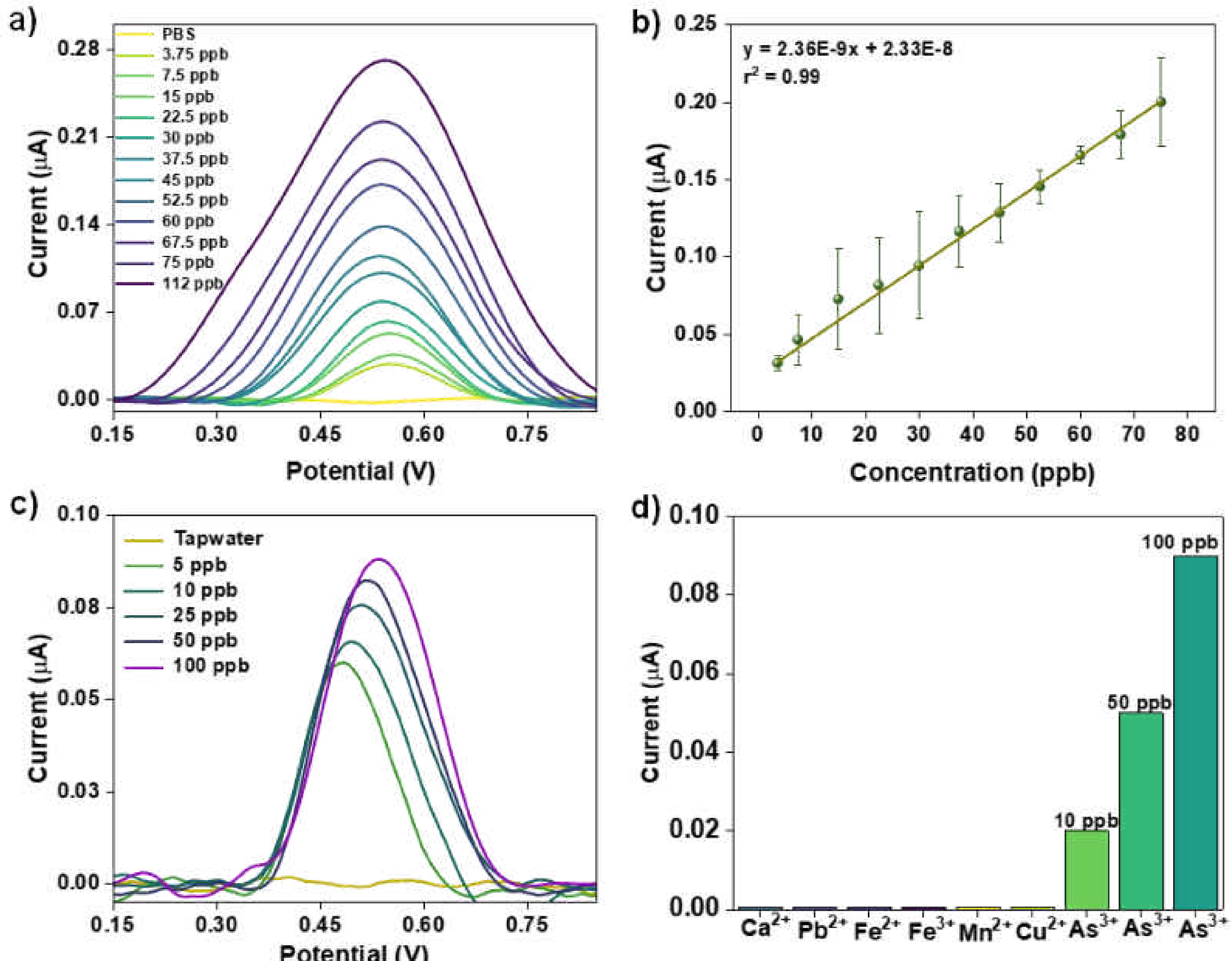


Electrospray deposition



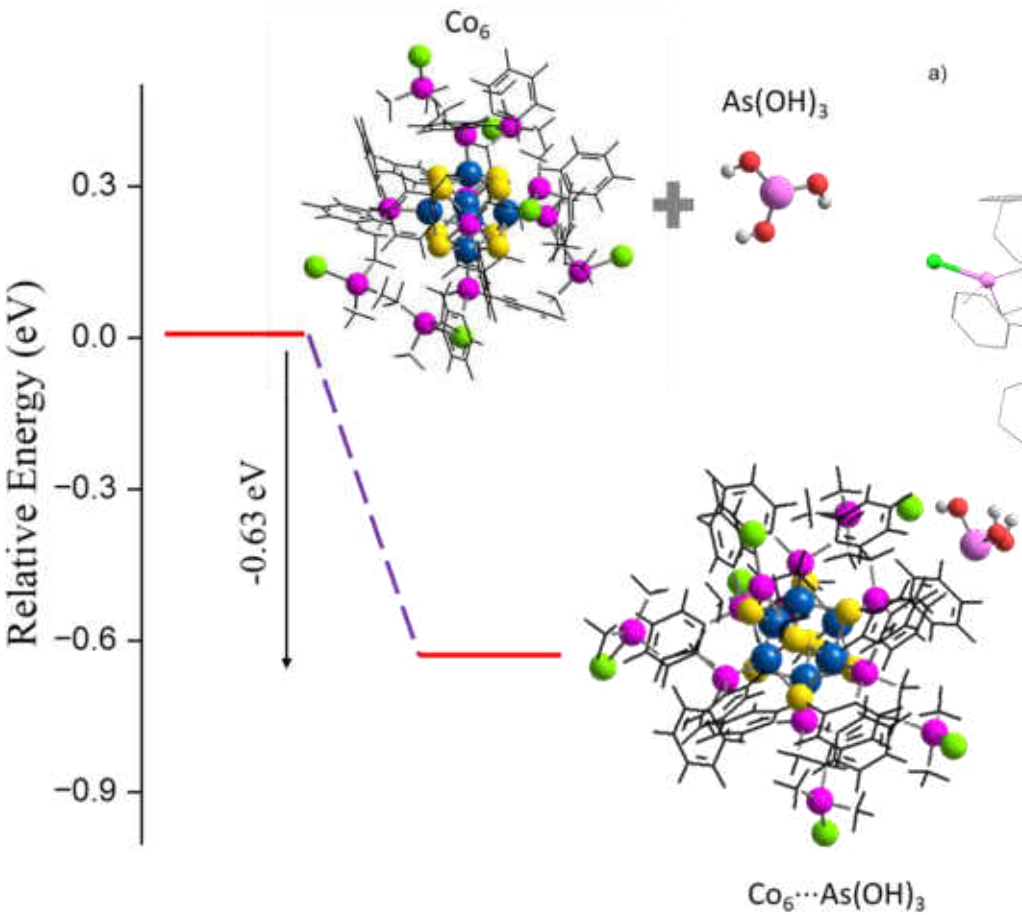
Anagha Jose et. al. ACS Mat. Lett. (2023)

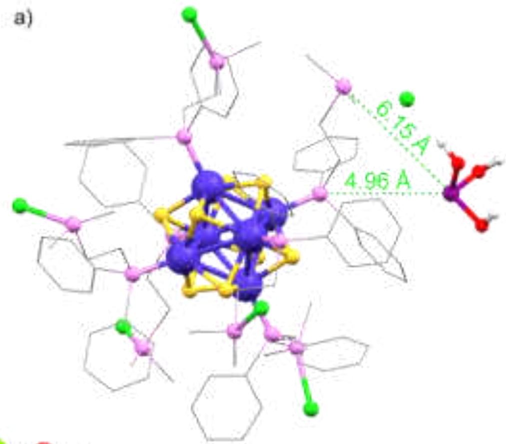
Sensing

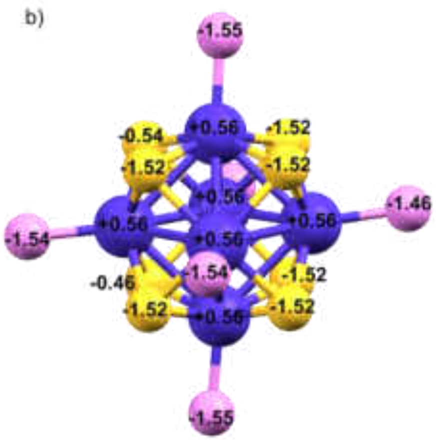


a)
PBS
3.75 ppb
7.5 ppb
15 ppb
22.5 ppb
30 ppb
37.5 ppb
45 ppb
52.5 ppb
60 ppb
67.5 ppb
75 ppb
112 ppb
Current (μA)
Potential (V)
b)
y = 2.36E-9x + 2.33E-8
r² = 0.99
Current (μA)
Concentration (ppb)
c)
Tapwater
5 ppb
10 ppb
25 ppb
50 ppb
100 ppb
Current (μA)
Potential (V)
d)
100 ppb
50 ppb
10 ppb
Current (μA)
Ca²⁺ Pb²⁺ Fe²⁺ Fe³⁺ Mn²⁺ Cu²⁺ As³⁺ As³⁺ As³⁺

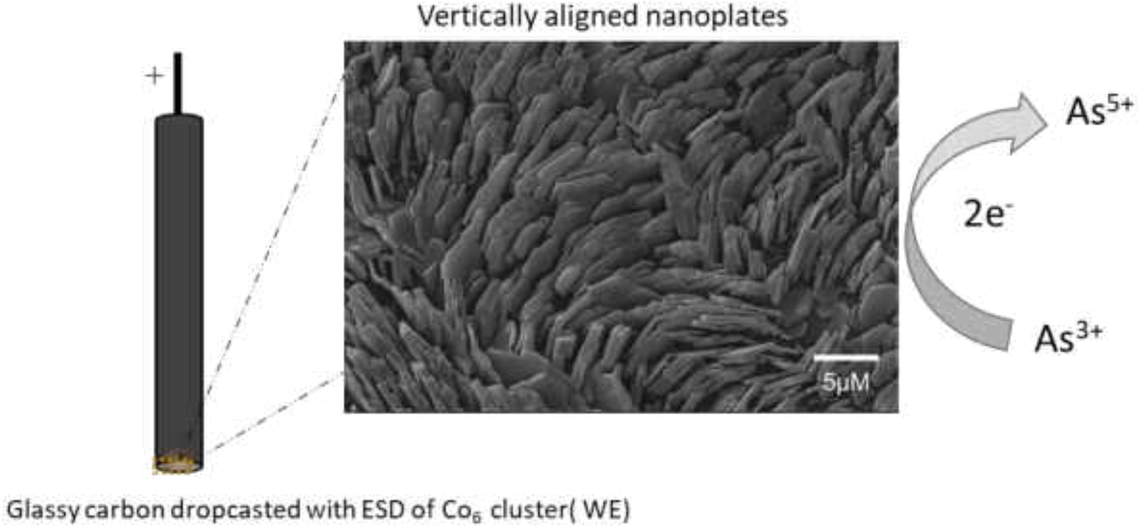
Computational insights

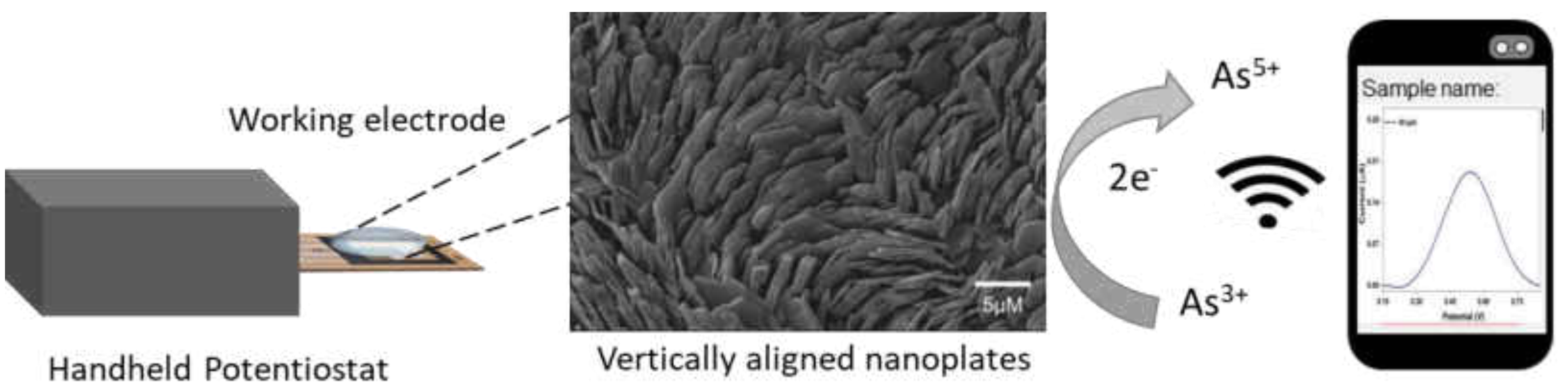




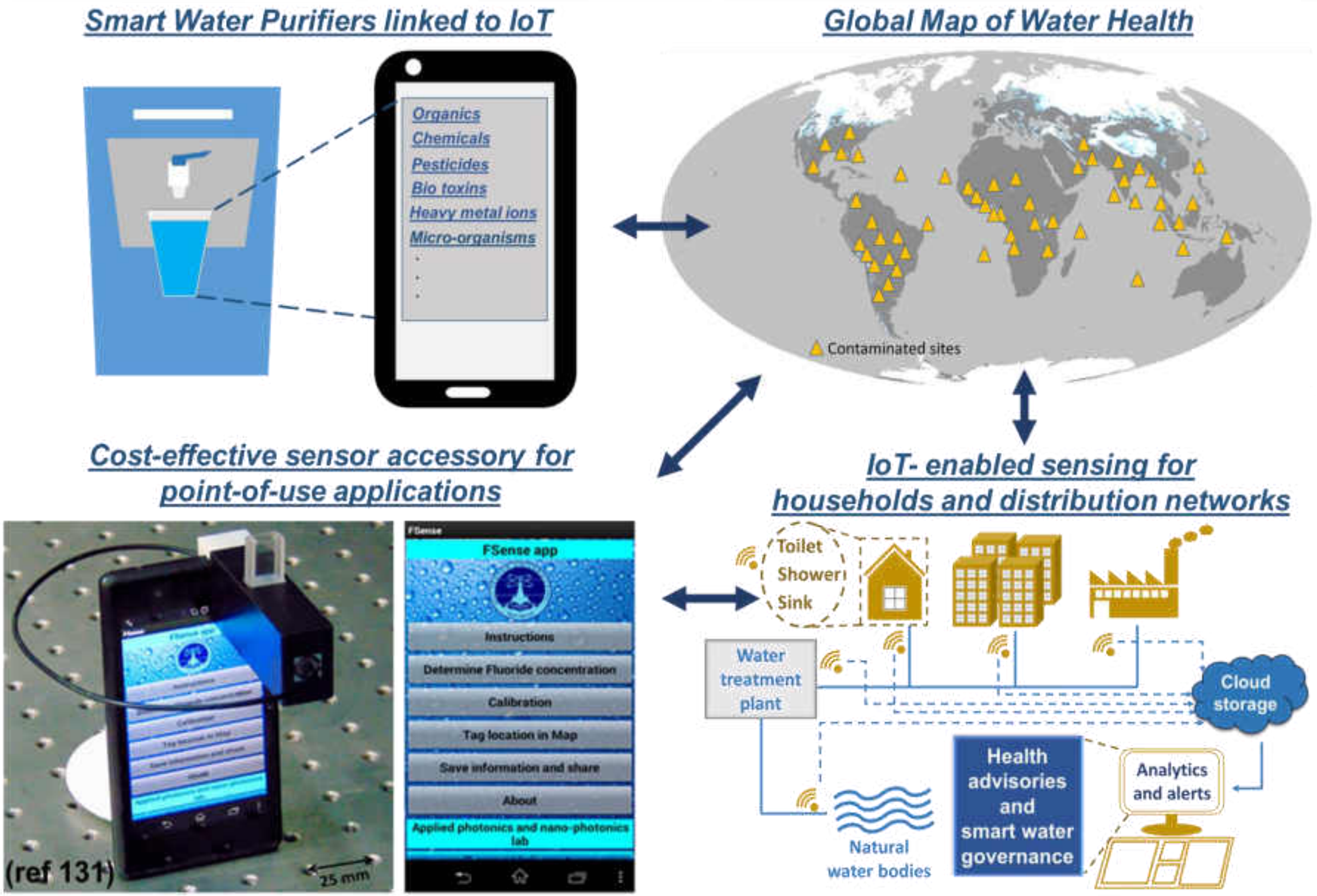


Working electrode





Smart water purifiers and big data



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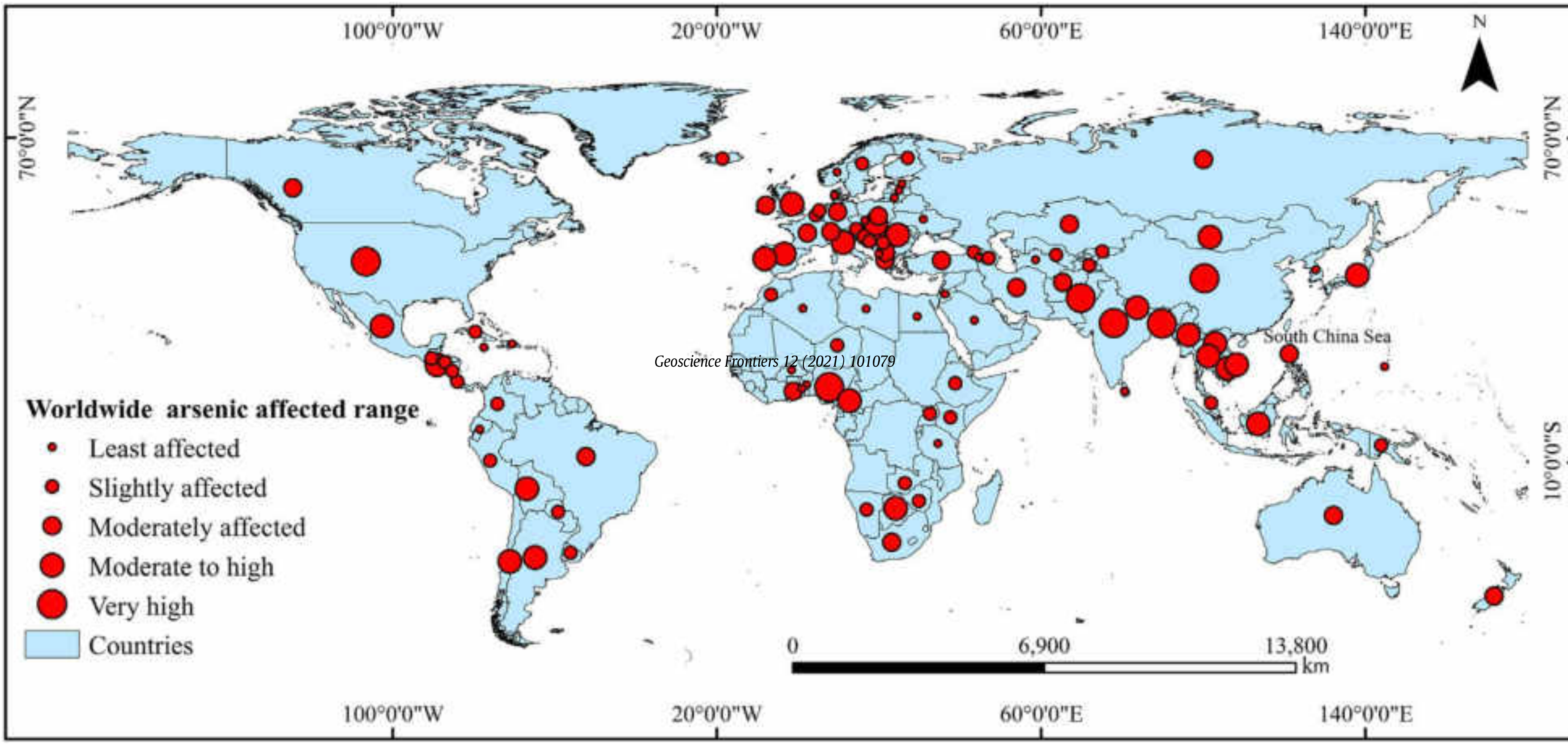
Arsenic poisoning across the world



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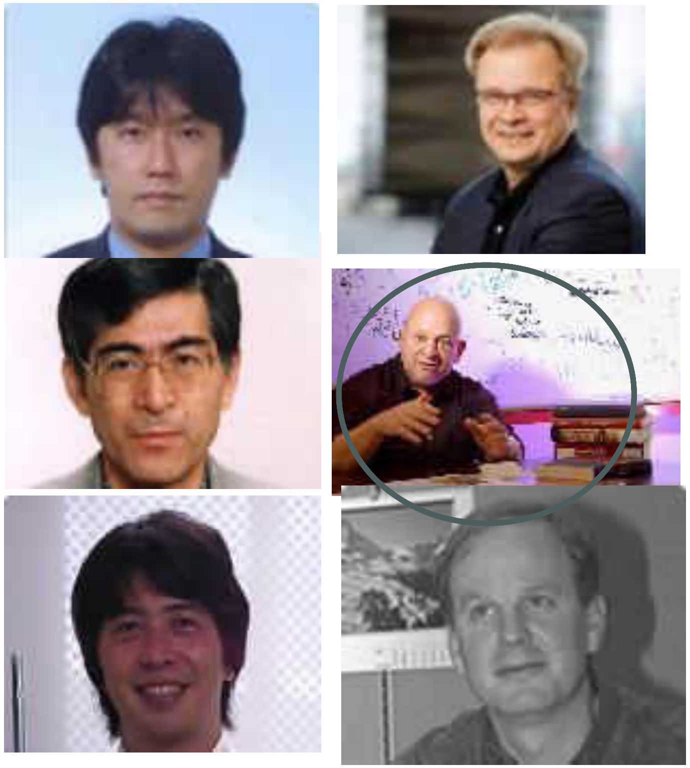
Collaborators



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Thank you all