



Since 1959

Atomically Precise Clusters

T. Pradeep

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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-in-charge

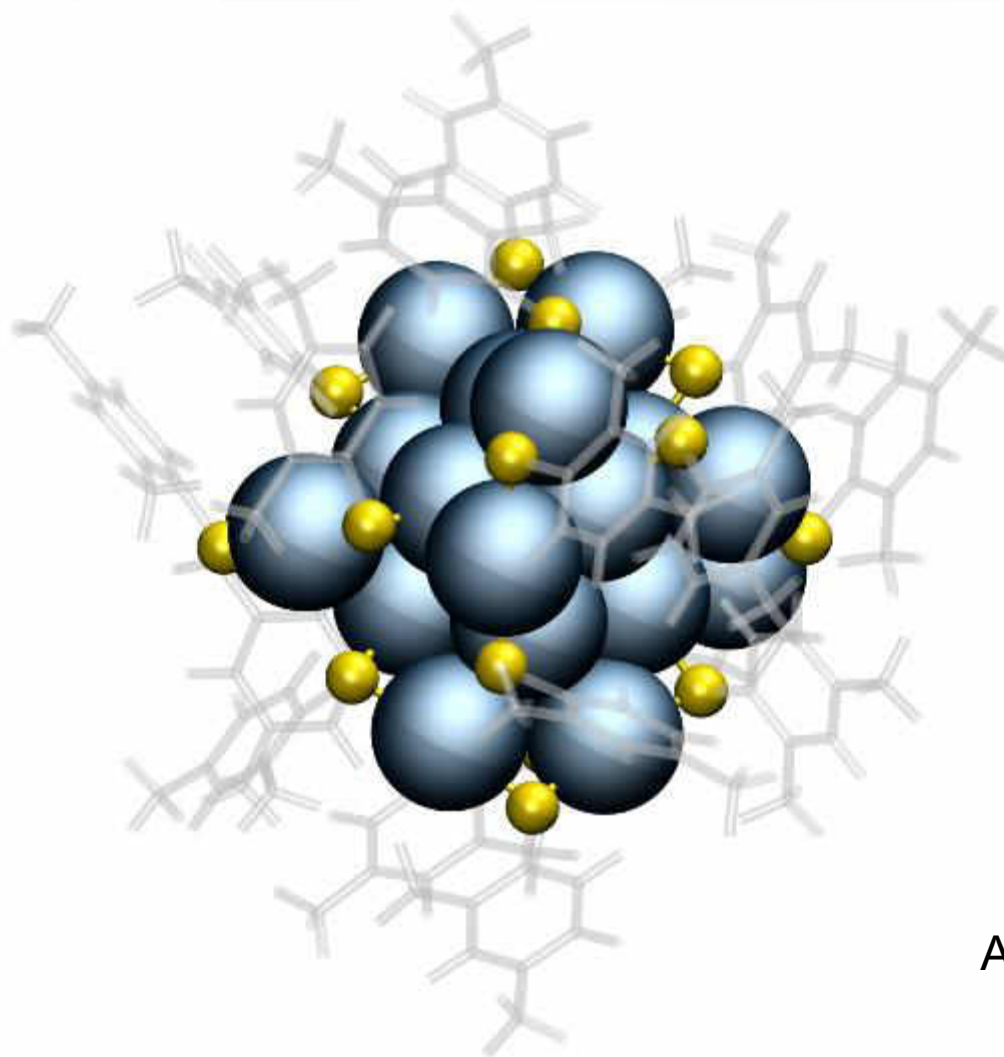


International Centre for Clean Water

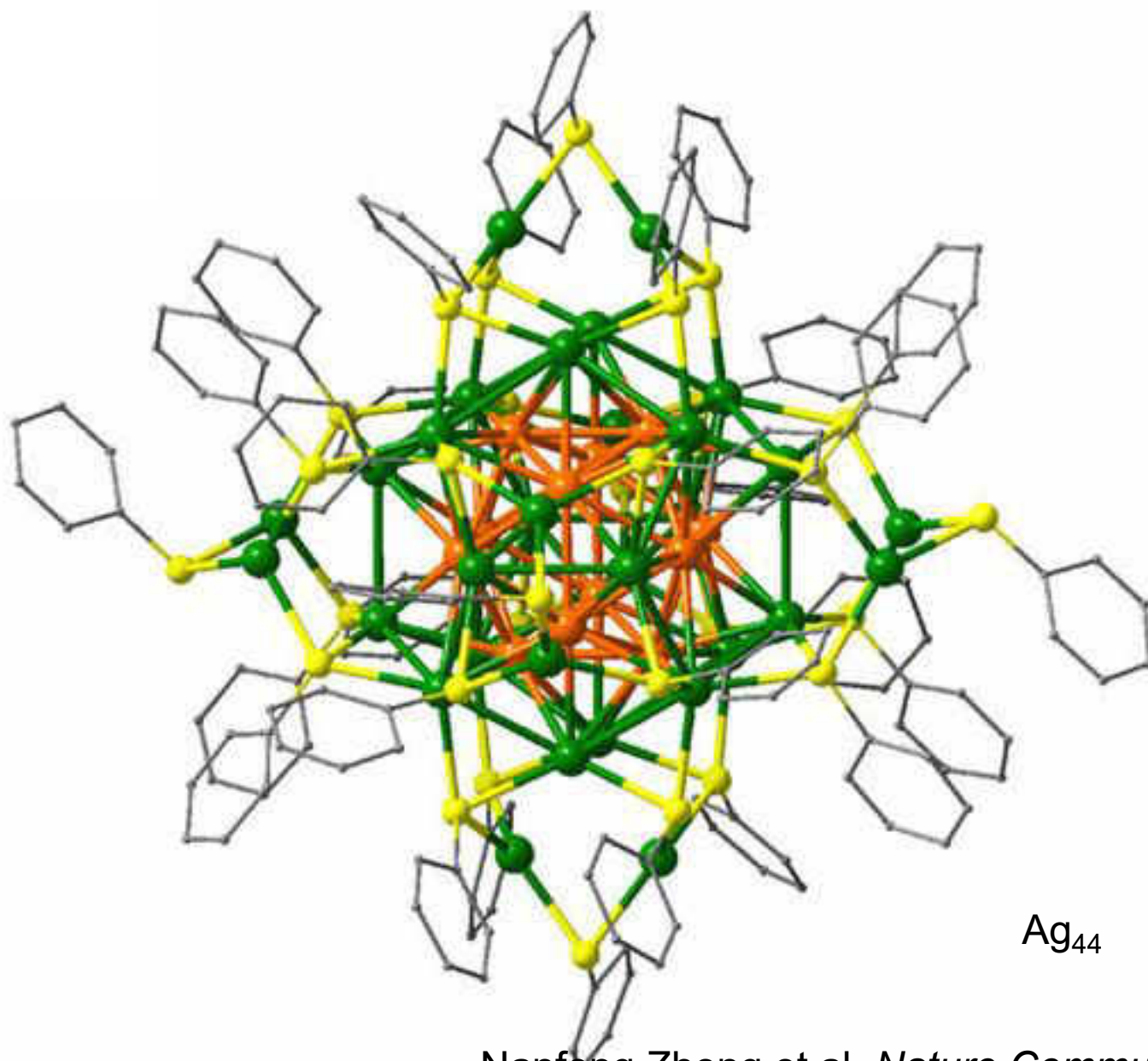


Rasayan 18, Christ University, Bengaluru, January 29-30, 2024

New molecules



$\text{Au}_{25}, \text{Ag}_{25}, \text{Ag}_{29}$

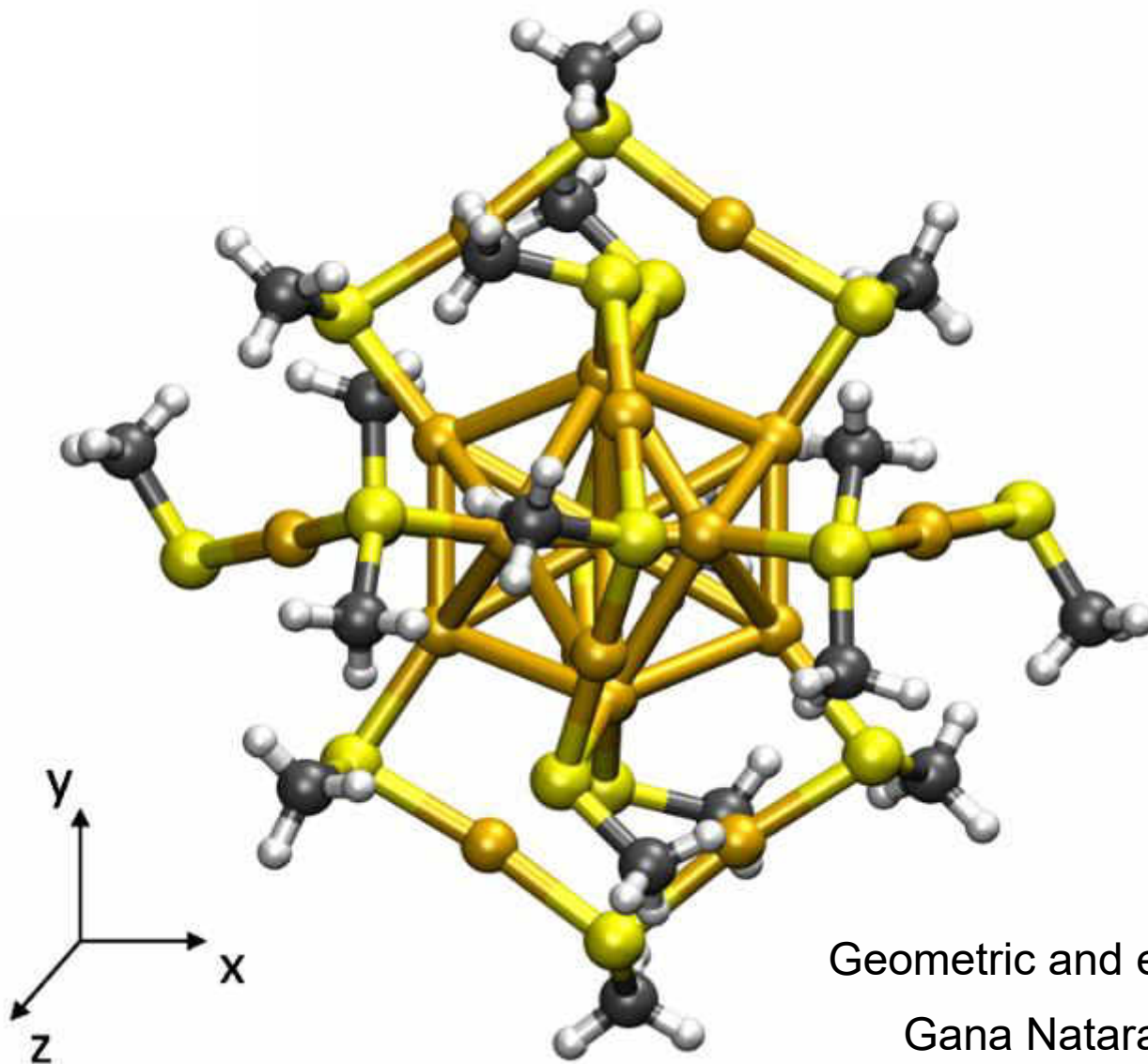


Nanfeng Zheng et al. *Nature Communications*, 2013
Terry Bigioni et al. *Nature* 2013

They make high quality crystals

50 μm

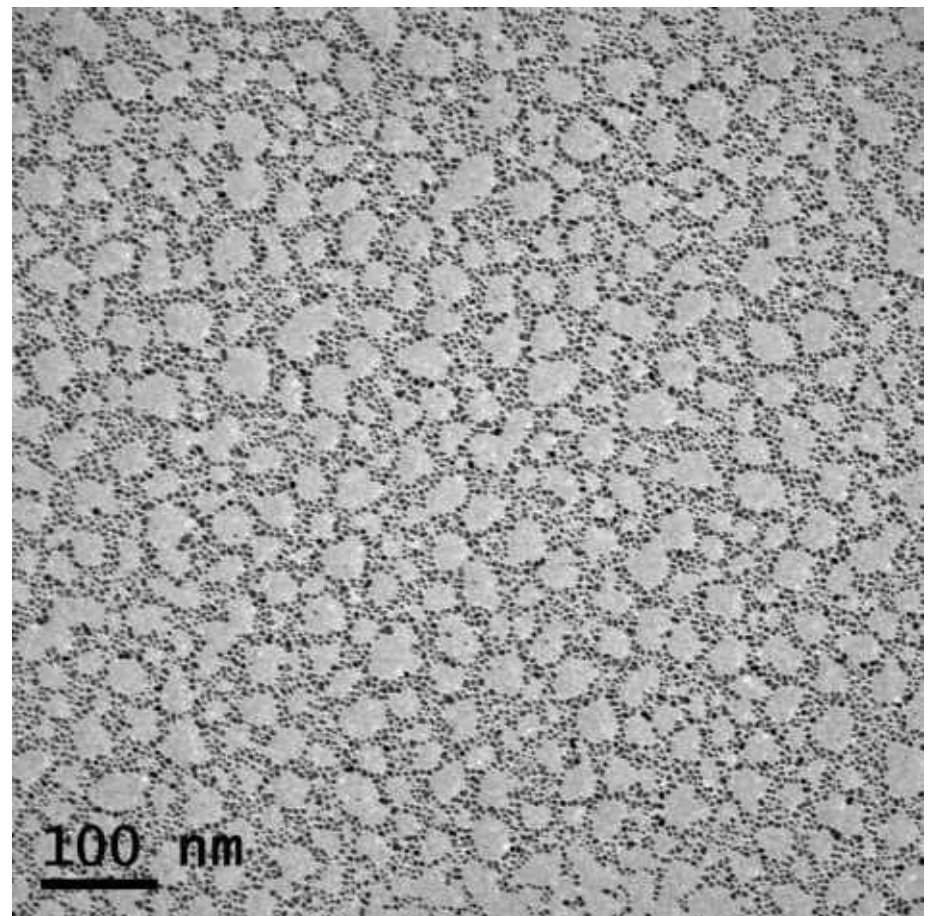
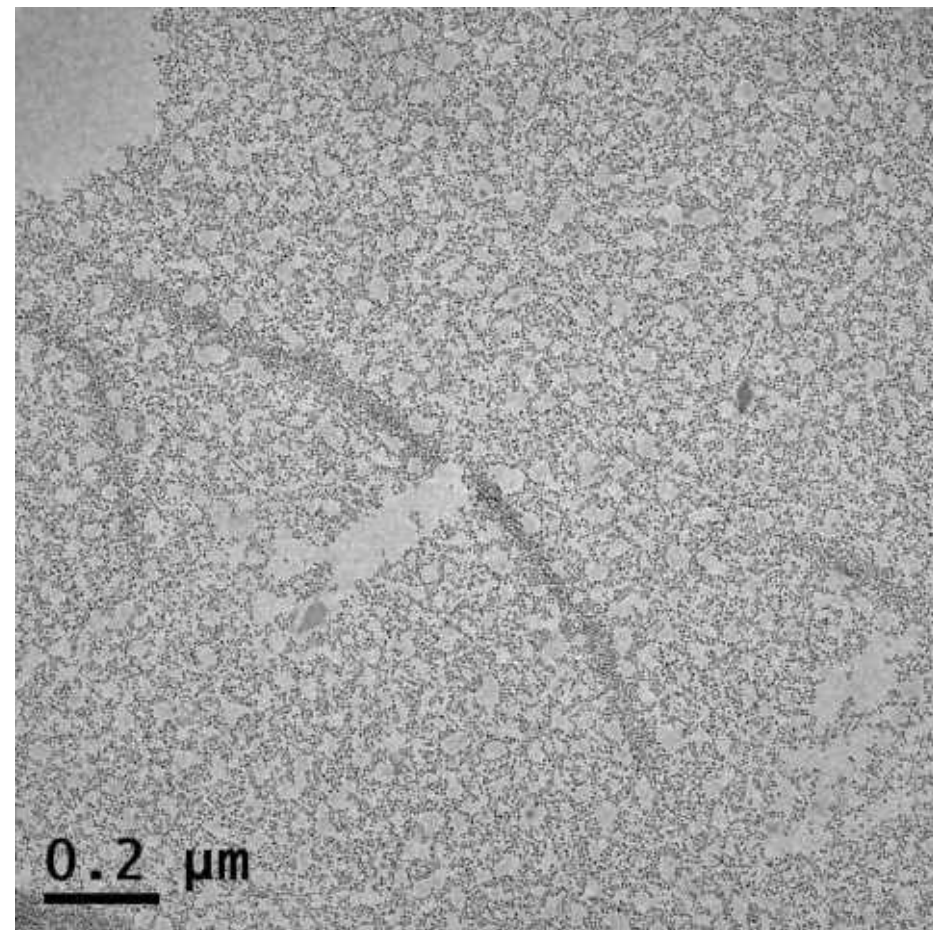
Molecular structure



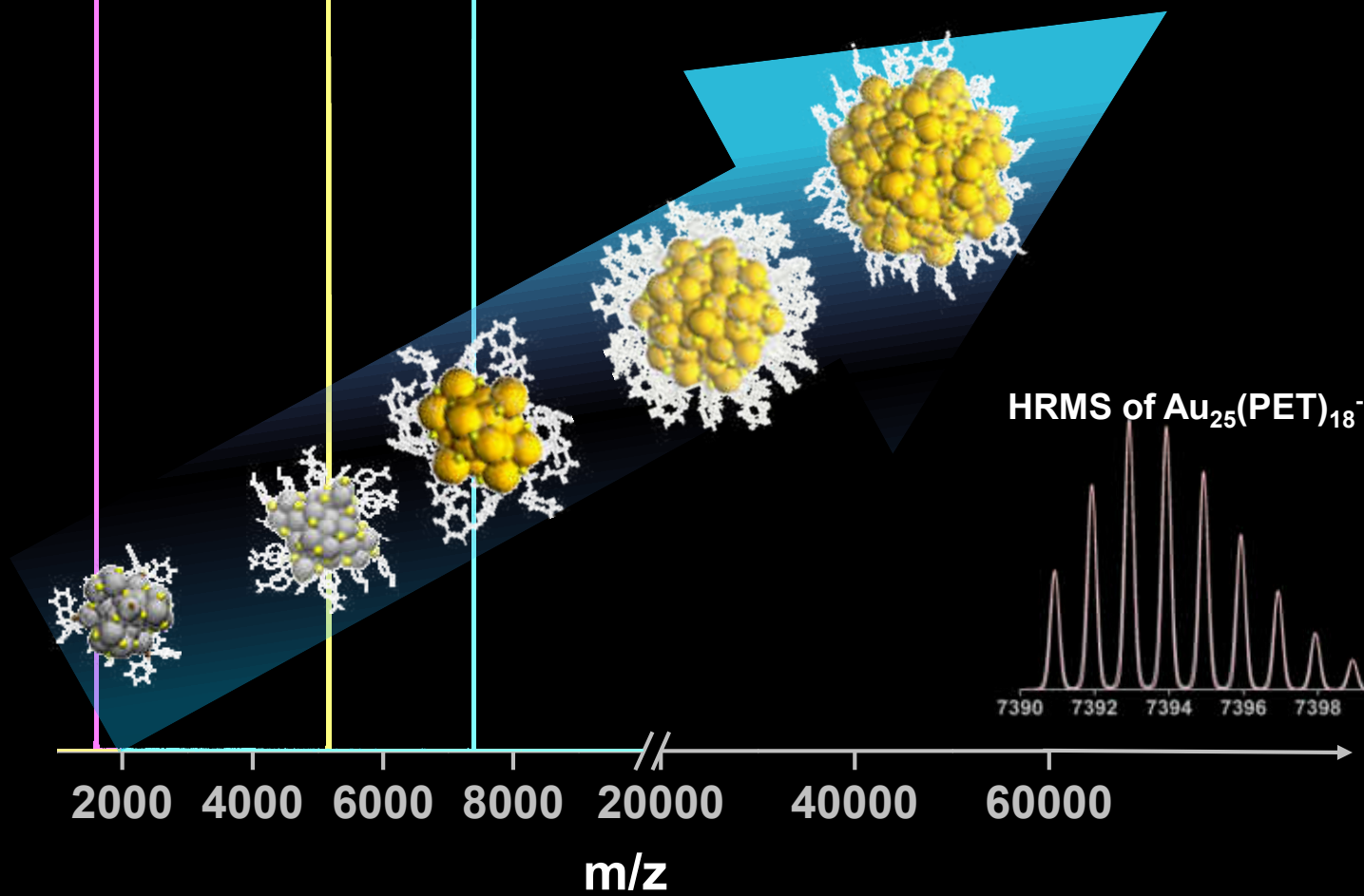
Geometric and electronic shells

Gana Natarajan

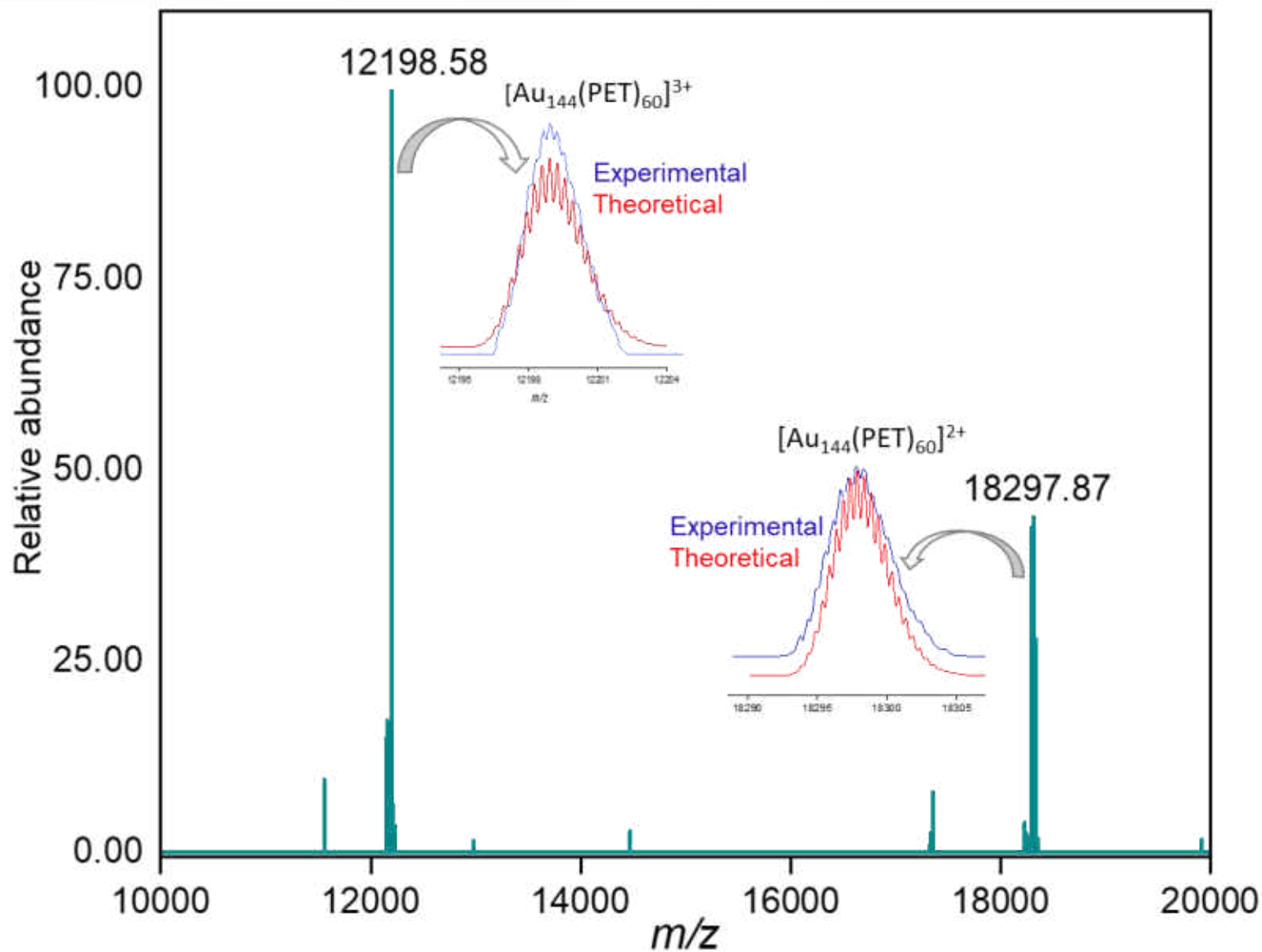
TEM images of Au₂₅ and Au₁₄₄



$\text{Ag}_{29}(\text{BDT})_{12}^{3-}$ $\text{Ag}_{25}(\text{DMBT})_{18}^{-}$ $\text{Au}_{25}(\text{PET})_{18}^{-}$



$\text{Au}_{144}(\text{PET})_{60}$



Molecular materials

ACCOUNTS

of chemical research

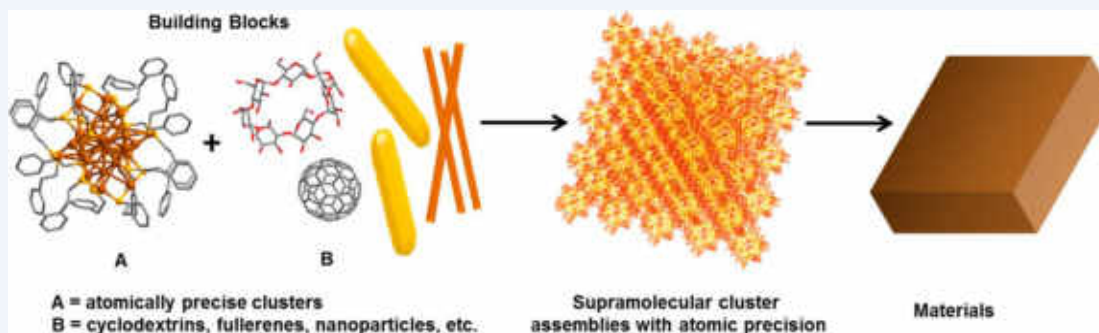
Article

pubs.acs.org/accounts

Approaching Materials with Atomic Precision Using Supramolecular Cluster Assemblies

Papri Chakraborty, Abhijit Nag, Amrita Chakraborty, and Thalappil Pradeep^{*ID}

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 ₂ O
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 emission

Molecular reactions

Molecular assembly

Molecular co-crystals

Ionization potential

Electron affinity

Phases - phase transitions

Physical properties

Electrical, magnetic

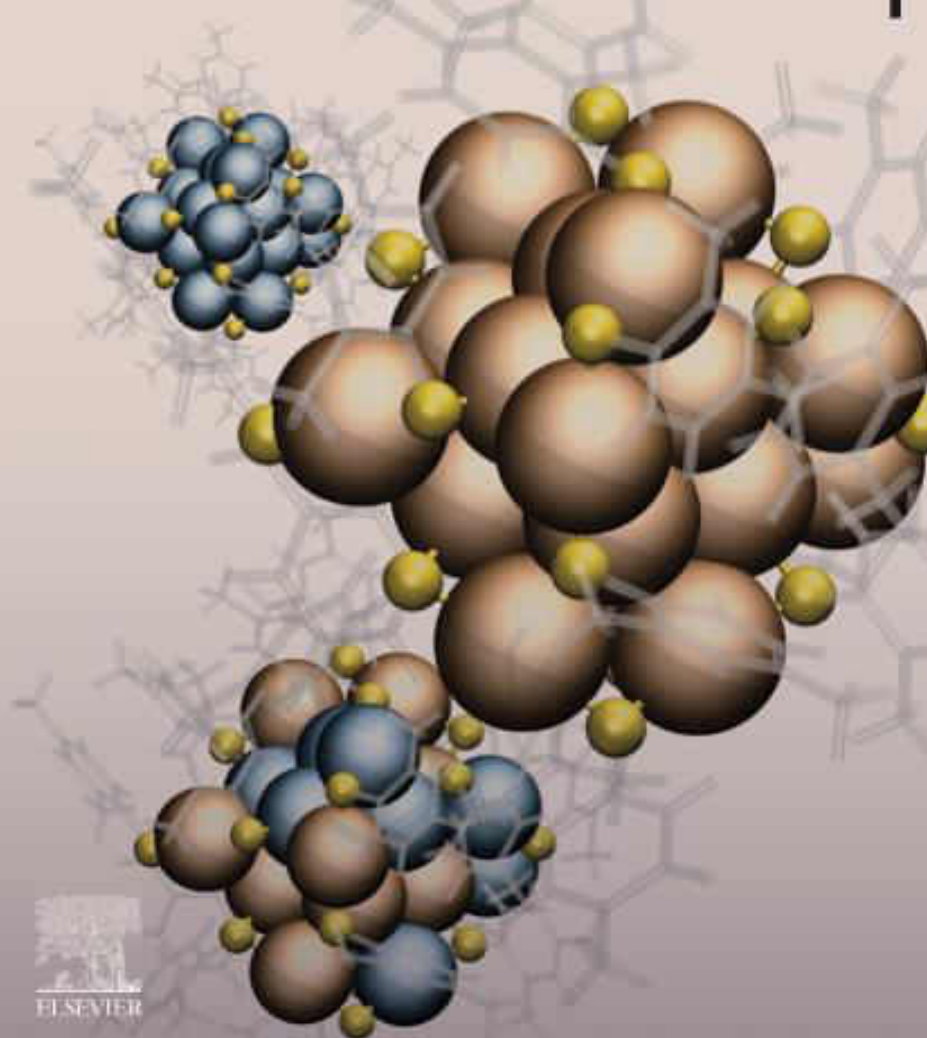
Mechanical properties

Electrochemical properties

Future?

Edited by
Thalappil Pradeep

ATOMICALLY PRECISE METAL NANOCCLUSERS



Molecular reactions



Reactions on clusters
Reactions between clusters

Inter-cluster reactions



Article

pubs.acs.org/JACS

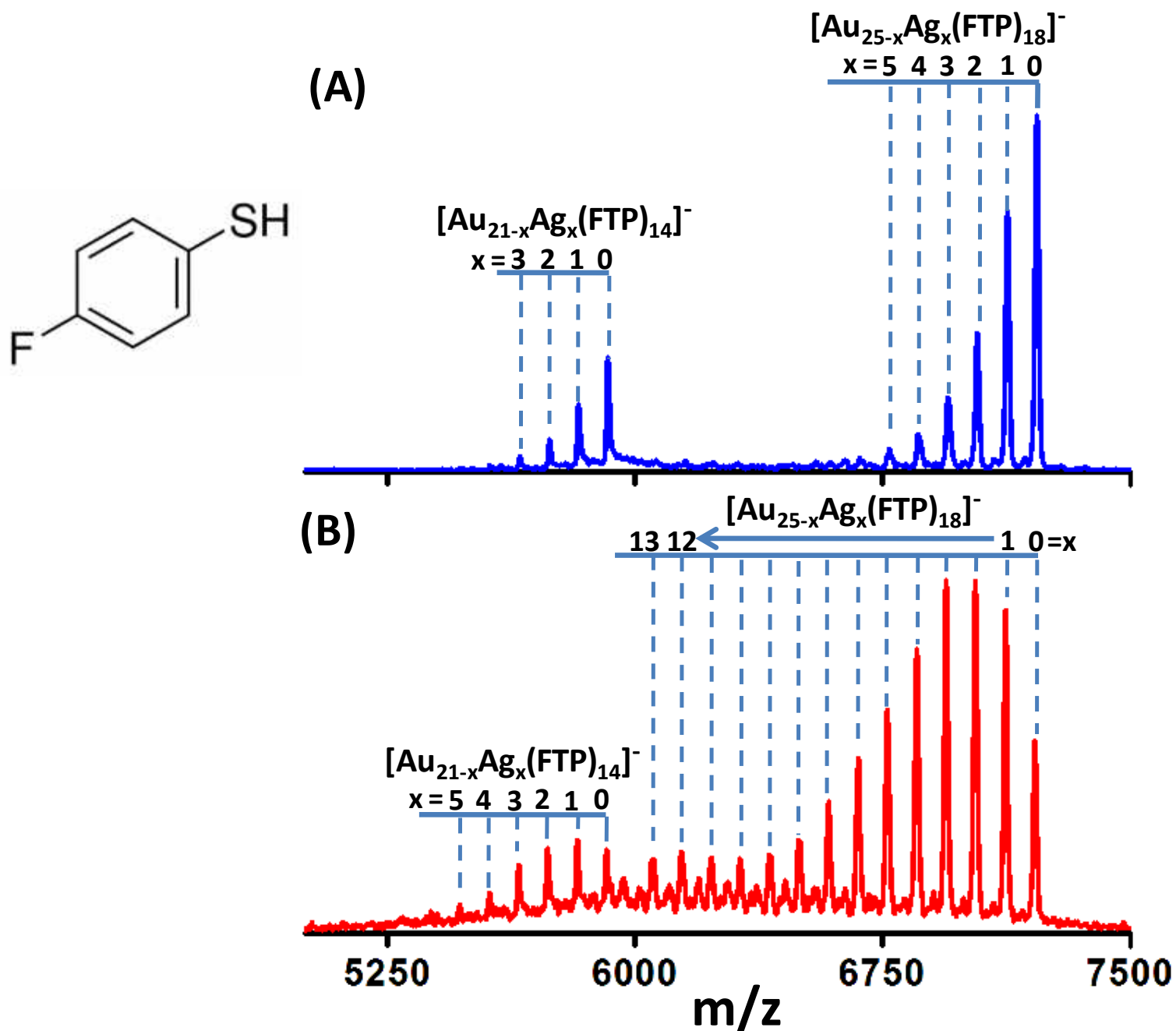
Intercluster Reactions between $\text{Au}_{25}(\text{SR})_{18}$ and $\text{Ag}_{44}(\text{SR})_{30}$

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



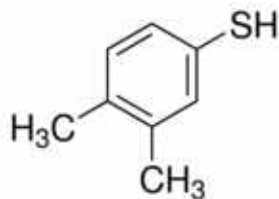


Ag₂₅-Au₂₅ experiments

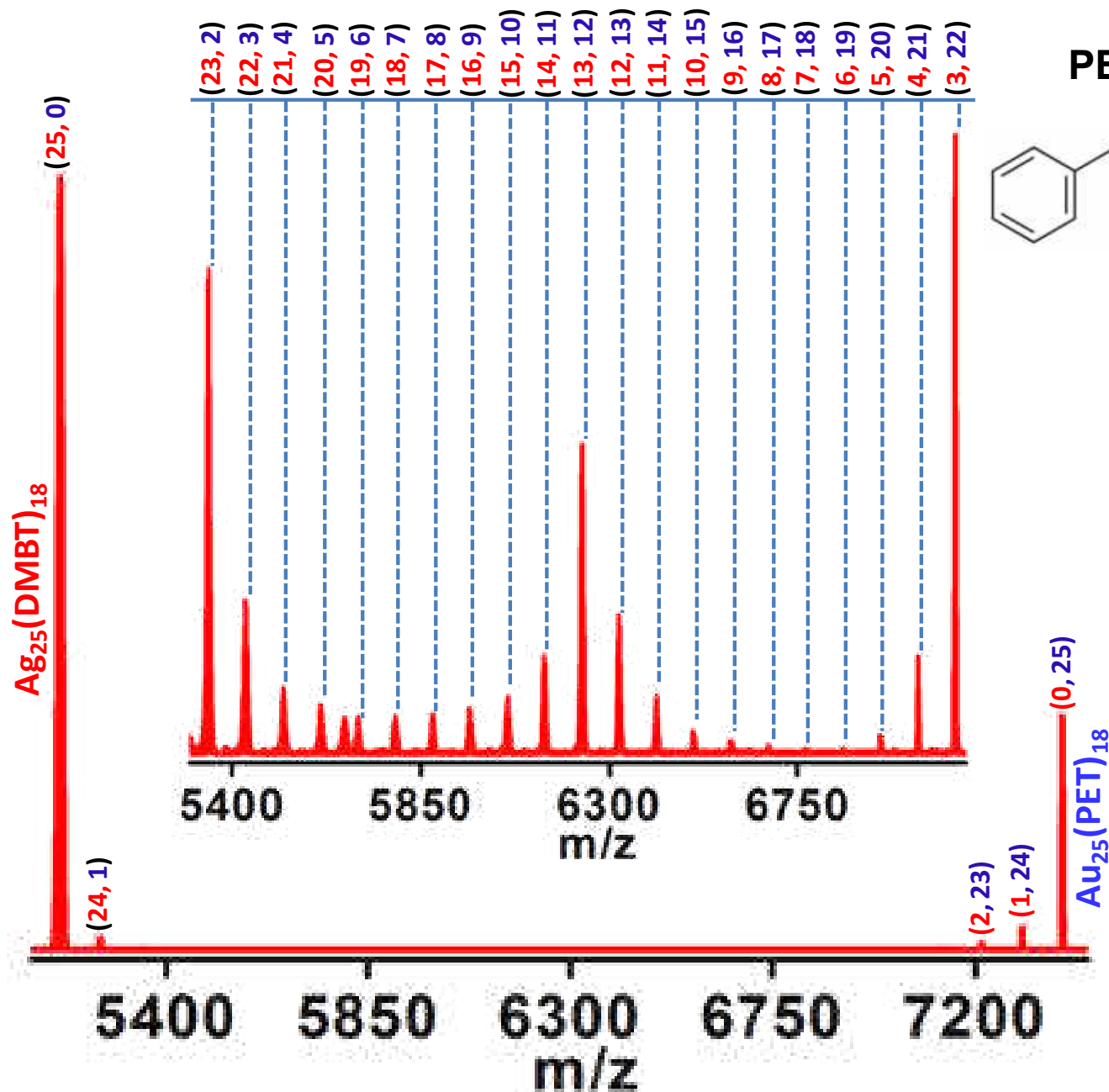
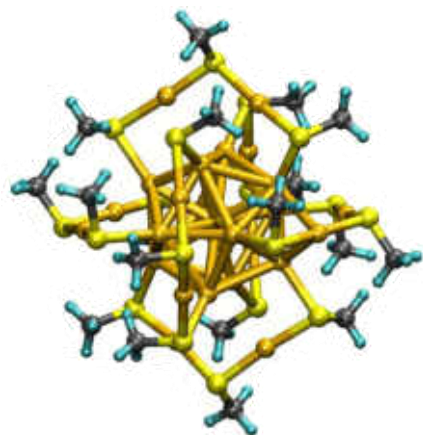
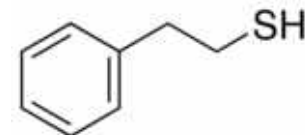
K. R. Krishnadas et al. *Nature Commun.* 2016

Reaction between $\text{Au}_{25}(\text{PET})_{18}$ and $\text{Ag}_{25}(\text{DMBT})_{18}$

DMBT

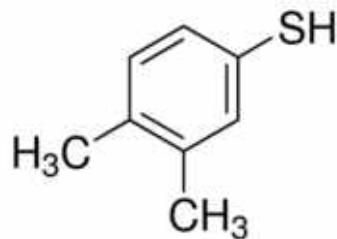


PET

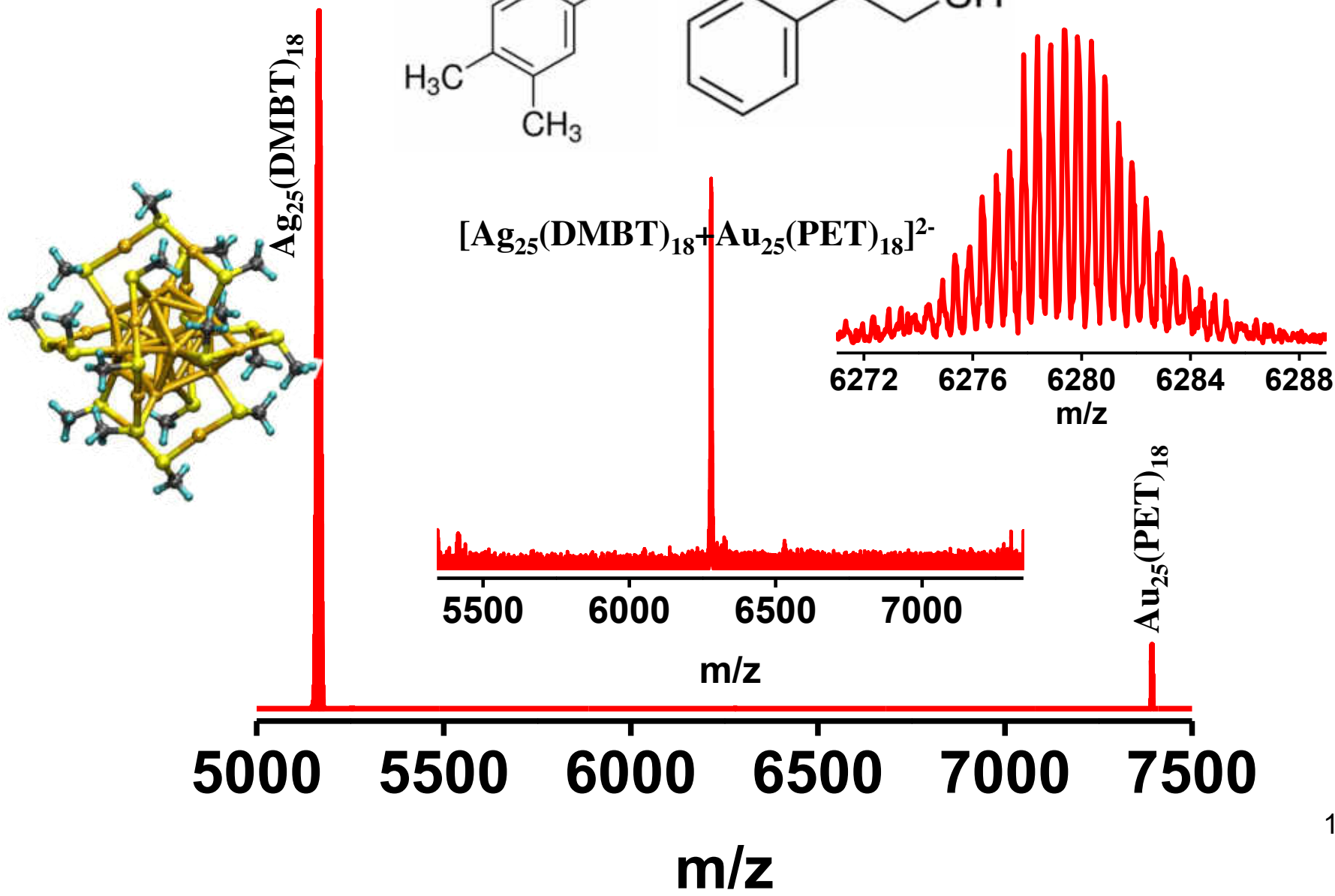
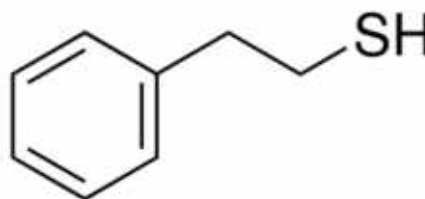




DMBT

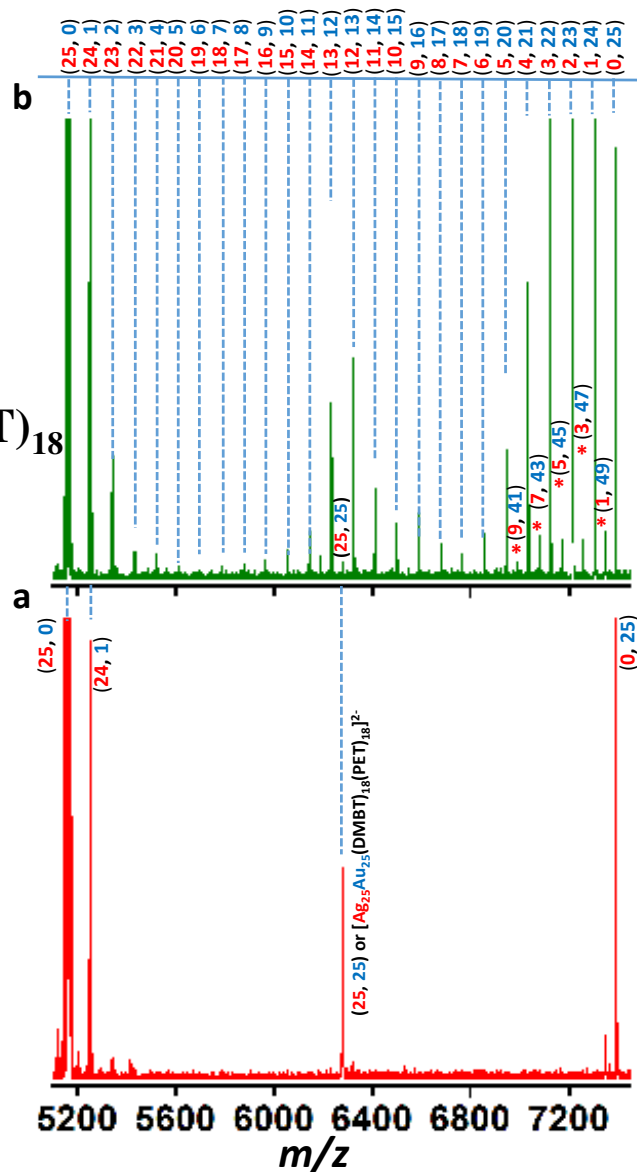


PET



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

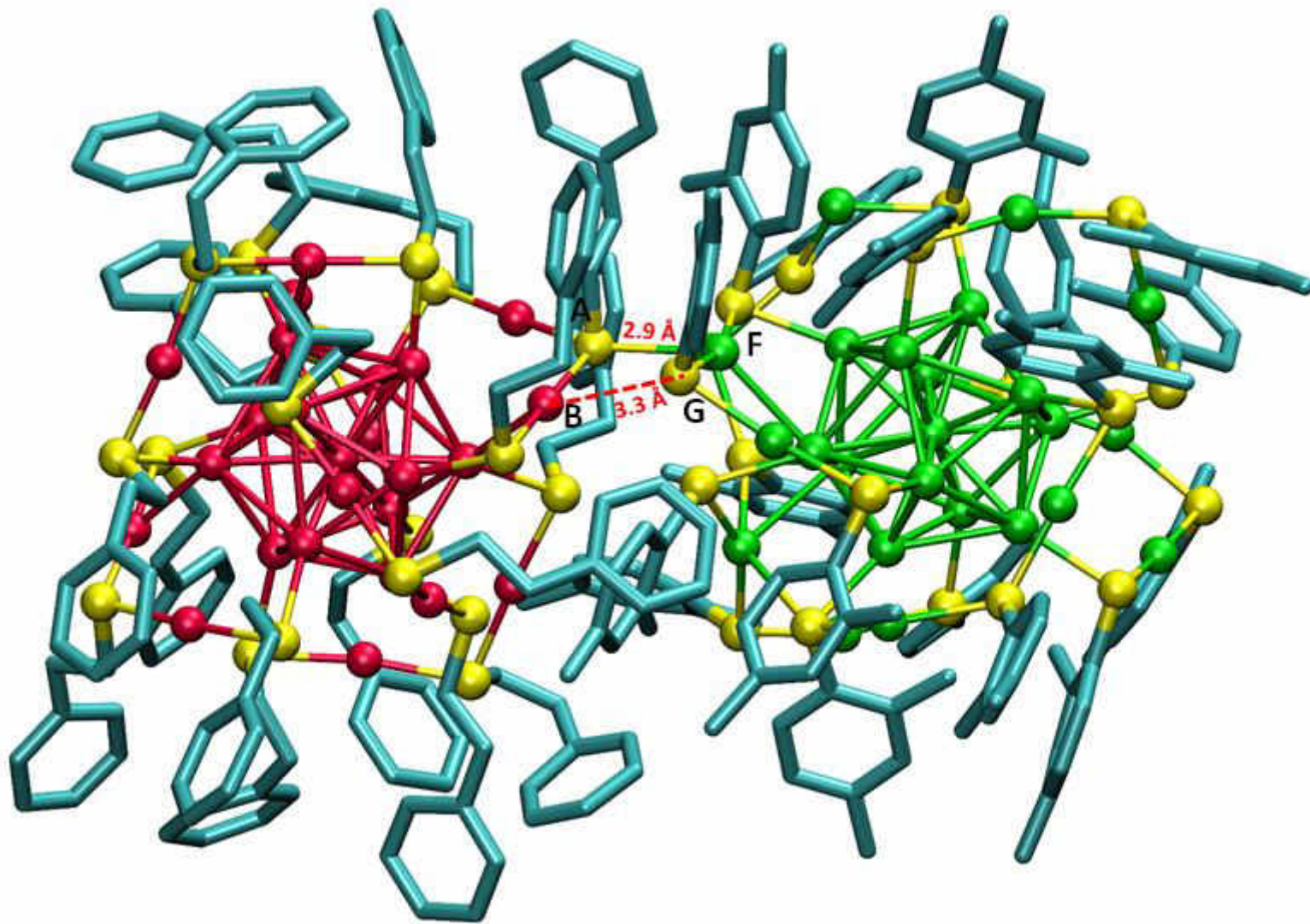
$\text{Ag}_{25}(\text{DMBT})_{18}:\text{Au}_{25}(\text{PET})_{18}$
 0.3:1.0

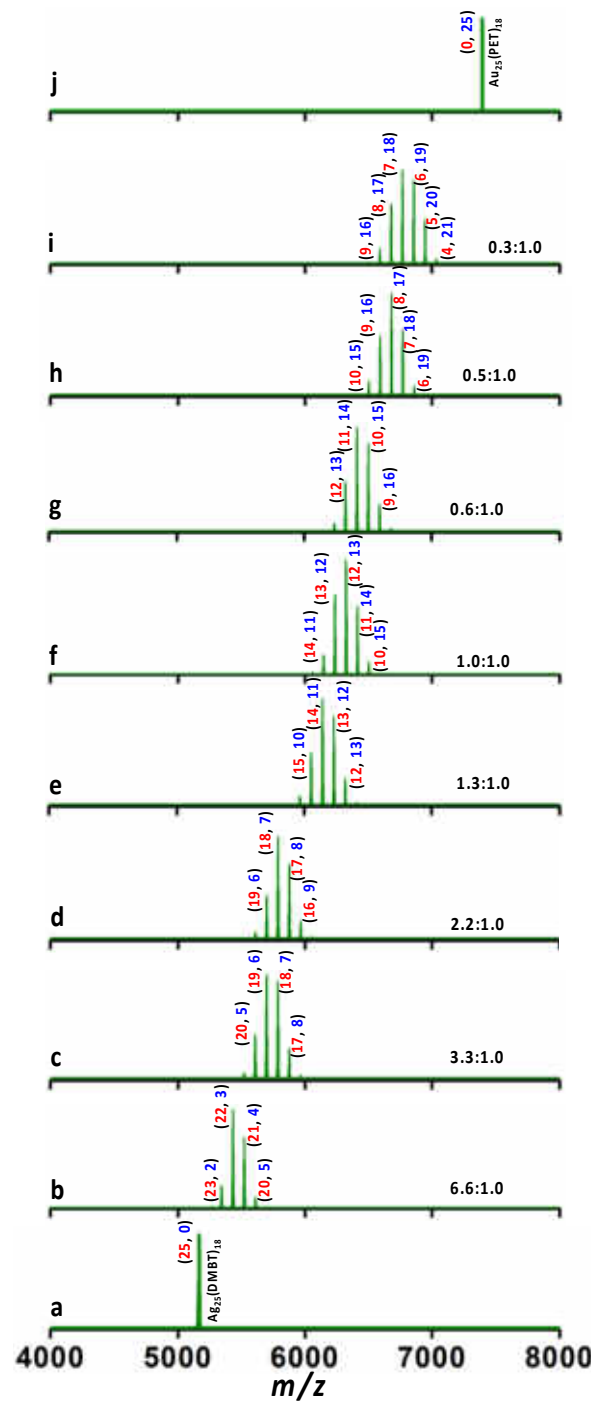


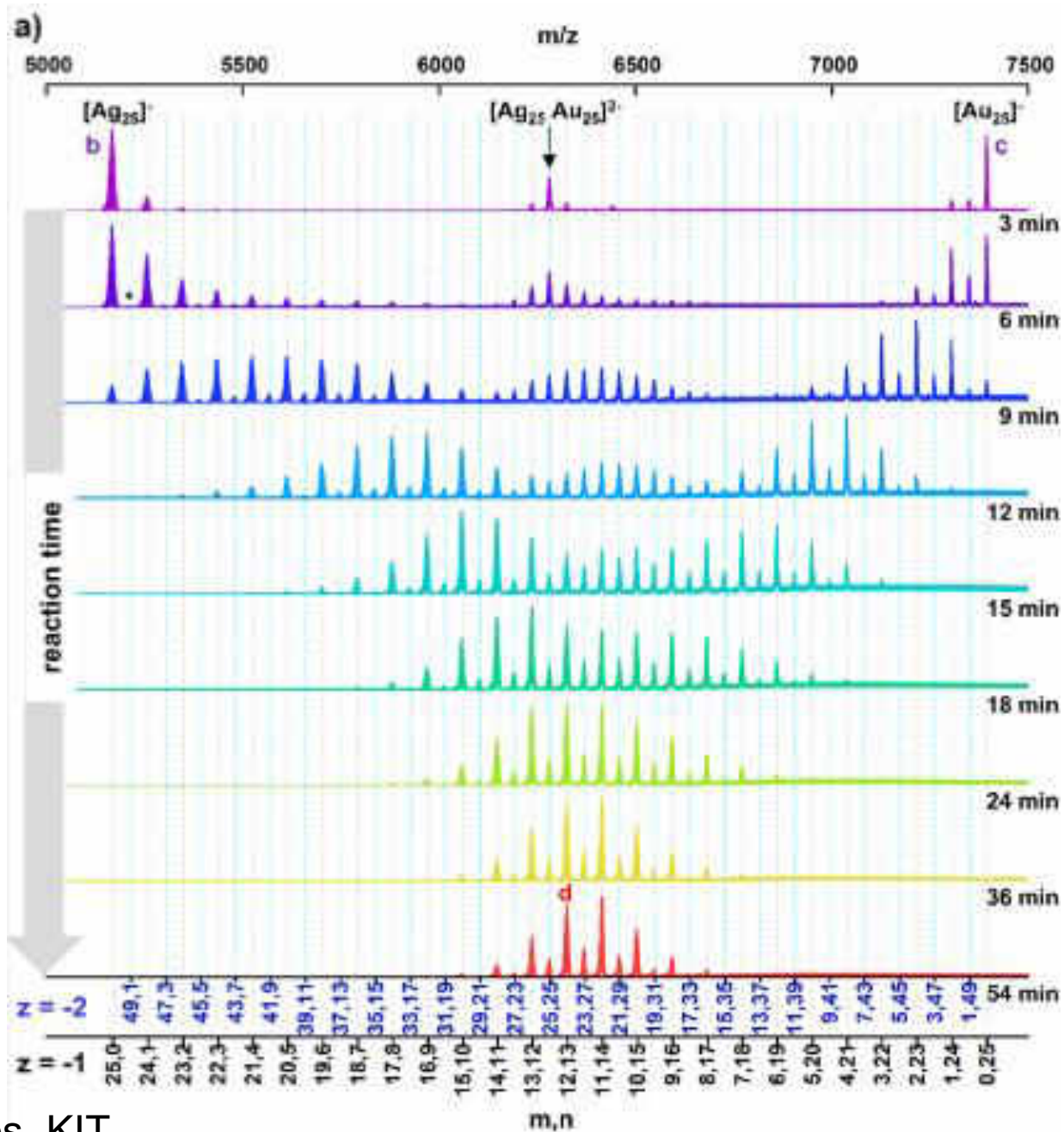
within 5 min

within 2 min

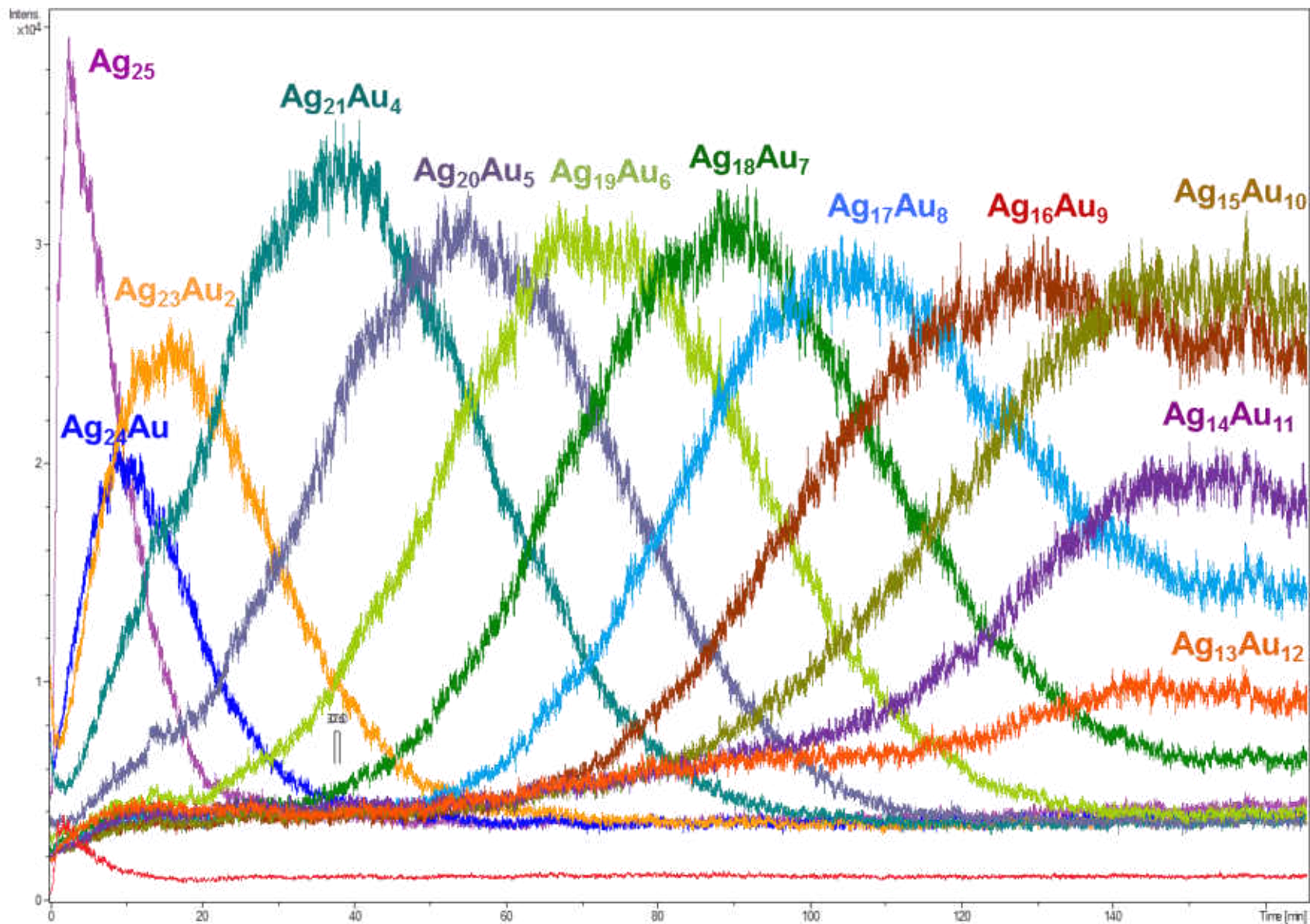
Optimized structure of $[\text{Ag}_{25}\text{Au}_{25}(\text{DMBT})_{18}(\text{PET})_{18}]^{2-}$



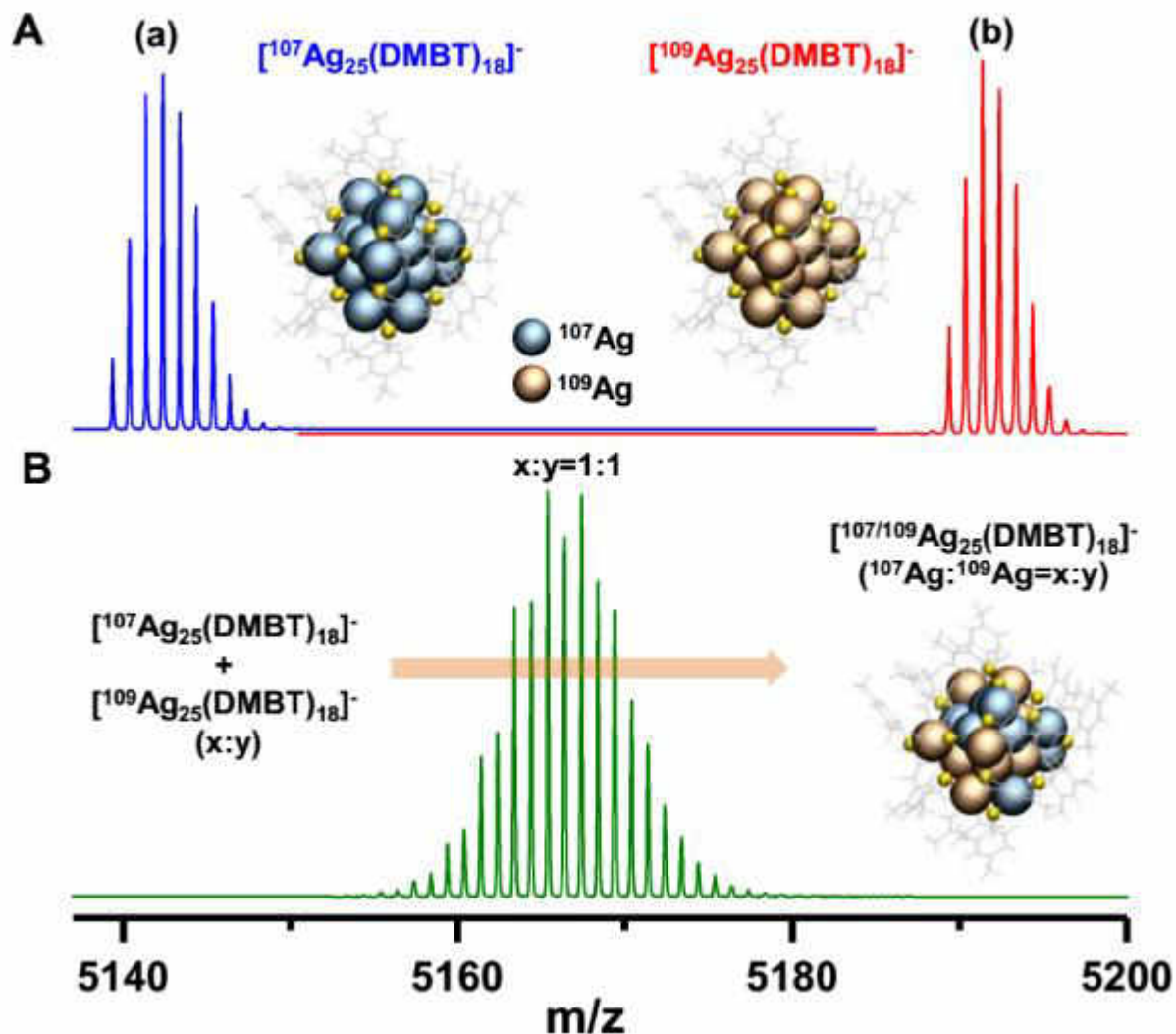




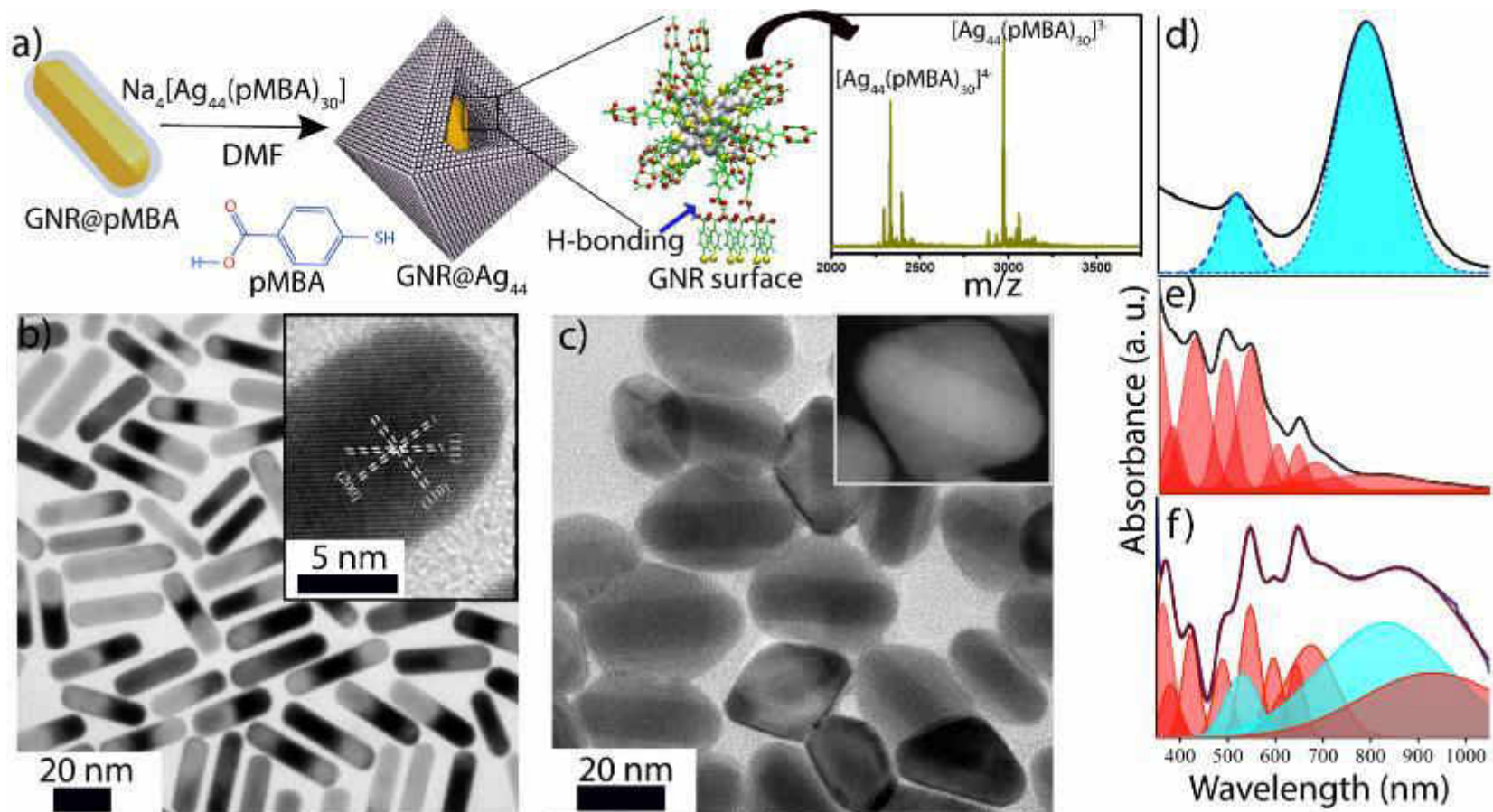
Kinetics of the exchange (monitored on the Ag₂₅ side)



Isotopic exchange



Atomically precise nanocluster assemblies encapsulating plasmonic gold nanorods



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

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

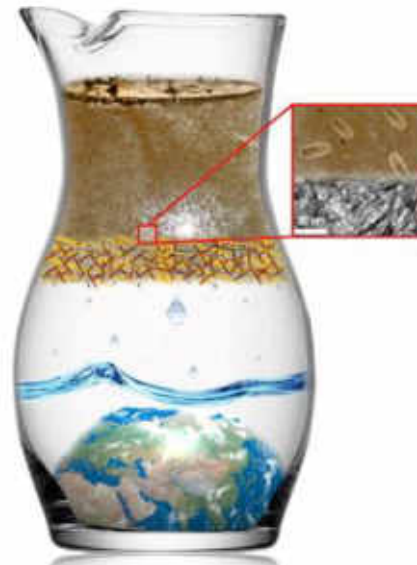
Mohan Udhaya Sankar¹, Sahaja Aigal¹, Shihabudheen M. Maliyekkal¹, Amrita Chaudhary, Anshup, Avula Anil Kumar, Kamalesh Chaudhari, and Thalappil Pradeep²

¹Unit of Nanoscience and Thematic Unit of Ex

Edited by Eric Hoek, University of California,

Creation of affordable materials for cons water is one of the most promising way 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 can 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 ility. The ability to prepare nanostructu ambient temperature has wide releva water purification.

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



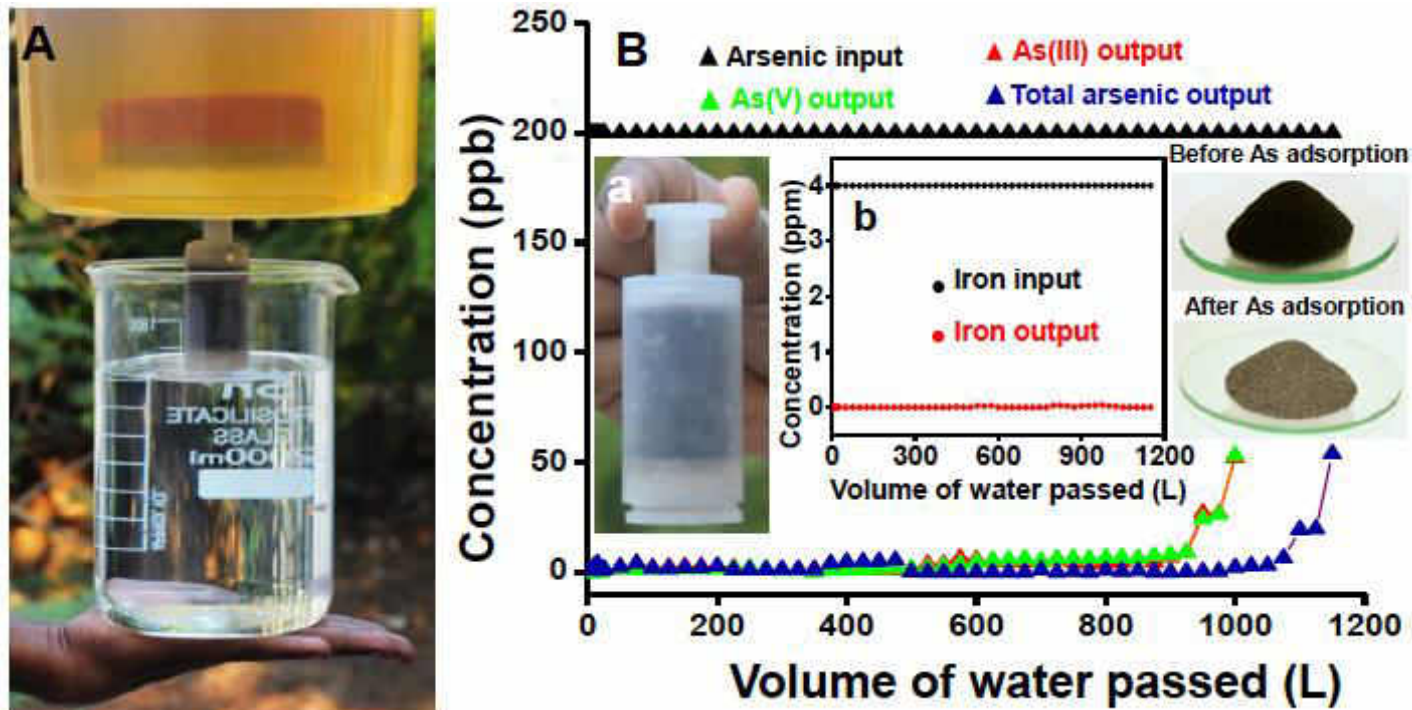
Madras, Chennai 600 036, India

(received for review November 21, 2012)

available; 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- und undergoing field trials in India, as :spread eradication of the waterborne

RESULTS AND DISCUSSION

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



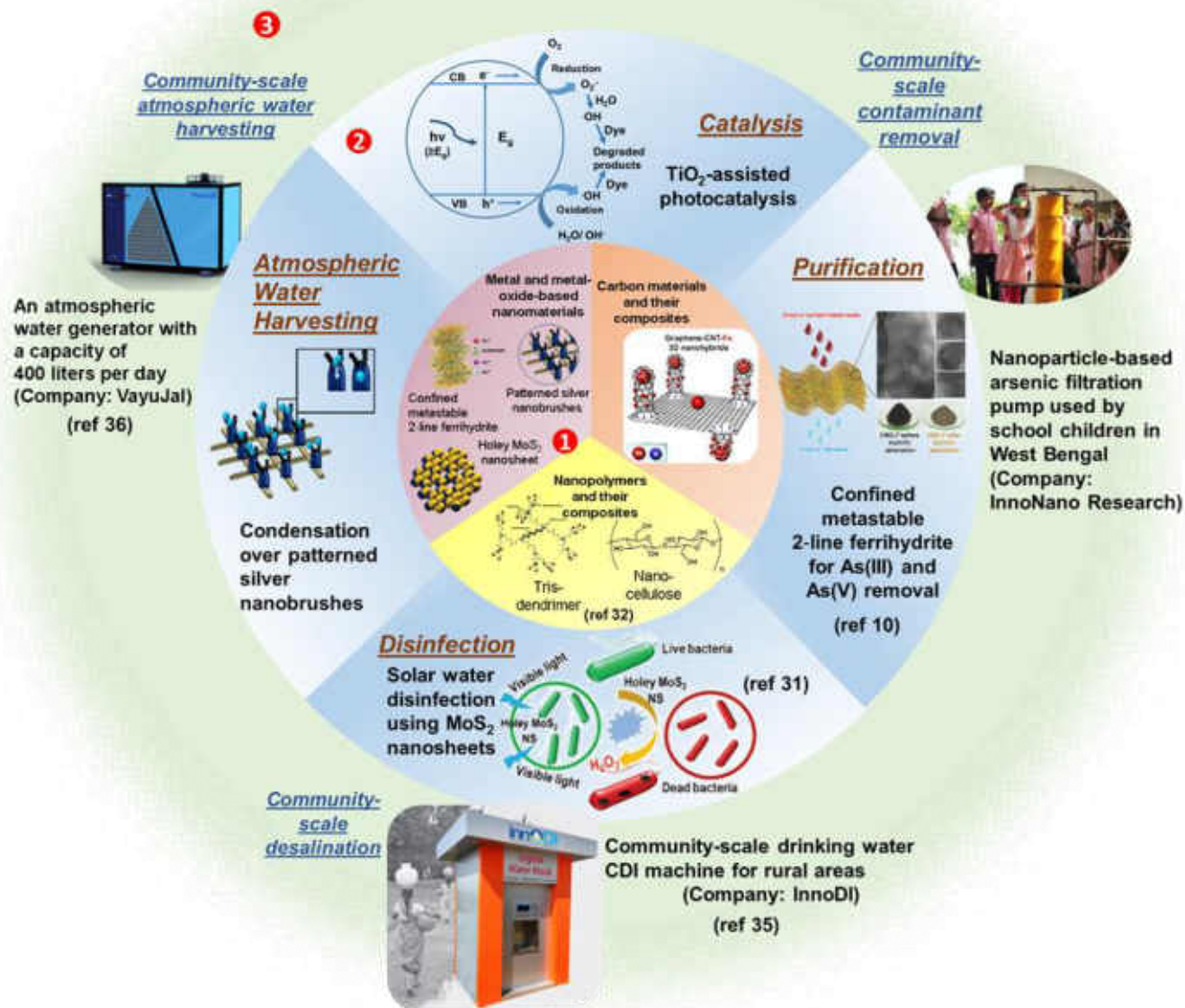
ACS Sustainable Chemistry & Engineering Editorial,
December 2016



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

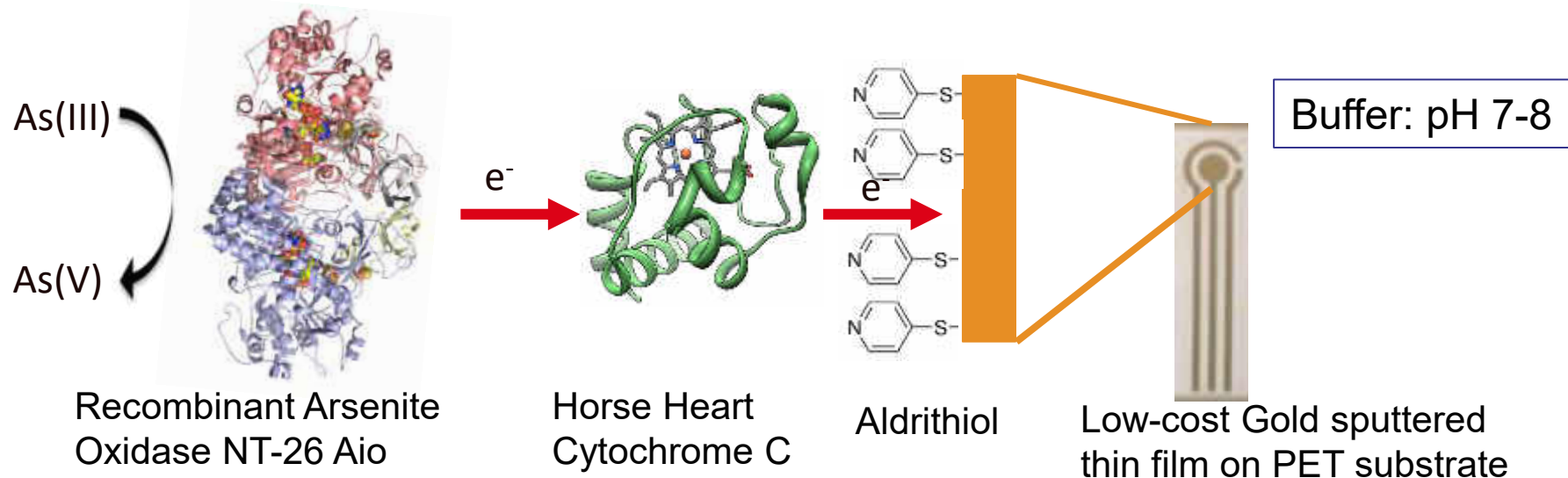
There are over 1700 community installations across the country, serving 1.3 million people with arsenic and iron-free water every day.

Evolution of materials to products

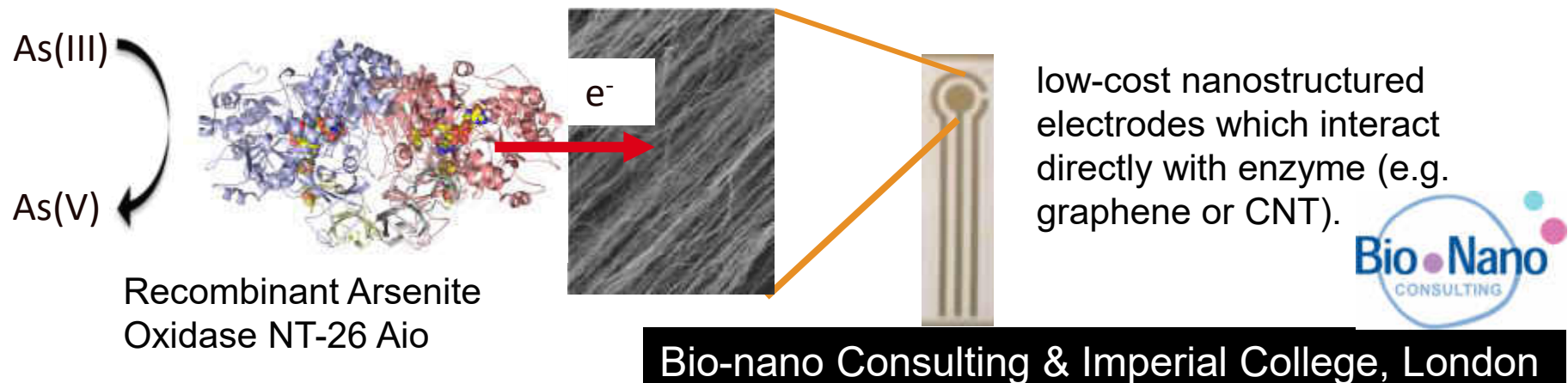


Biosensor Design

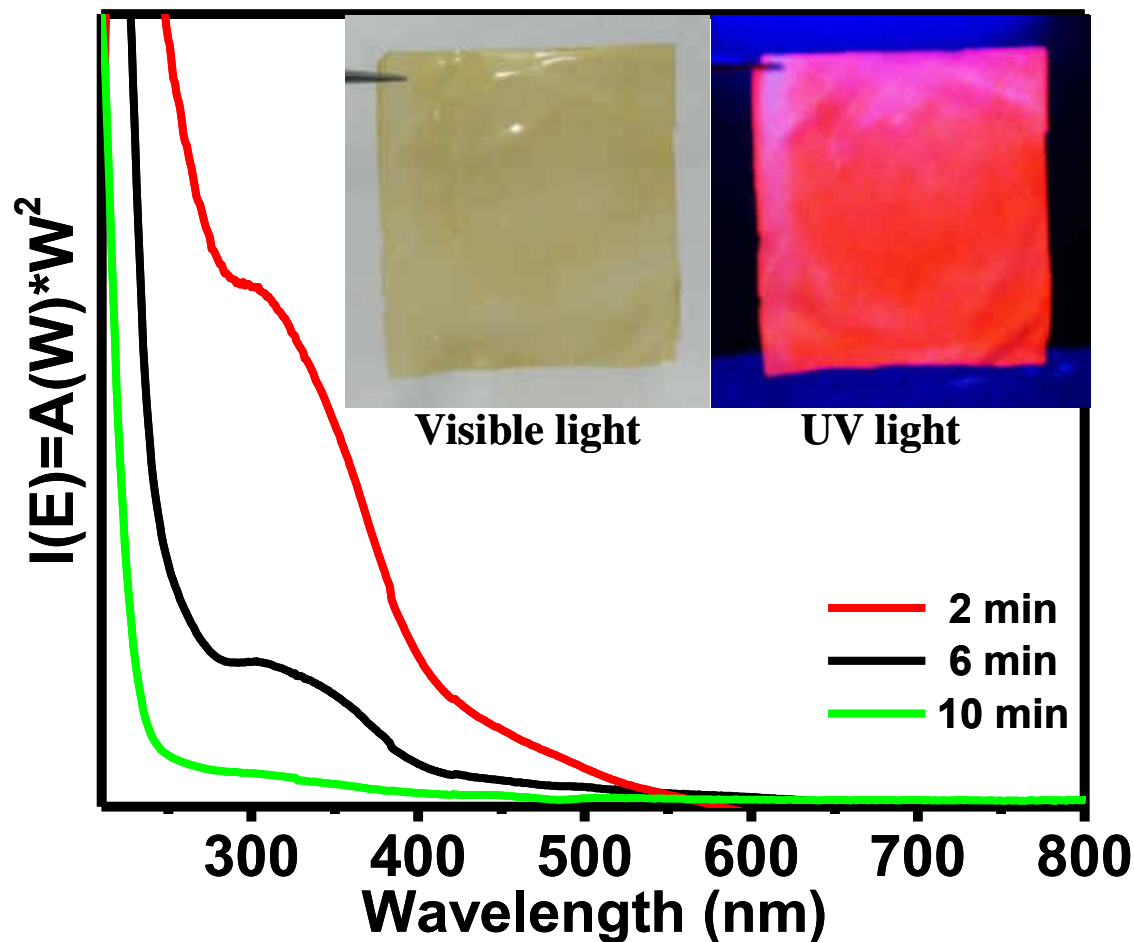
1st Generation Design (Mediated Electrochemistry)



2nd Generation Design (Direct Electron Transfer)

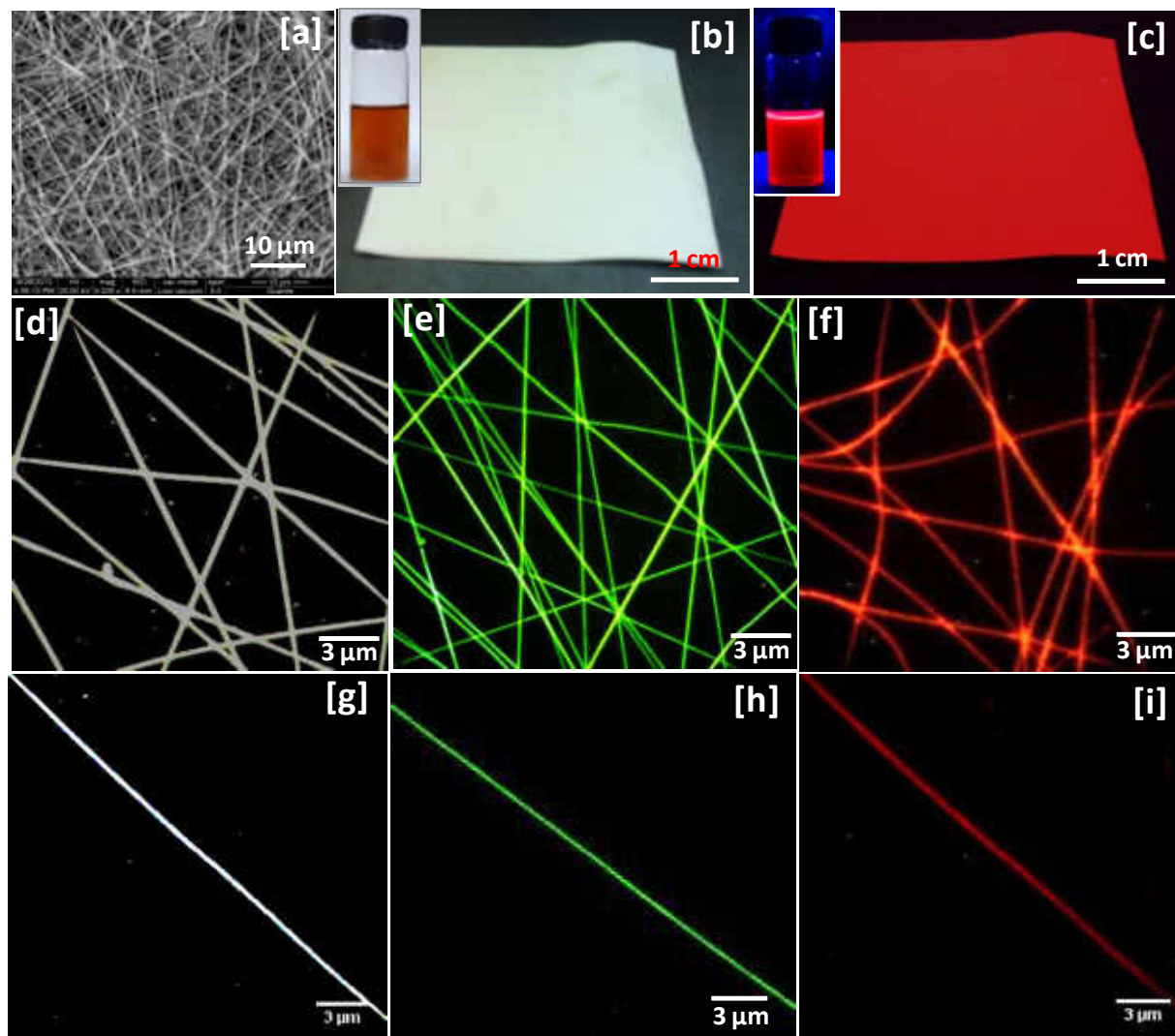


Cluster-based metal ion sensing

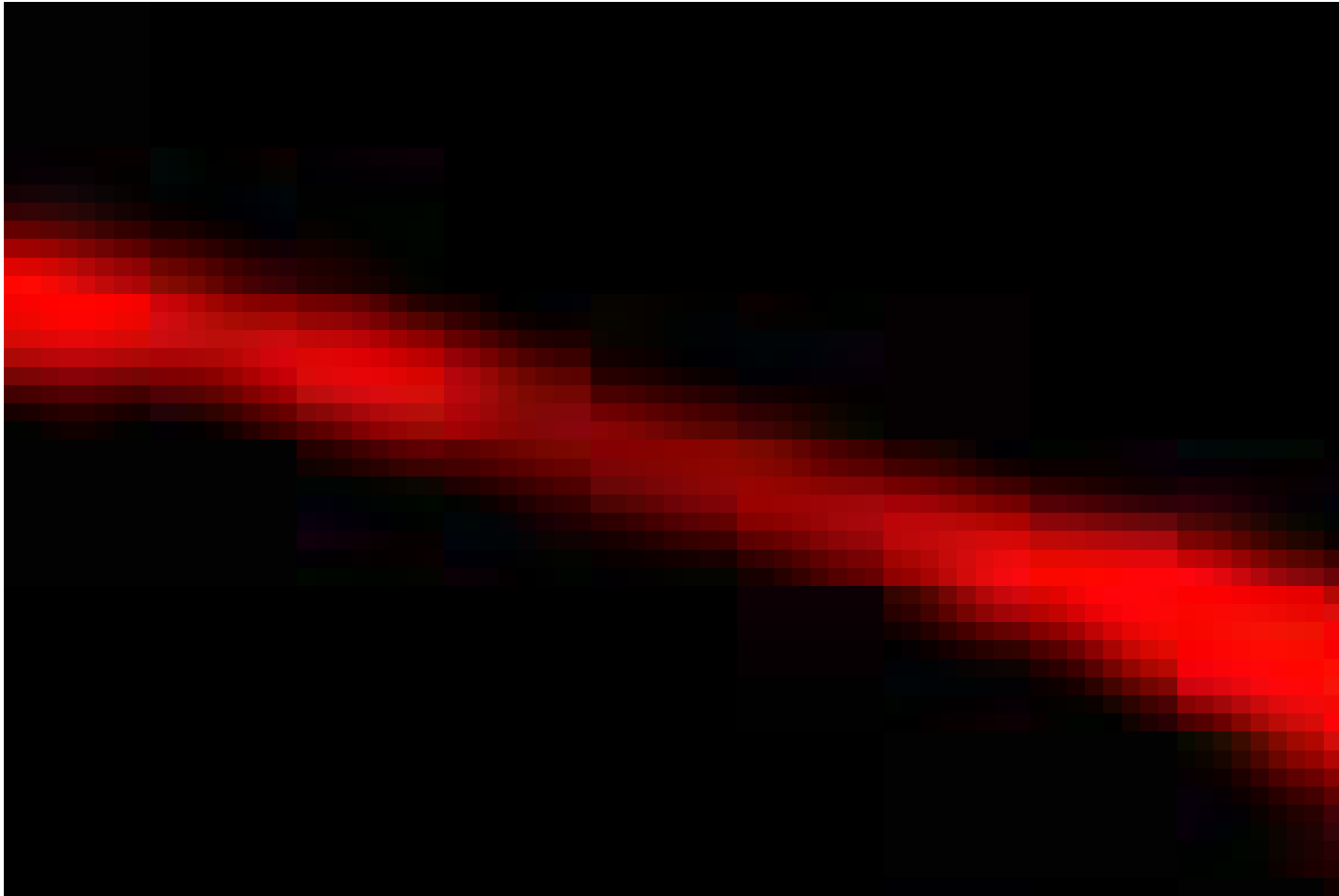


Decrease in the absorption of Au_{15} as a biofilm is dipped into the cluster solution. Inset: Free standing quantum cluster loaded film in visible light and UV light.

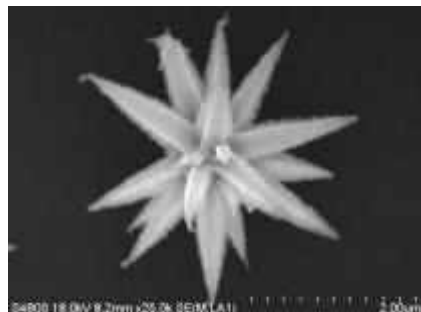
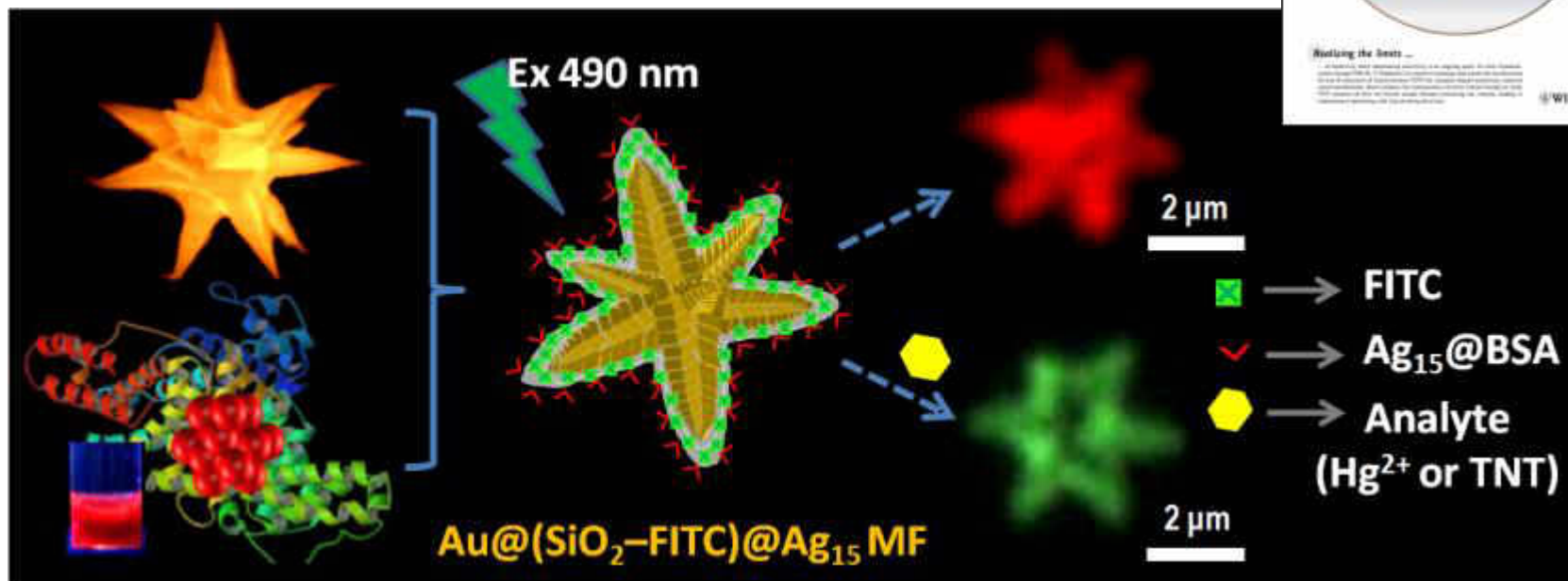
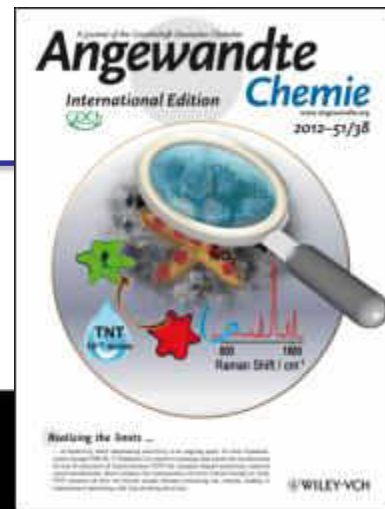
Approaching detection limits of tens of Hg^{2+}



Mercury quenching experiment using nanofiber



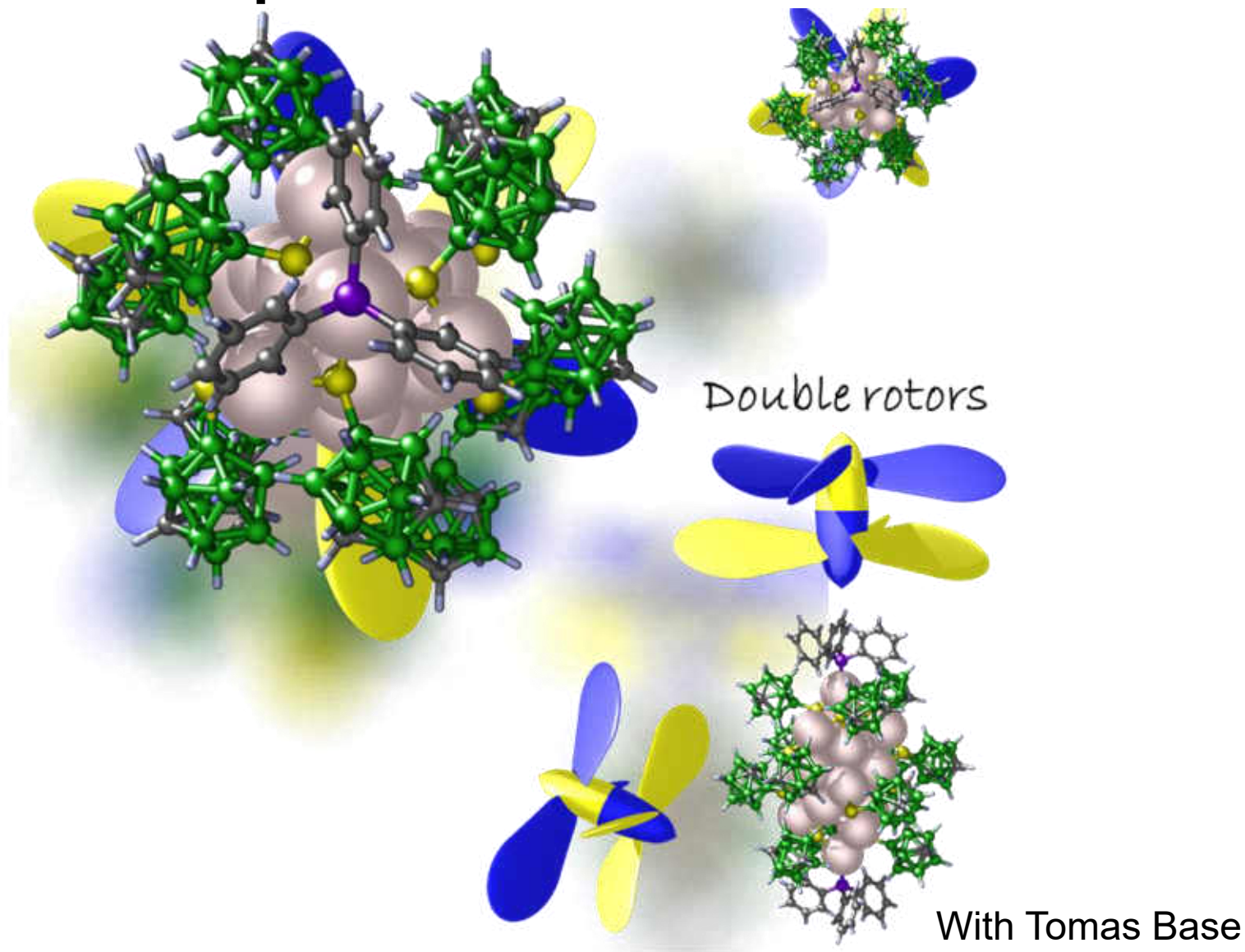
Sub-zeptomolar detection

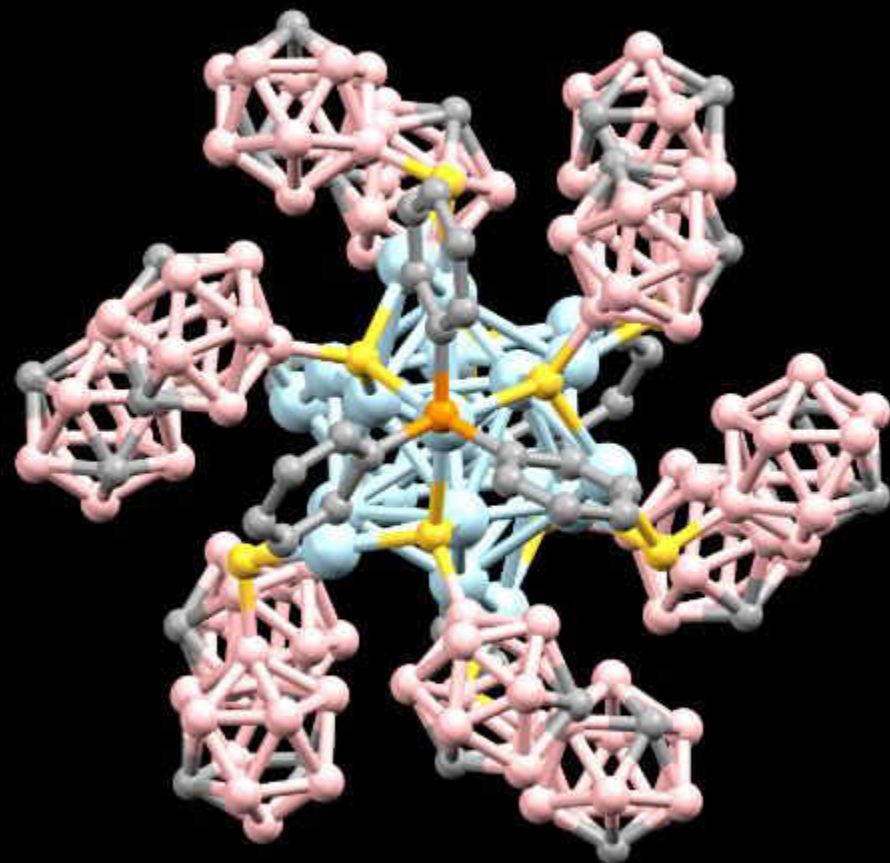
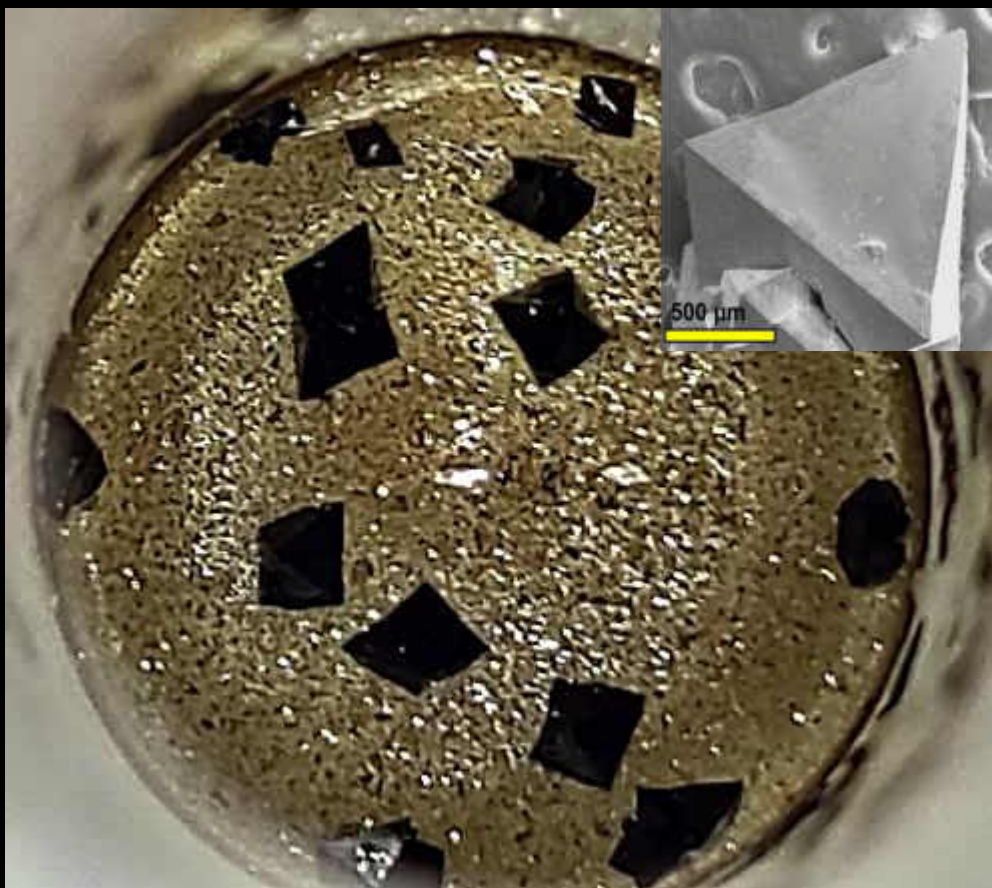


Featured in:
The Hindu, Telegraph, Times of India, etc.
C&E News
and many others

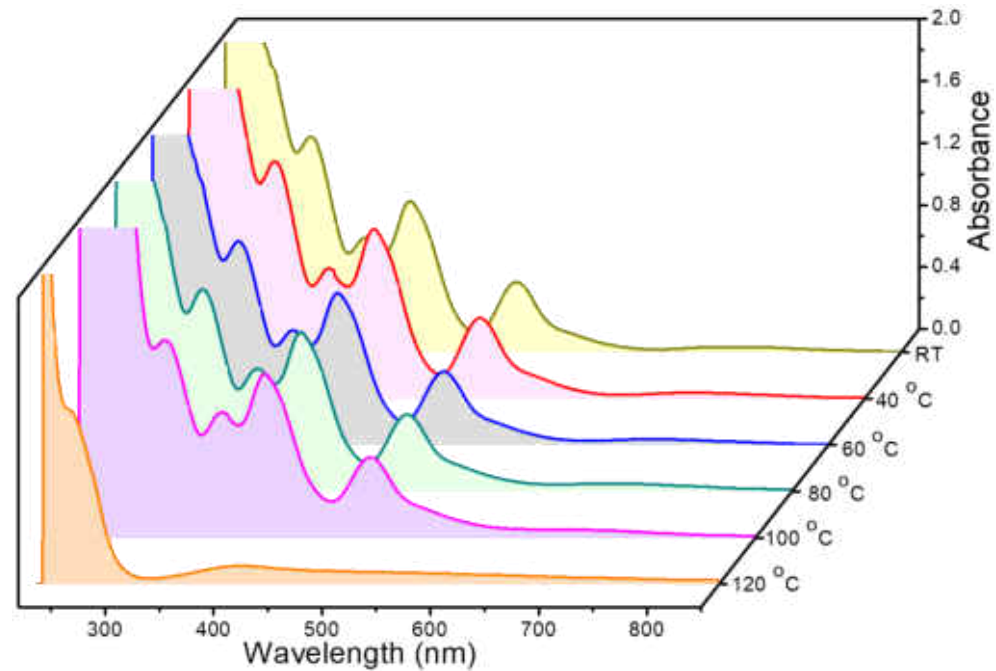
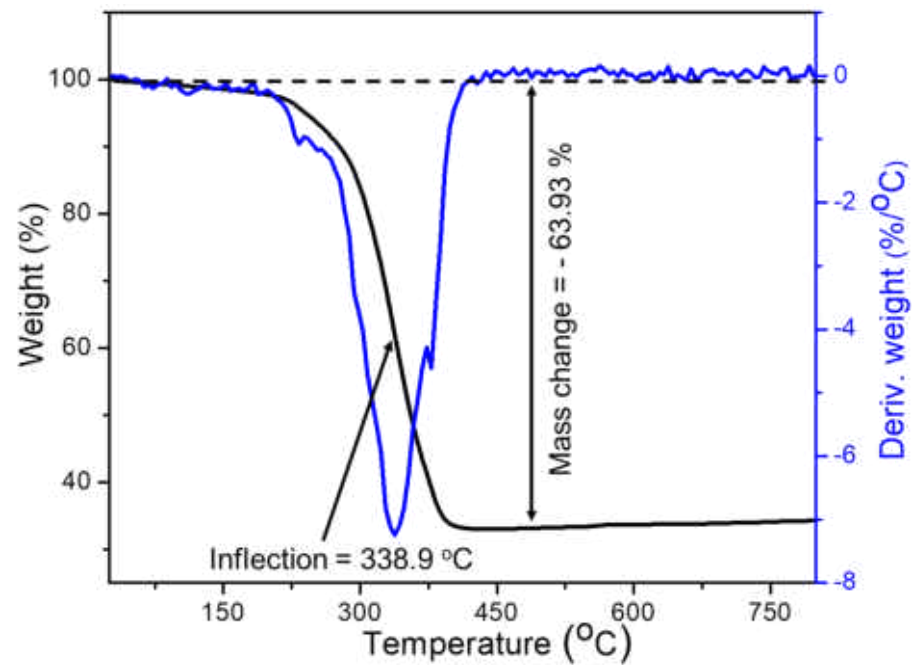
Ammu Mathew, et al. Angew. Chem. Int. Ed. 2012

Carborane-thiol protected silver nanomolecule

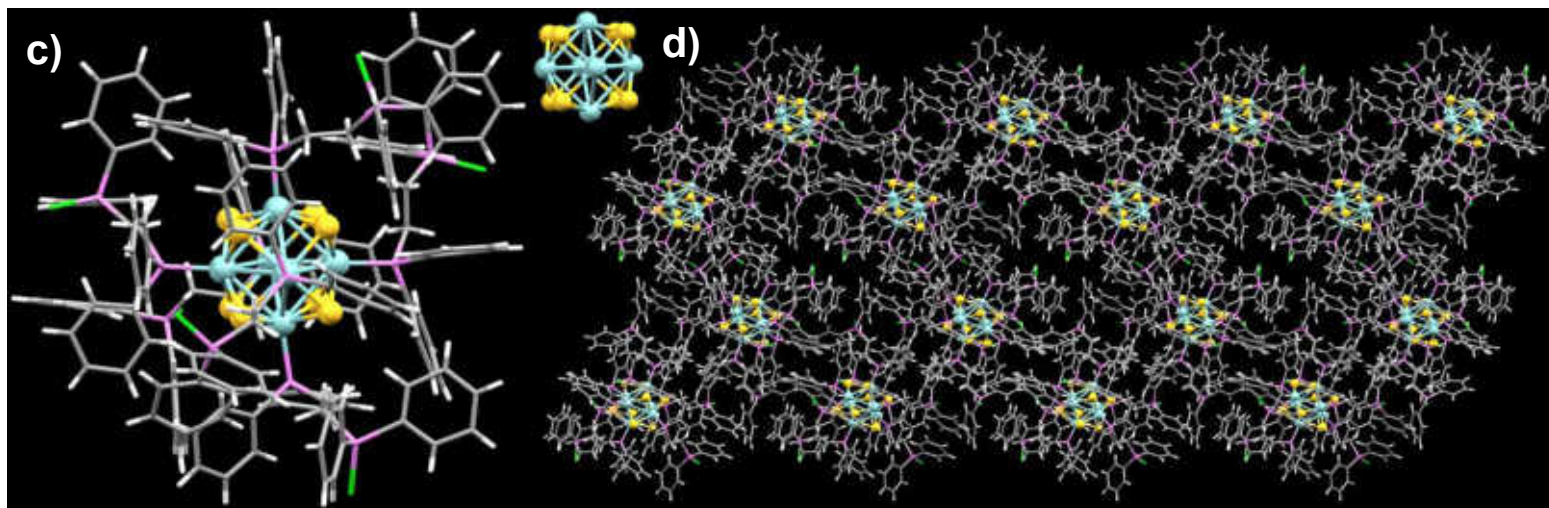
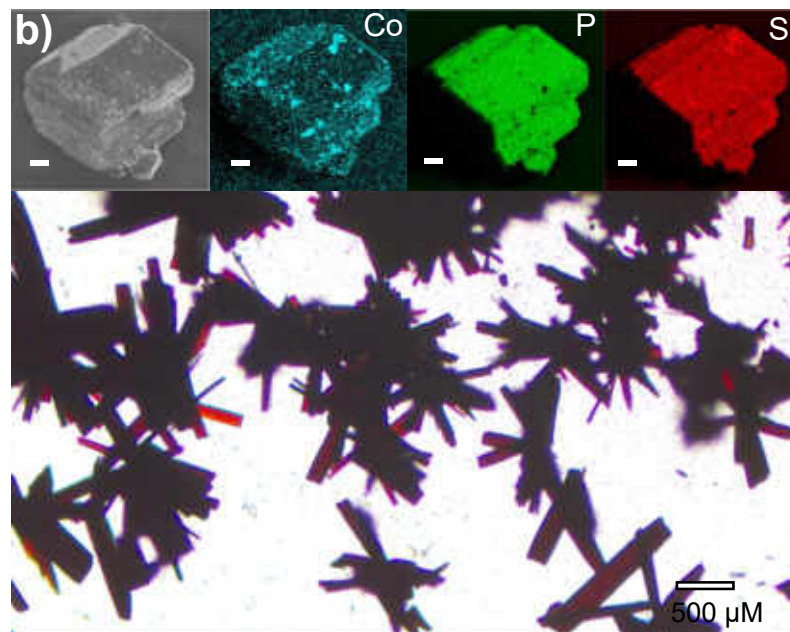
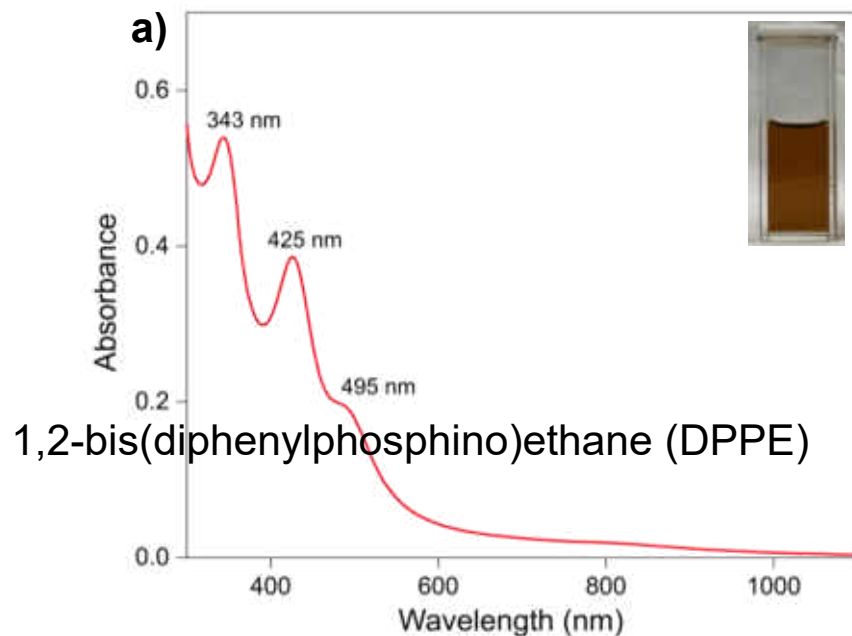




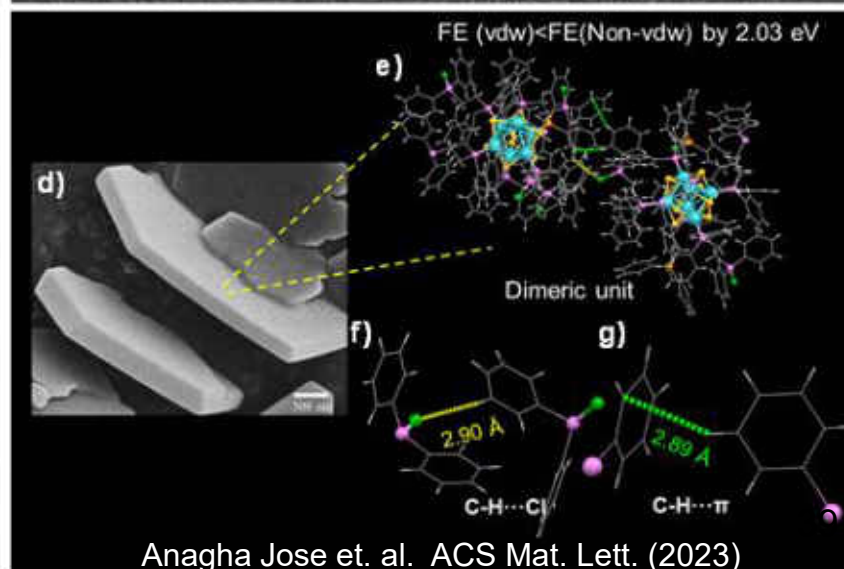
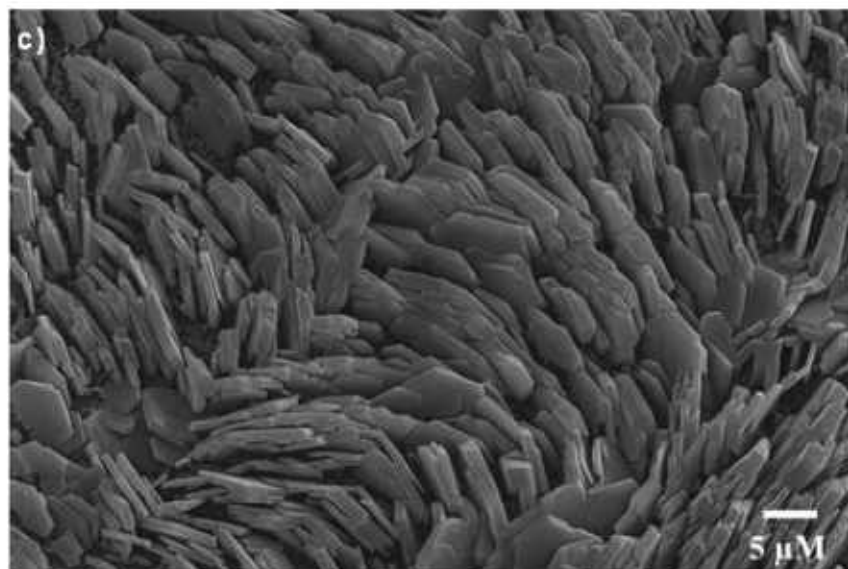
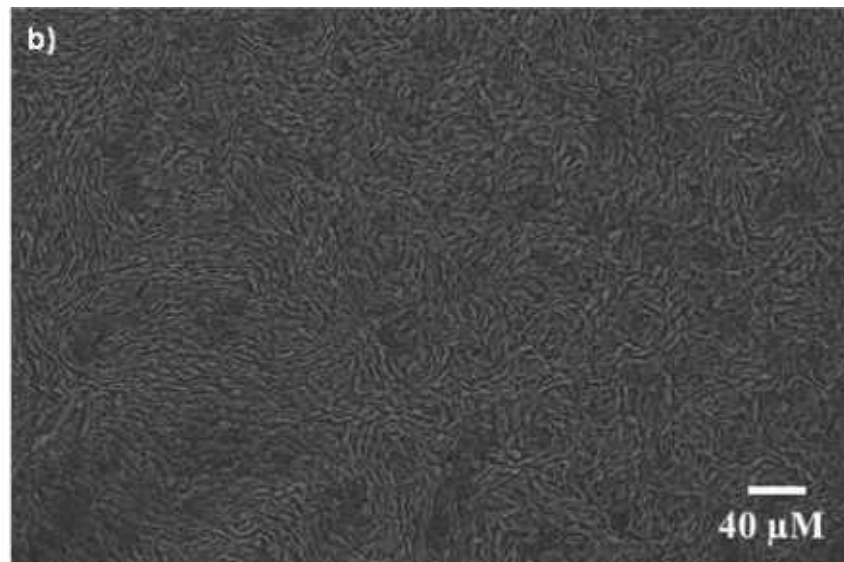
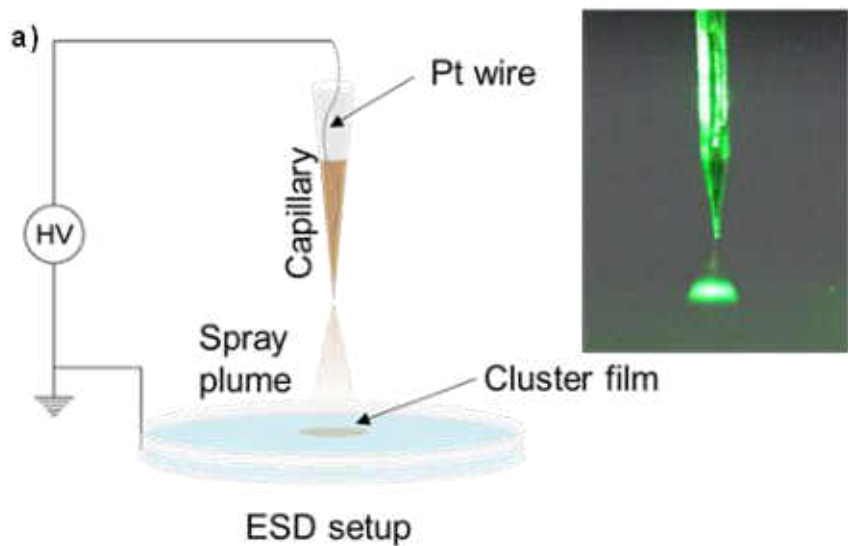
Thermal stability



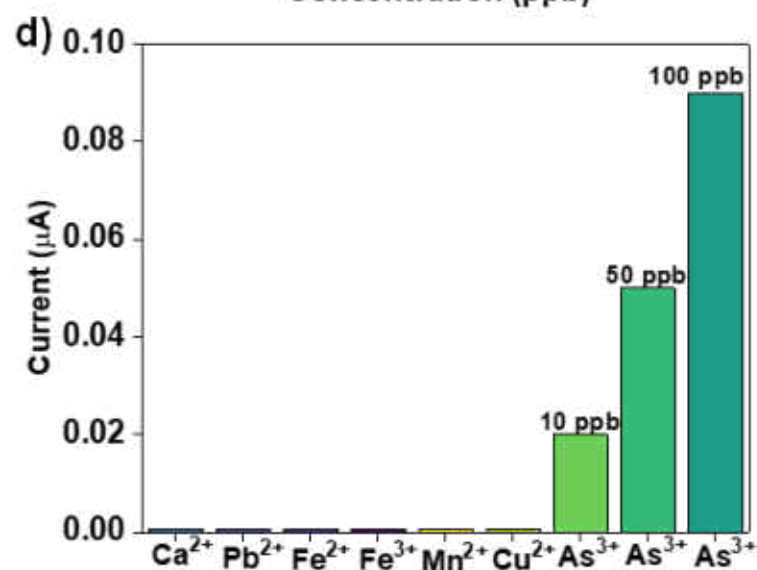
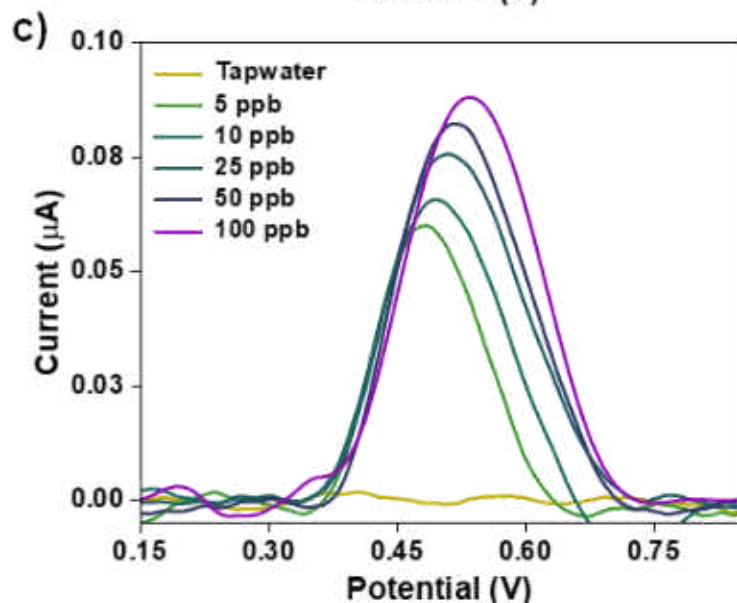
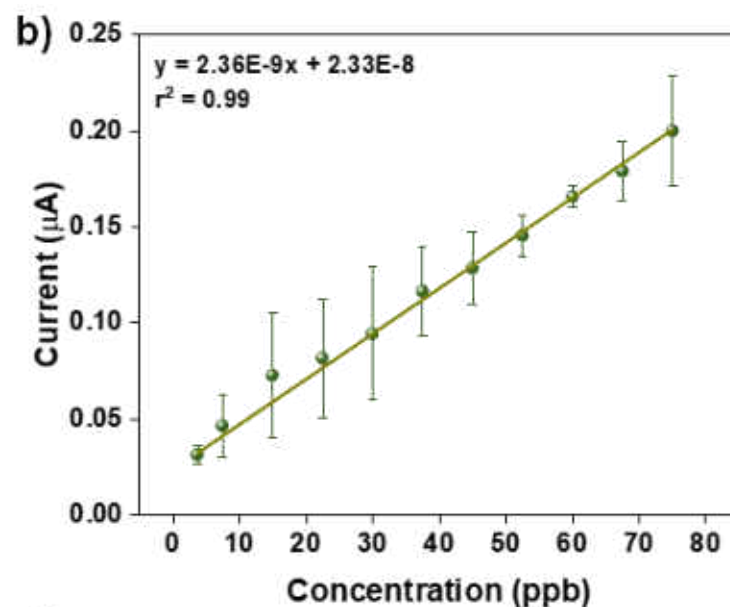
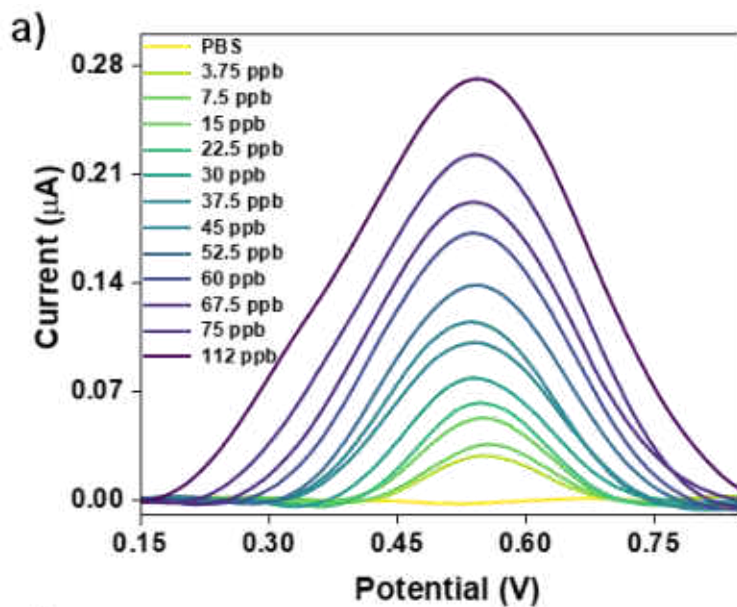
New electrodes - Aligned nanoplates of Co_6S_8



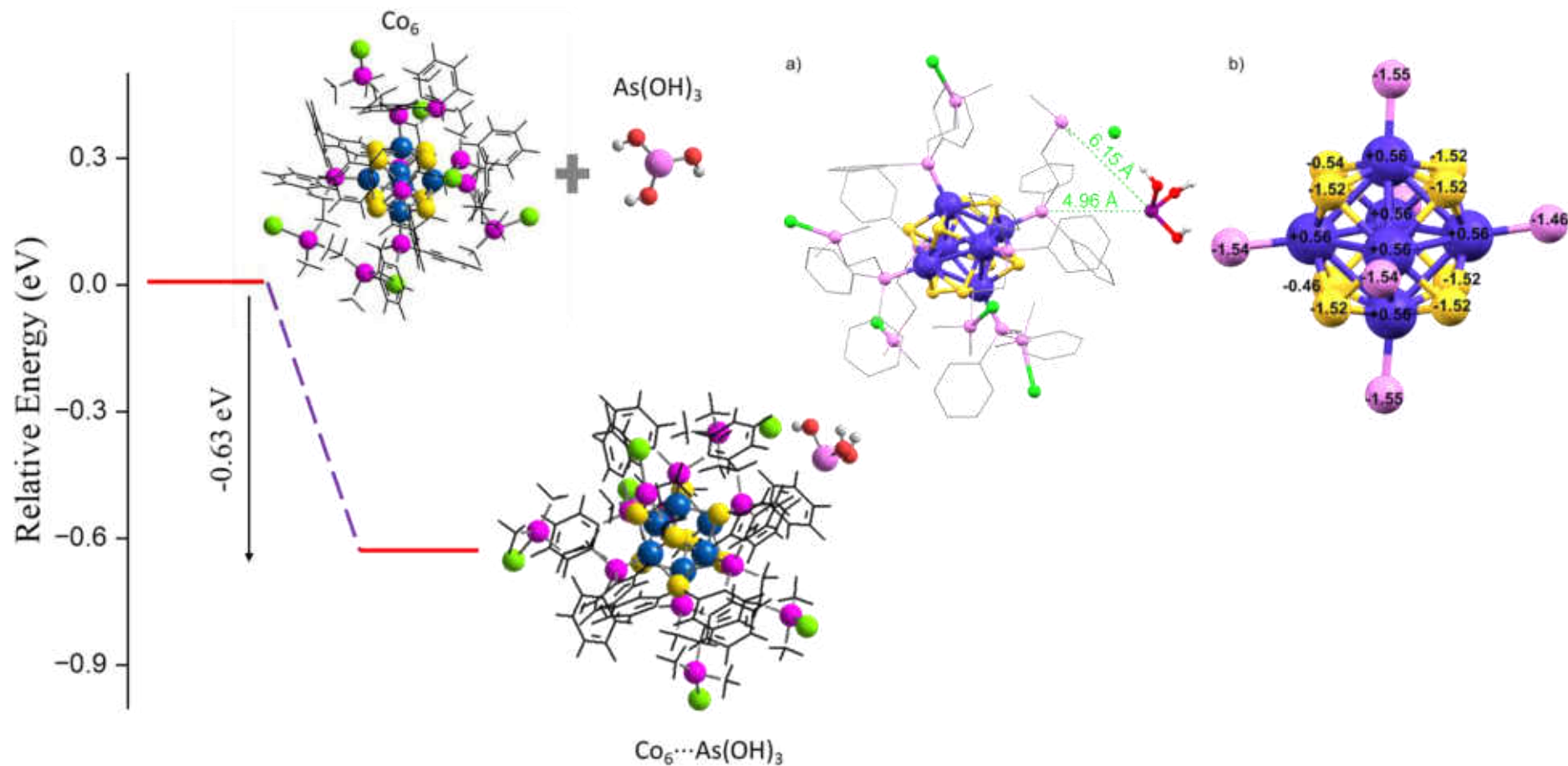
Electrospray deposition



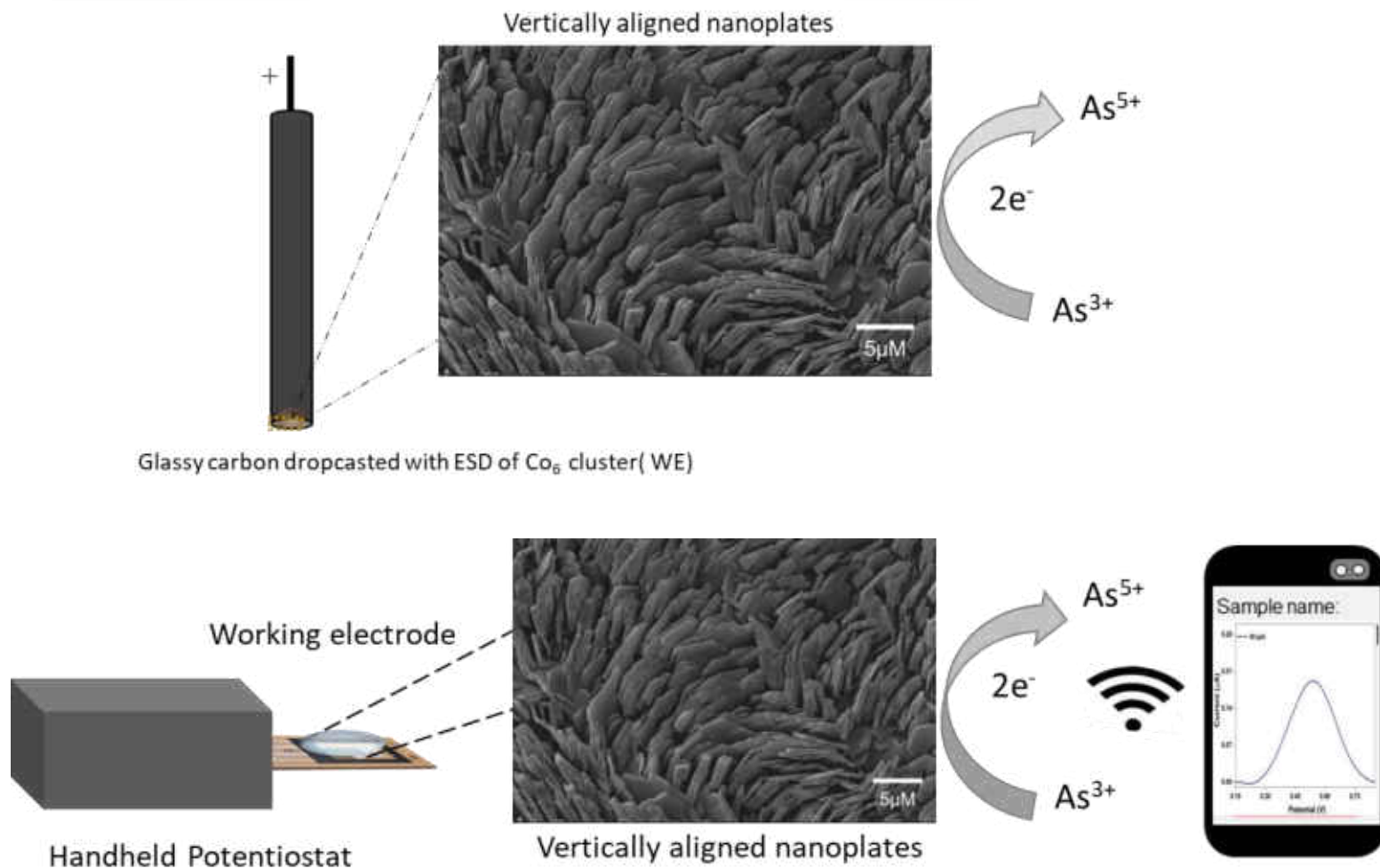
Sensing



Computational insights

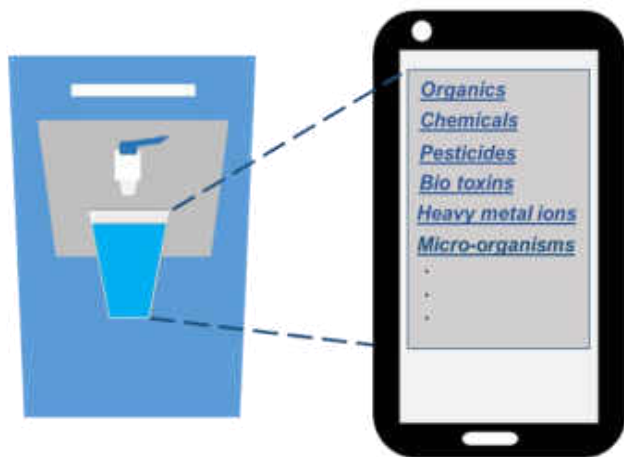


Working electrode



Smart water purifiers and big data

Smart Water Purifiers linked to IoT



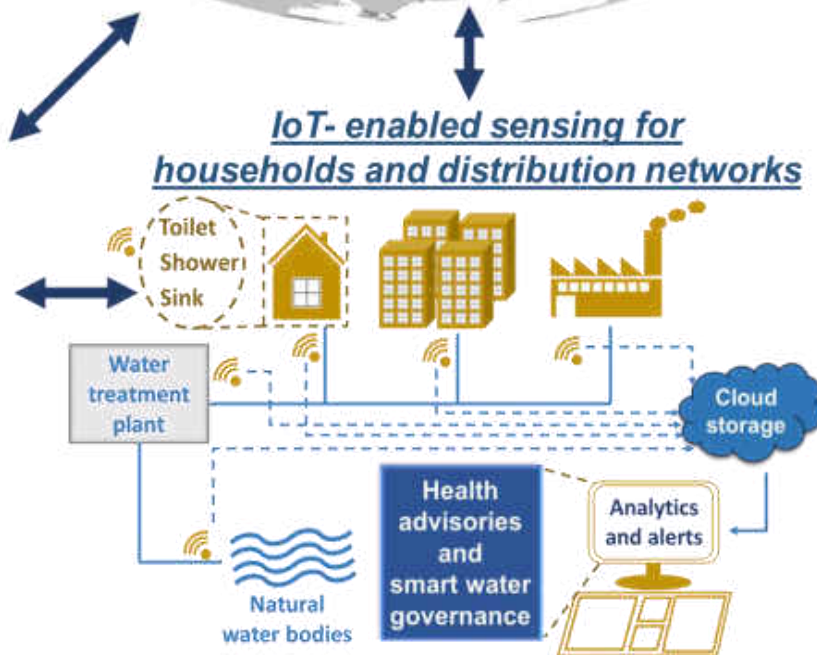
Cost-effective sensor accessory for point-of-use applications



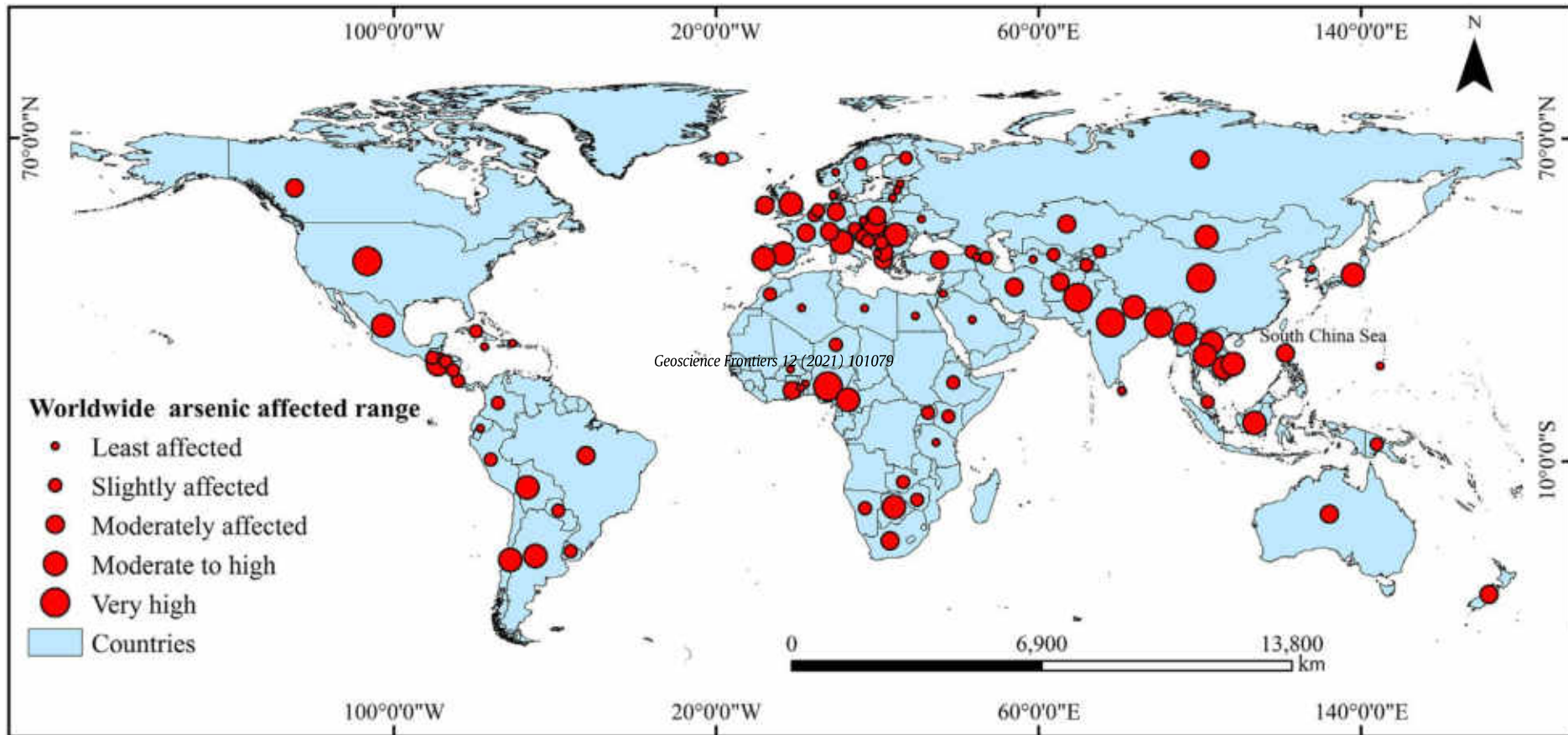
Global Map of Water Health



IoT-enabled sensing for households and distribution networks



Arsenic poisoning across the world



Collaborators



Tatsuya Tsukuda
Keisaku Kimura
Yuichi Negishi
Uzi Landman
Hannu Hakkinen
Rob Whetten

Shiv Khanna



Robin Ras



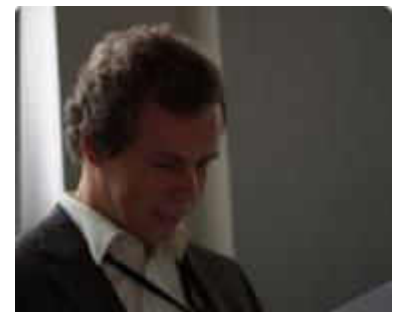
Manfred Kappes



Nonappa



Olli Ikkala



Tomas Base



Horst Hahn



Biswarup Pathak



K. V. Adarsh



G. U. Kulkarni



Vivek Polshettiwar





Department of Science and Technology

Collaborators: Tatsuya Tsukuda, Keisaku Kimura, Yuichi Negishi, Uzi Landman, Rob Whetten, Hannu Hakkinen, Robin Ras, Manfred Kappes, Horst Hahn, Tomas Base, Nonappa, Shiv Khanna, Umesh Waghmare, Chandrabhas Narayana, Giridhar U. Kulkarni, Reji Philip, Vivek Polshettiwar, R. Mukhopadhyay, K. V. Adarsh, Biswarup Pathak, Chaitanya Sharma Yamijala

Thank you all