Now in the 66th y
ear

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Co-founder

InnoNano Researc

InnoDI Water Tech

VayuJAL Technolo

Aqueasy Innovations Pvt. Ltd.

Hydromaterials Pvt. Ltd.

EyeNetAqua Solutions Pvt. Ltd.

DeepSpectrum

Associate Editor

ACS Sustainable Resource Management

Professor-in-charge

ICCW INTERNATIONAL CENTRE FOR CLEAN WATER

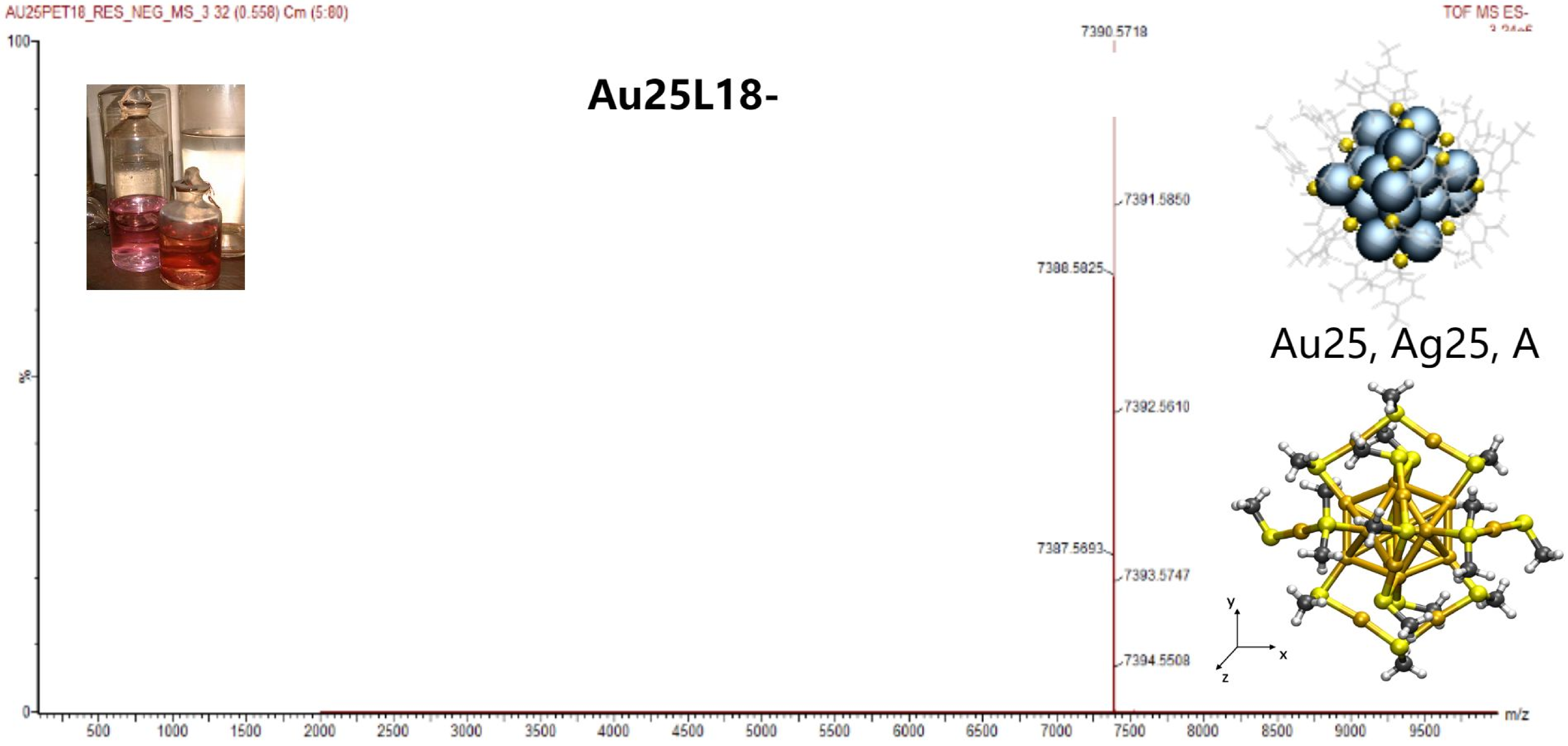
International Centre for Clean Wa
ter

Pradeep RESEARCH GROUP

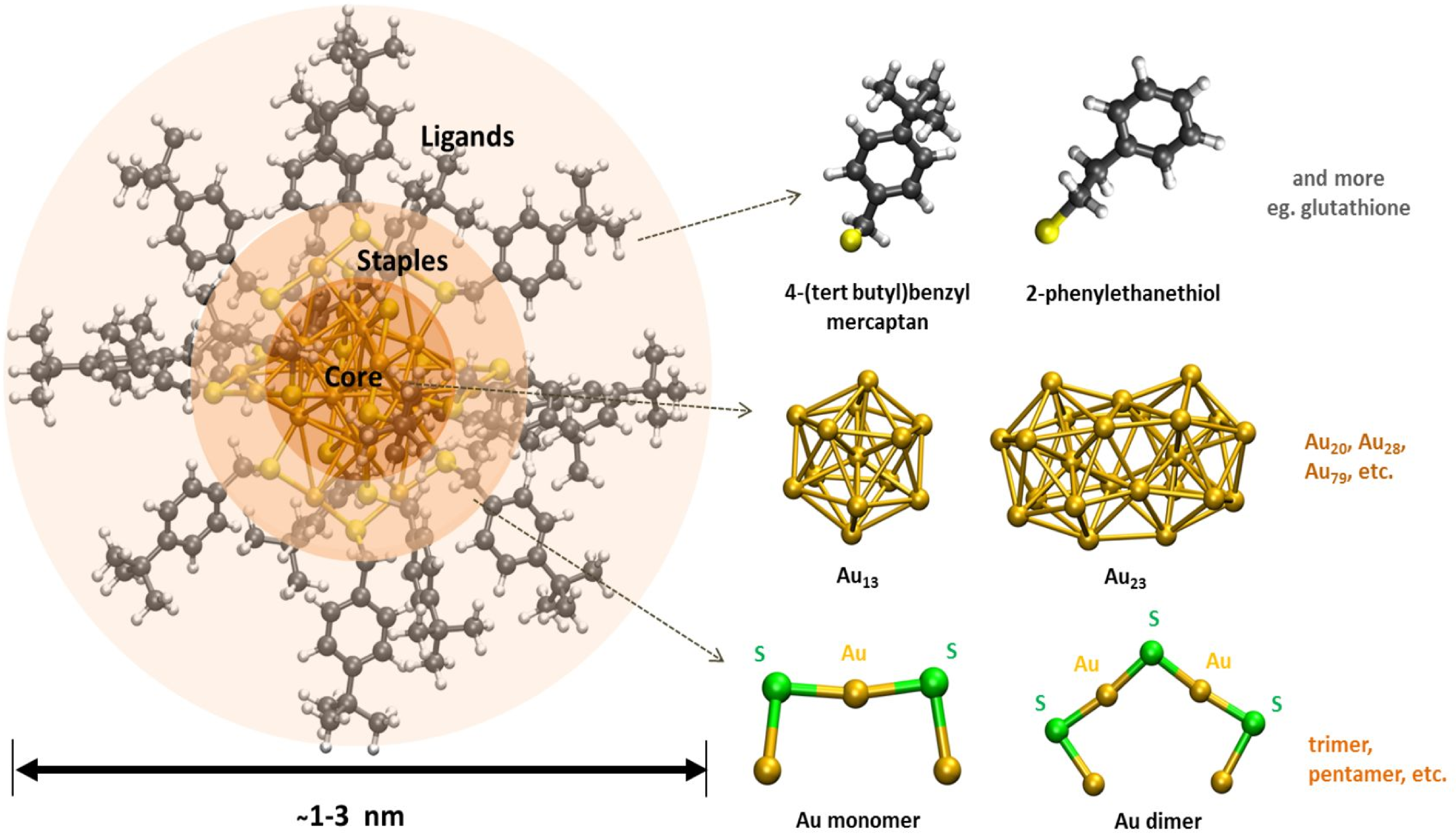
THEMATIC UNIT OF EXCELLENCE

CiHS, IIT Madras, September 8, 2025

Atomically precise metal clusters as material
s



T. Pradeep et. al. *Acc. Chem. Res.* 2018; 201
9

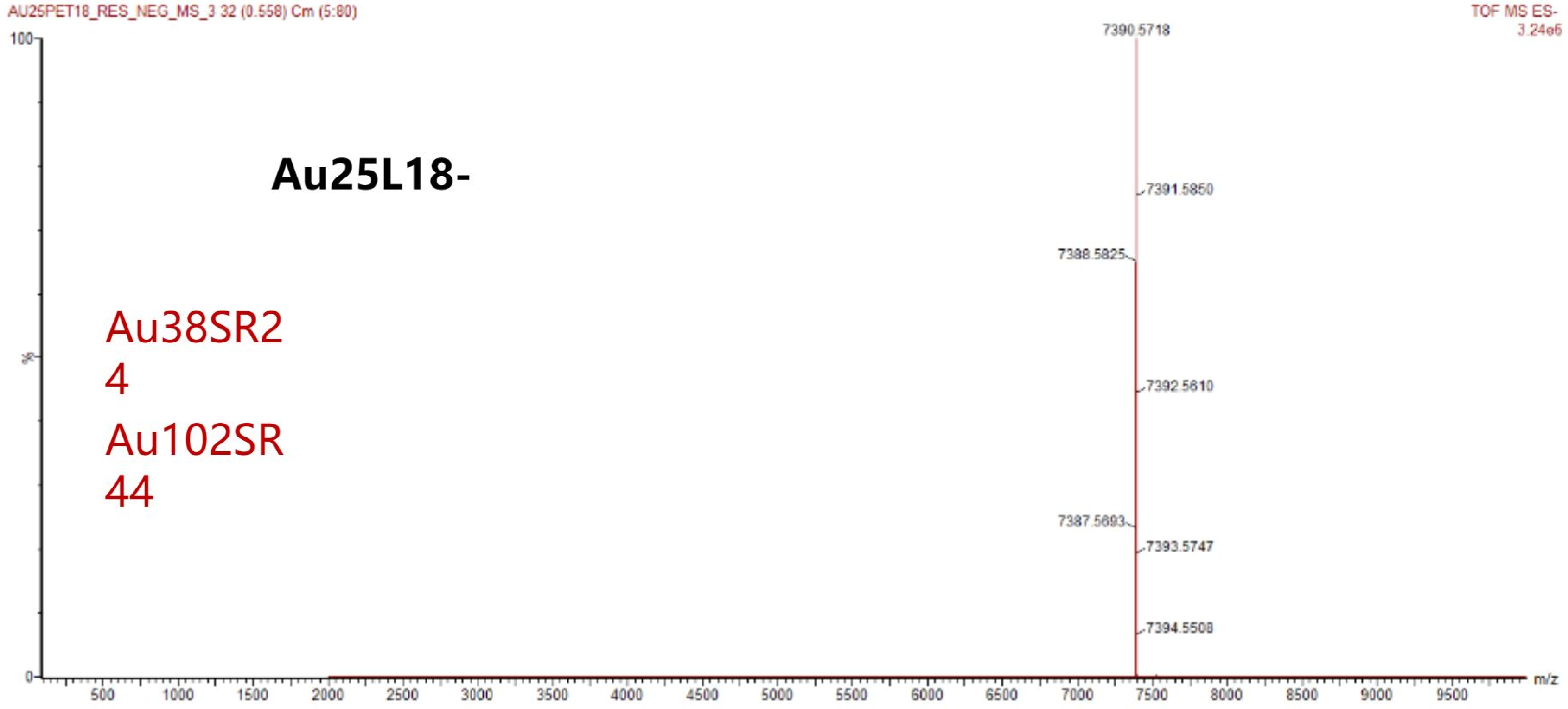


Ligands
Staples
Core
~1-3 nm
4-(tert butyl)benzyl mercaptan
2-phenylethanethiol
and more
eg. glutathione
Au_{13}
Au_{23}
Au_{20}, Au_{28},
Au_{79}, etc.
S
Au
S
Au monomer
S
Au
Au
S
S
Au dimer
trimer,
pentamer, etc.

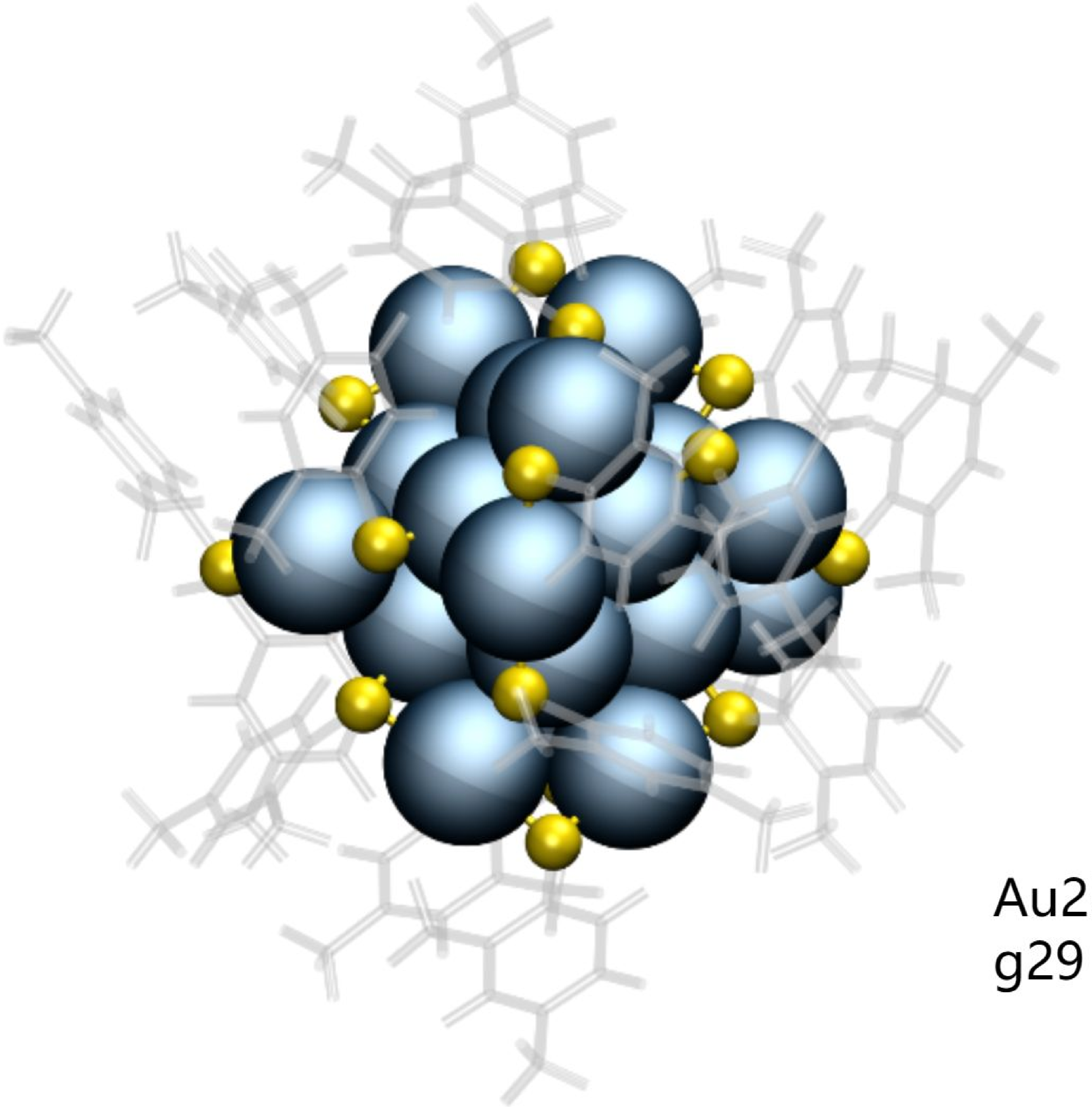
Citations: >220
0

Also the pioneering work of R. W. Murray, Robert L. Whetten, Uzi Landman, Robert Dickson, Tatuya Tsukuda, Yuichi Negishi, Hannu Hakkinen, Rongchao Jin, Nanfeng Zheng, Terry Bigioni, Osman Bakr, Kornberg, Jianping Xie, C. M. Aikens, Thomas Buergi, Amala Dass, Ackerson, De-en Jiang, ... A. W. Castle man Jr., H. Schmidbauer, ... Robin Ras, Olli Ikkala....

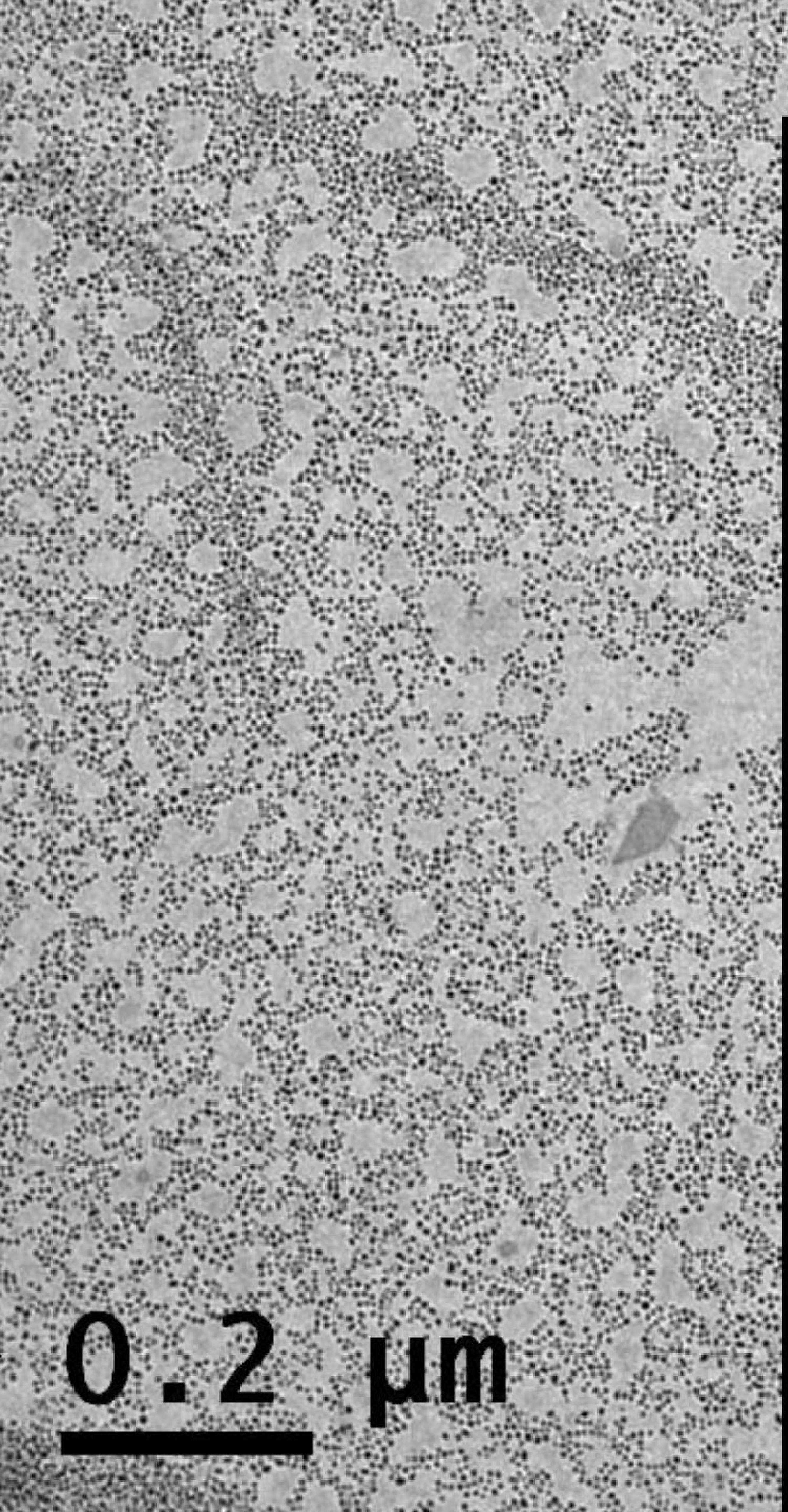
Molecular formula, Molecular weight

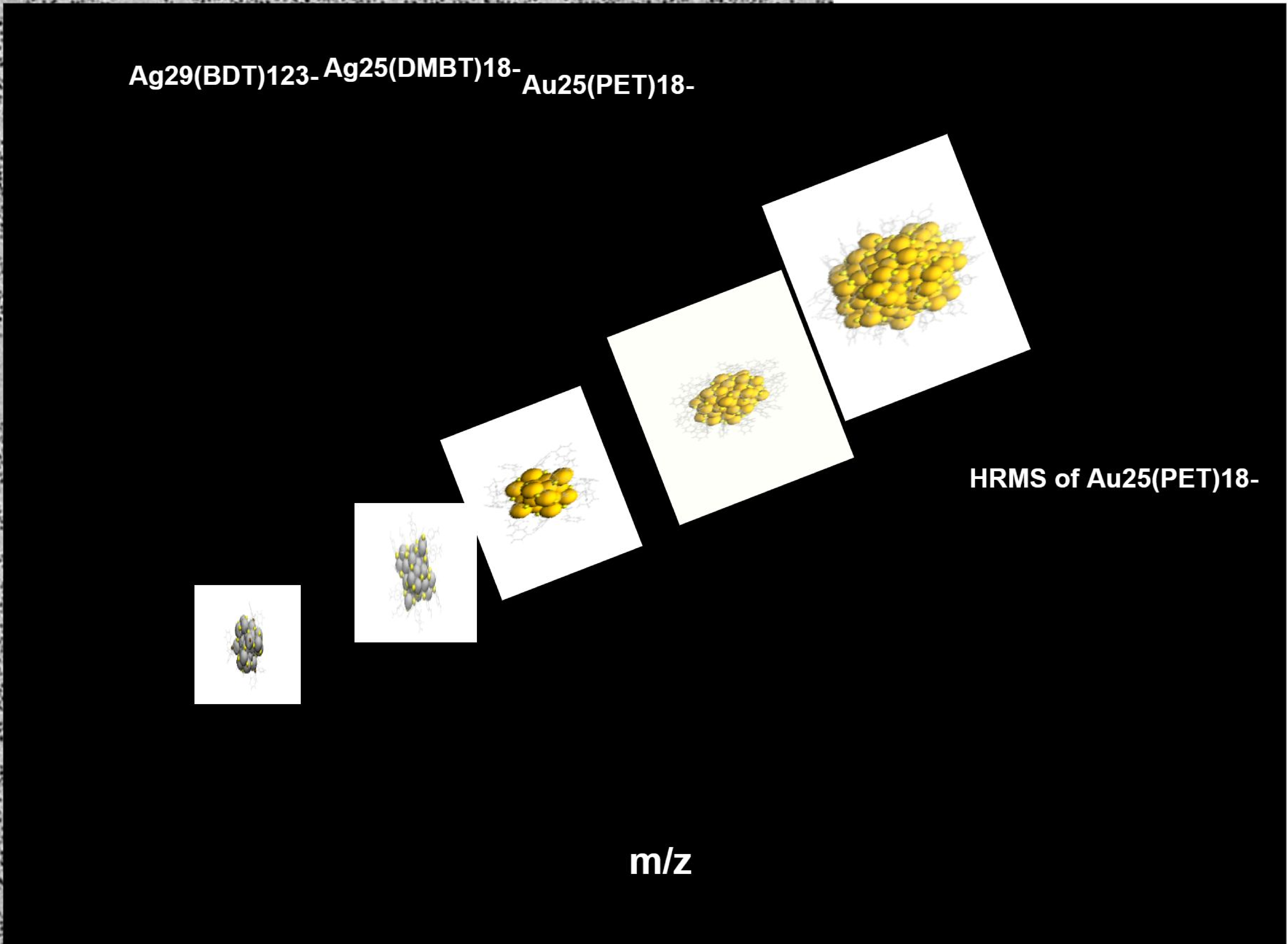


New molecules



Au25, Ag25, Ag29


0.2 µm


Ag29(BDT)123-
Ag25(DMBT)18-
Au25(PET)18-
HRMS of Au25(PET)18-
m/z

Molecular materia
ls

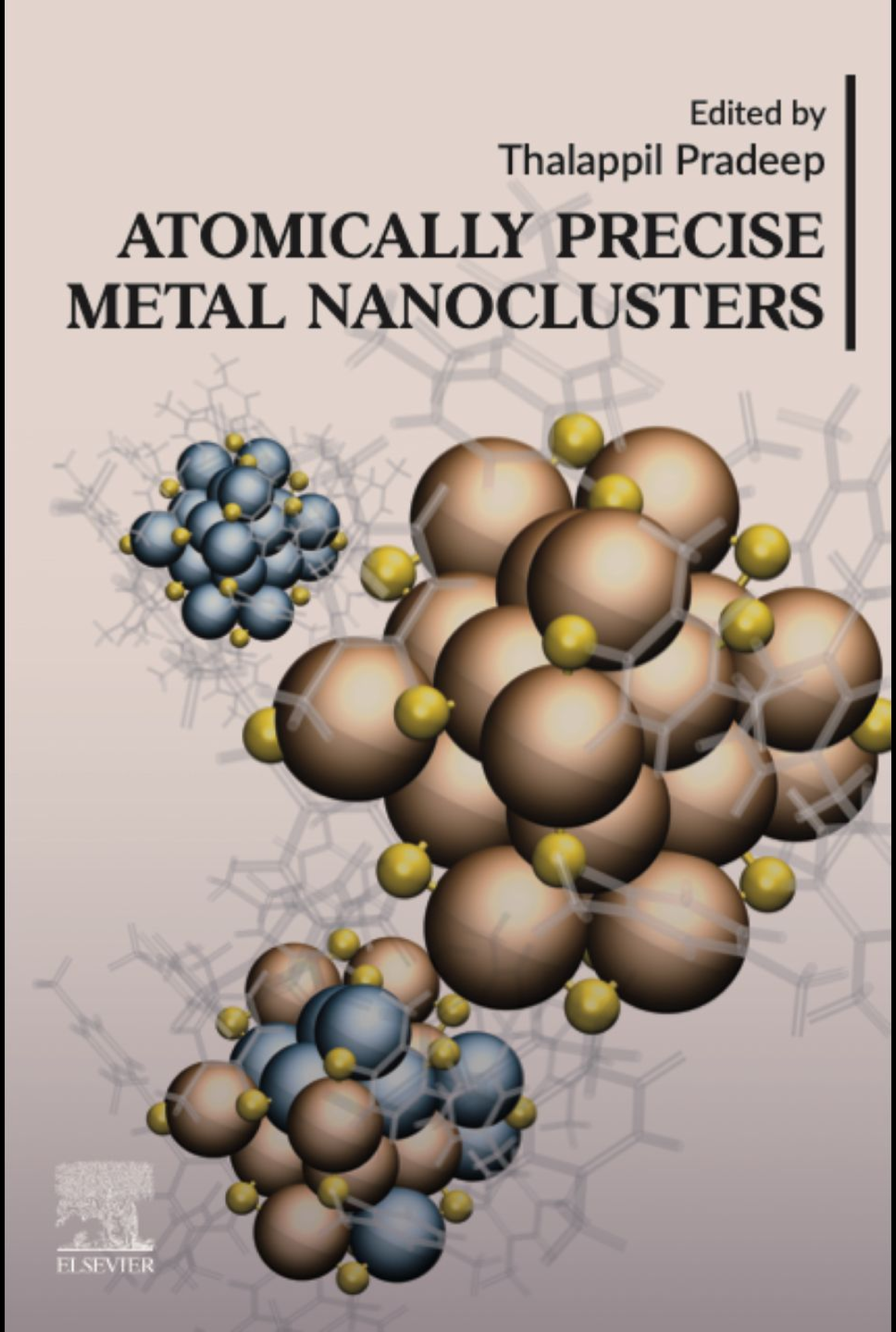
Molecules and their properties

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

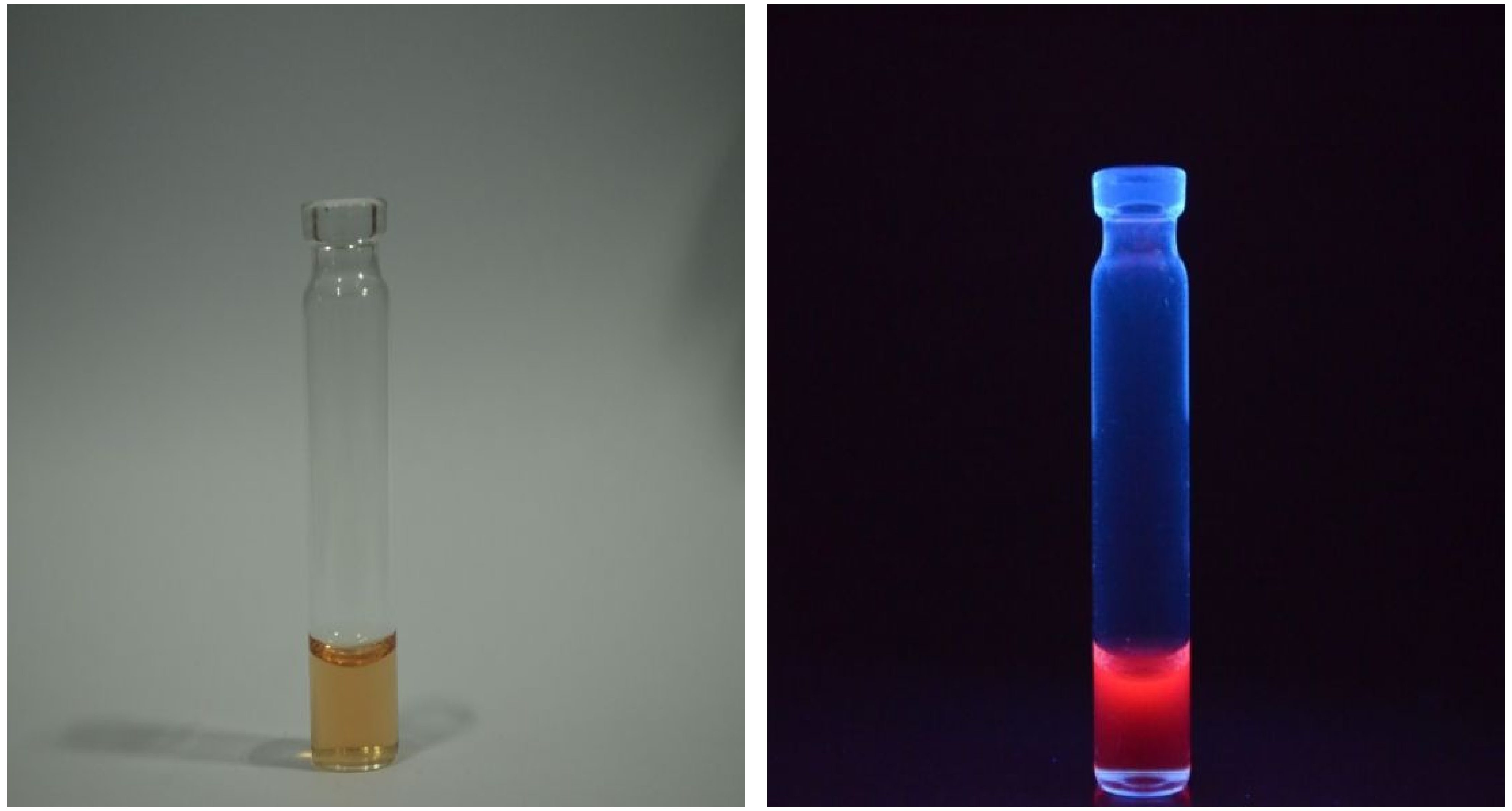
Phases - phase transitions
Physical properties
Electrical, magnetic
Mechanical properties
Electrochemical properties

Future?



Gordon Research Conference

Molecular reactions



Reactions on clusters

Reactions between clusters

Inter-cluster reactions

J|A|C|S
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
Article
pubs.acs.org/JACS

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

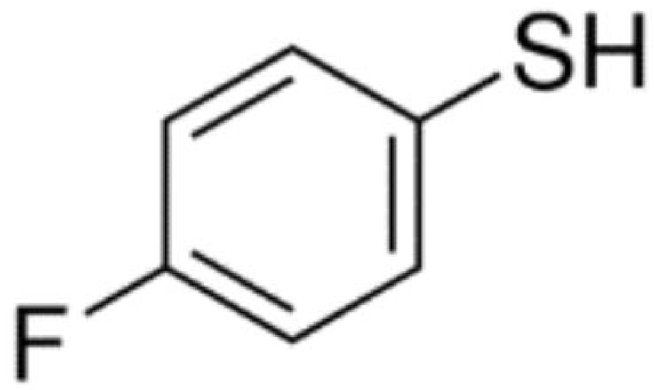
K. R. Krishnadas, Atanu Ghosh, Ananya Baksi, Indranath Chakraborty,[†] Ganapati Natarajan, and Thalappil Pradeep*

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

$A + B \rightarrow C + D$

Au25(FTP)18 + Ag44(FTP)30 Au25-xAgx(FTP)18



Energies for the substitution reaction of (A) Au in $Ag_{44}(SR)_{30}$, (B) Ag in $Au_{25}(SR)_{18}$ and (C) the overall reaction energies (in eV) as a function of their positions in product clusters, $Au_xAg_{44-x}(SR)_{30}$ and $Au_{25-x}Ag_x(SR)_{18}$ 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, $[Ag_{25}Au_{25}(DMBT)_{18}(PET)_{18}]^{2-}$

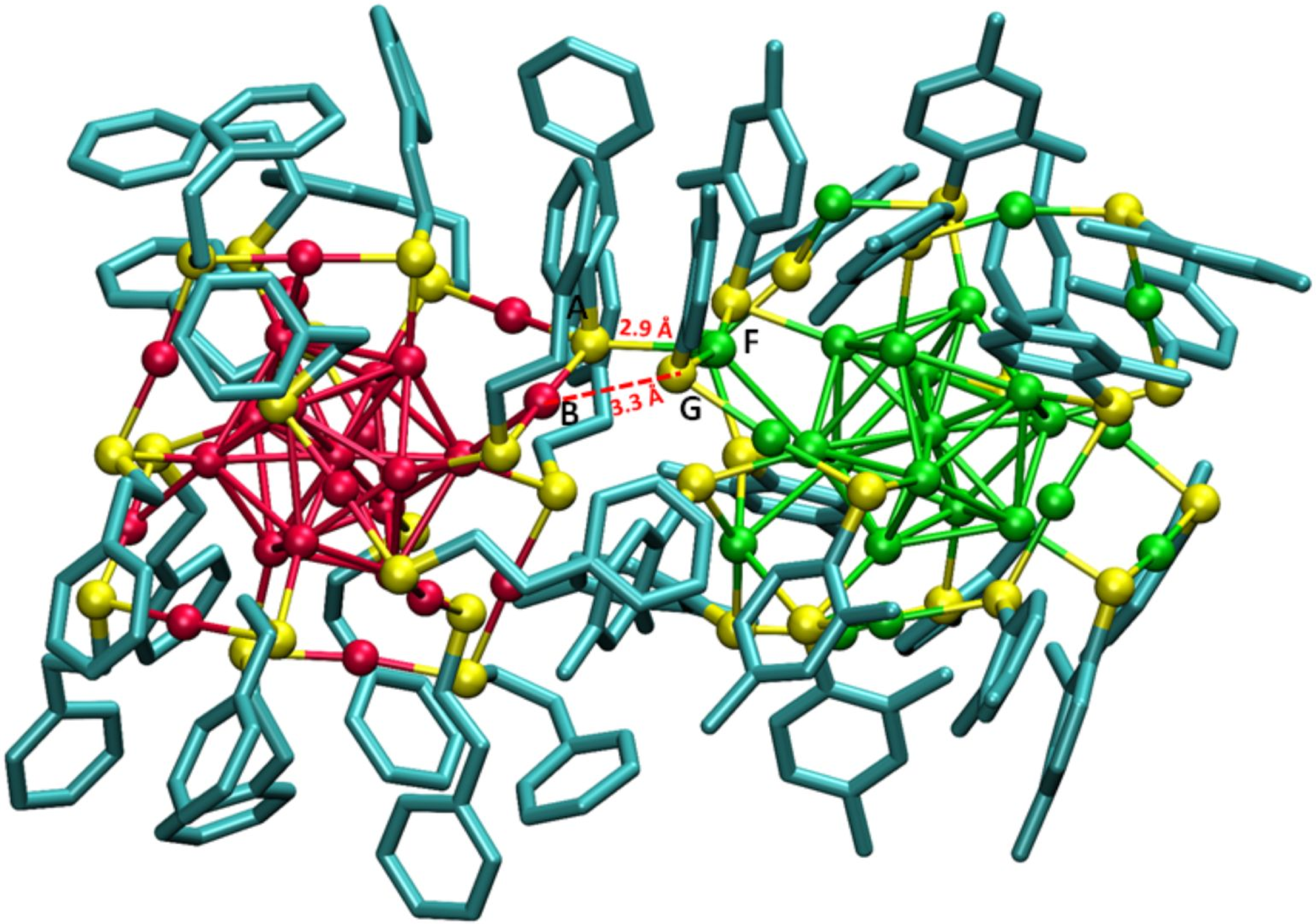
within 5 min

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

0.3:1.0

within 2 min

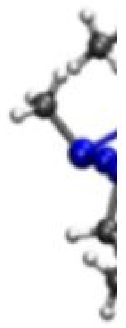
Optimised structure of [Ag25Au25(DMBT)18(PET)18]2-



How do we comprehend this?

Nomenclature

i)



ii)

32°

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PROJECTS

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- ADVICE FOR PROJECT REVIEWERS
- PROJECT REVIEW PROCEDURE
- INFORMATION FOR TASK GROUP CHAIRS

Naming naked and monolayer protected atomically precise metal nanoclusters

Project No.:	2024-014-2-500
Start Date:	1 Apr 2025
End Date:	
Cite:	https://iupac.org/project/2024-014-2-500
Division:	Analytical Chemistry Division

Objective | Description | Progress | Partners

Objective

The subject of atomically precise clusters (APCs), especially the sub-group of atomically precise metal clusters, and even more specifically, atomically precise noble metal clusters, is expanding tremendously. From the discovery of new APCs and their characterisation, the subject is expanding to their properties and applications.

This project will attempt the development of a systematic method for understanding APCs in terms of their (a) classification into various chemical groups, (b) terminologies and (c) naming, taking diverse views into consideration. As the field is growing to include distinct groups of chemical substances in

Chair

Thalappil Pradeep

Members

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Tomas Base
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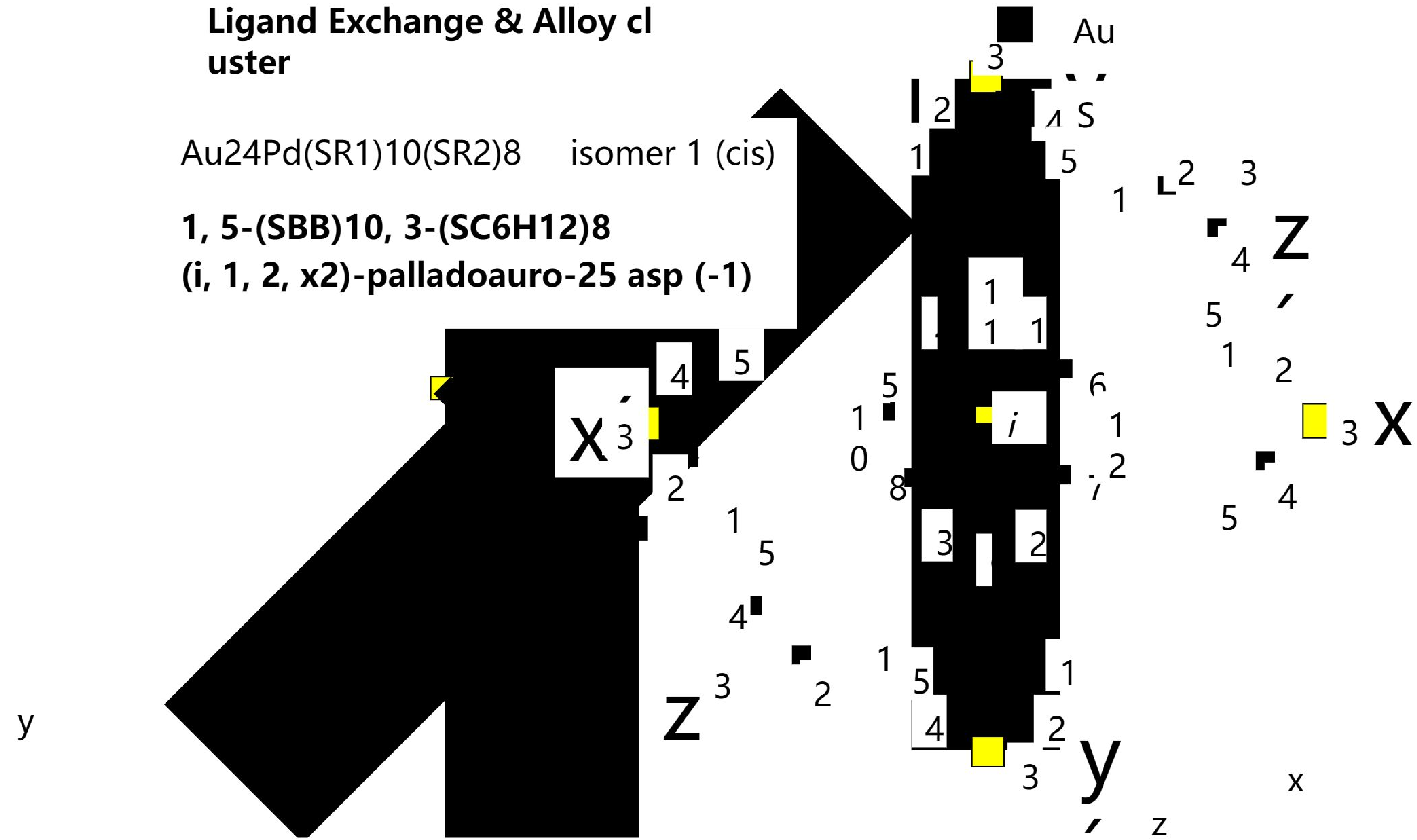
Nonappa Nonappa
Joanna Olesiak-Banska
Sarah Sunah Park
Di Sun
Tatsuya Tsukuda
Robert L. Whetten
Jianping Xie

Aspicule
s

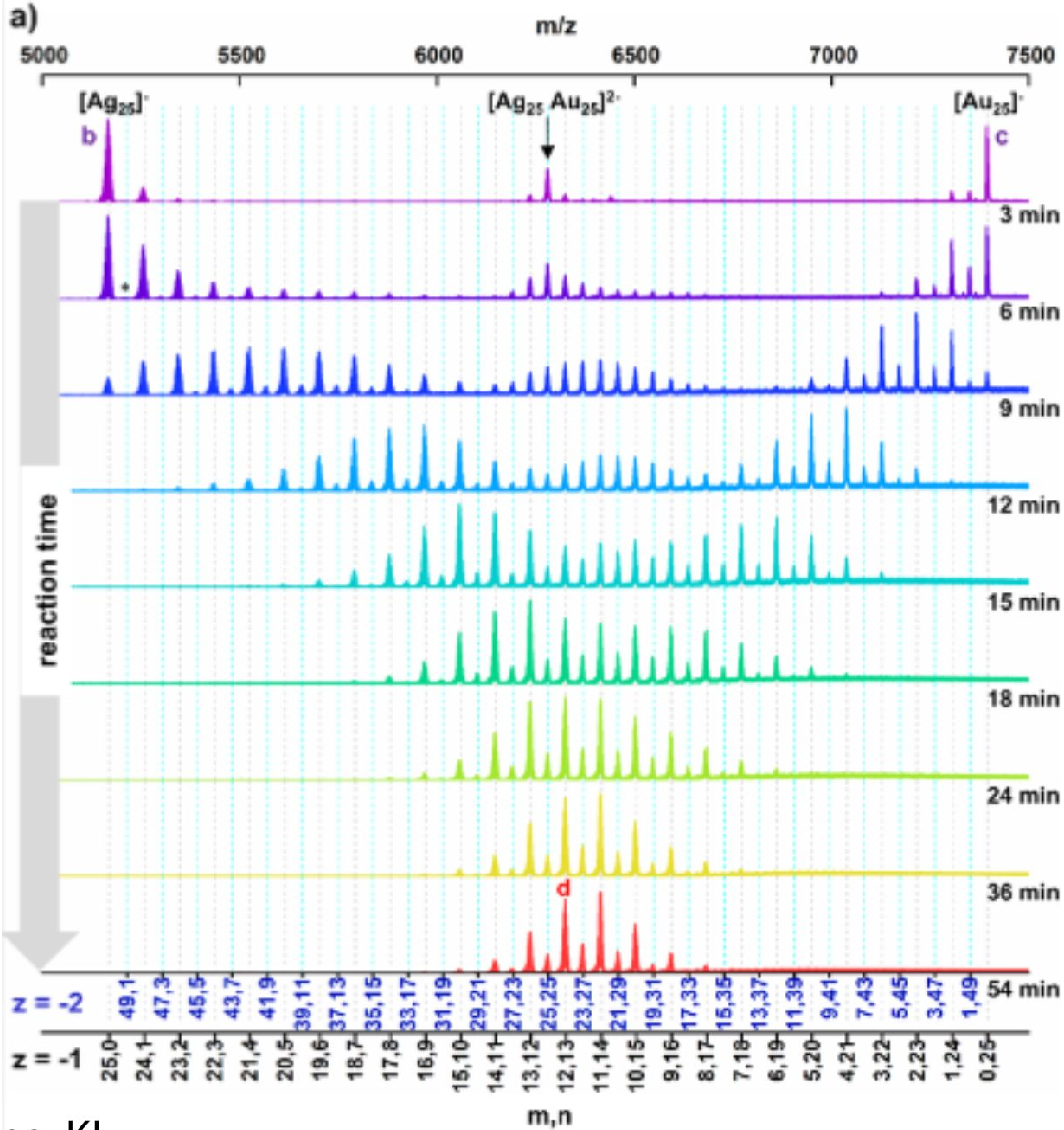
Ligand Exchange & Alloy cl uster

Au24Pd(SR1)10(SR2)8 isomer 1 (cis)

1, 5-(SBB)10, 3-(SC6H12)8
(i, 1, 2, x2)-palladoauro-25 asp (-1)



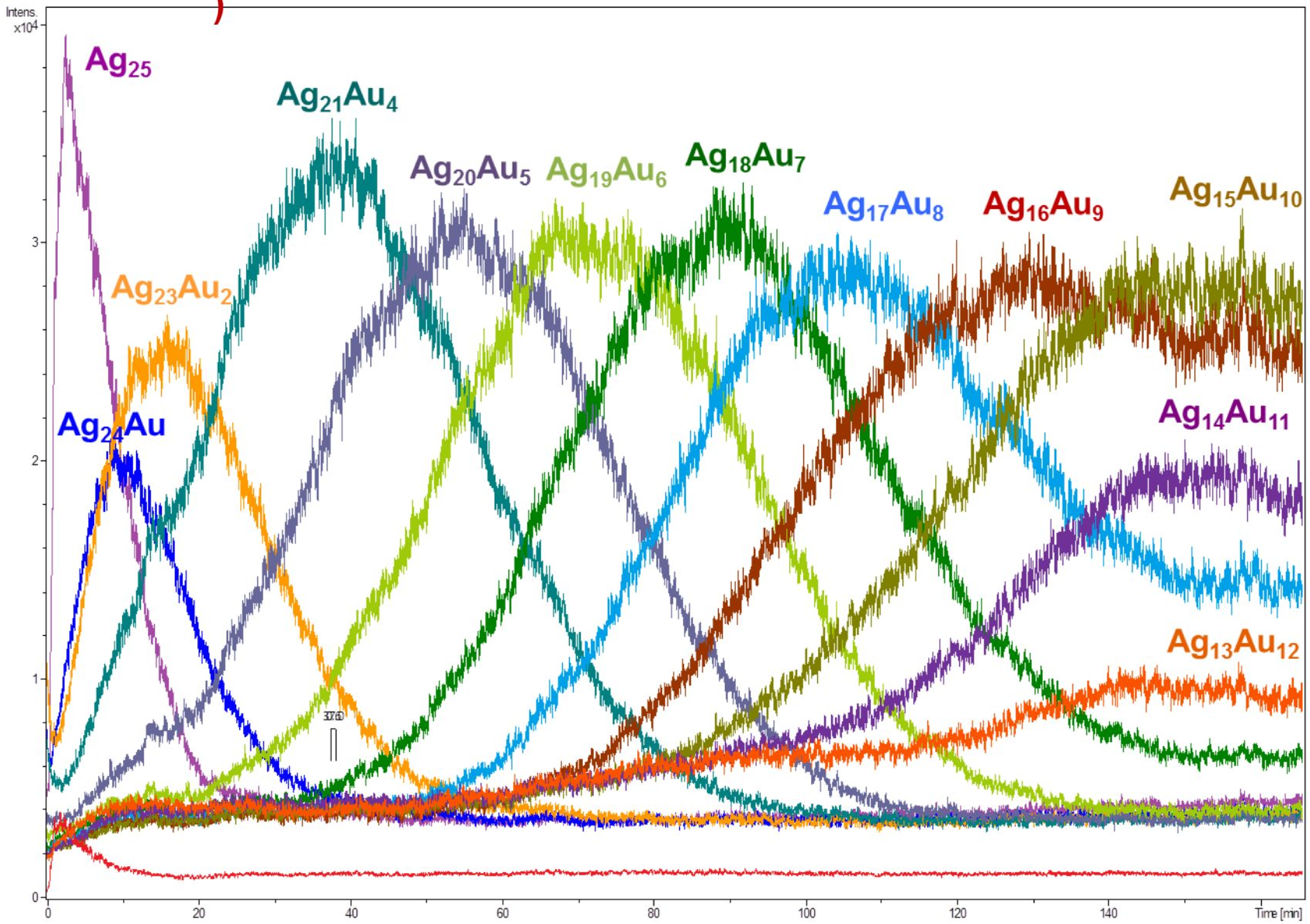
(D1-3,D2-3)-di(2-phenylethylthiolato),16(methylthiolato)-auro-25 aspicul e(1-)



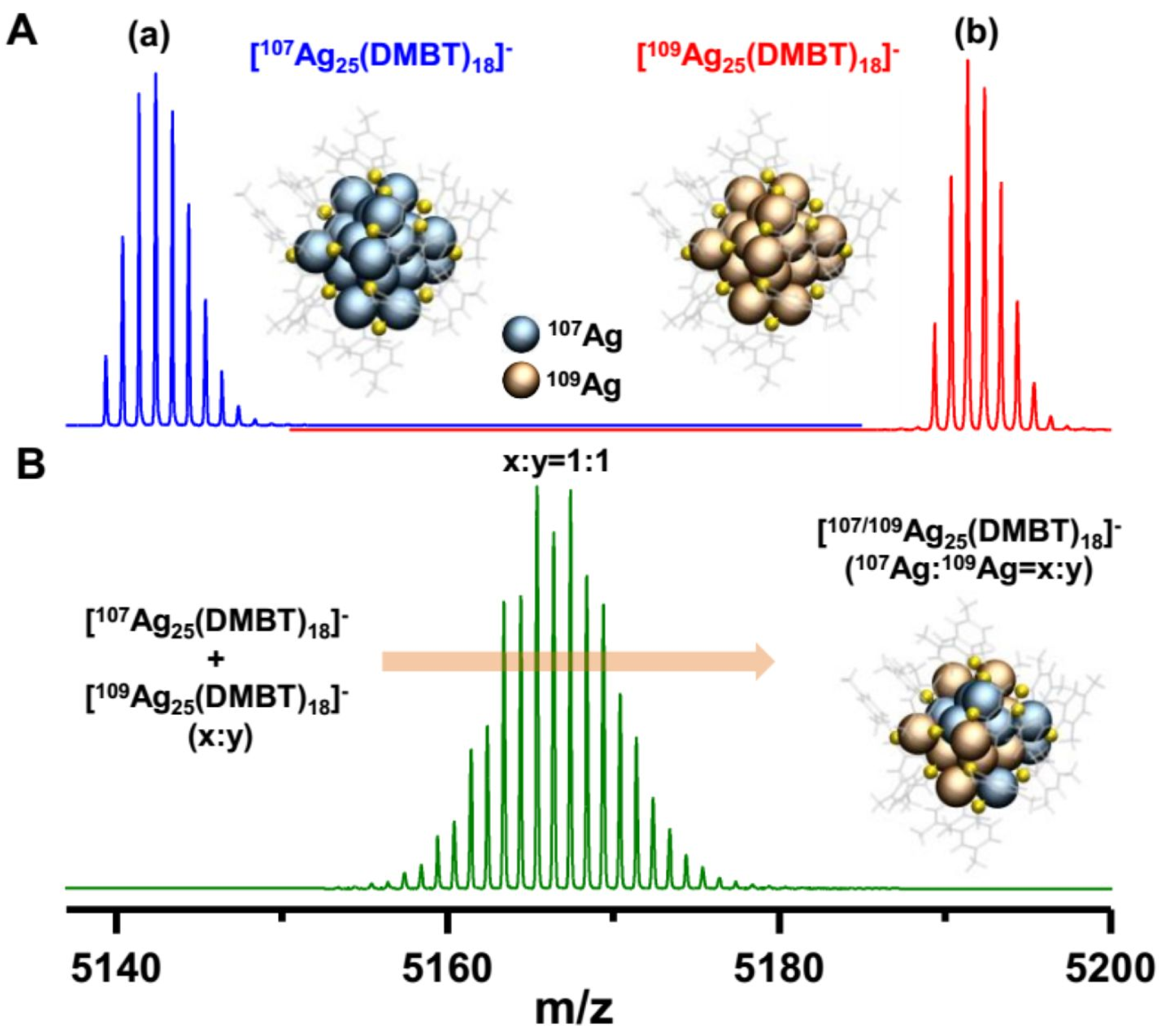
Manfred Kappes, KIT

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

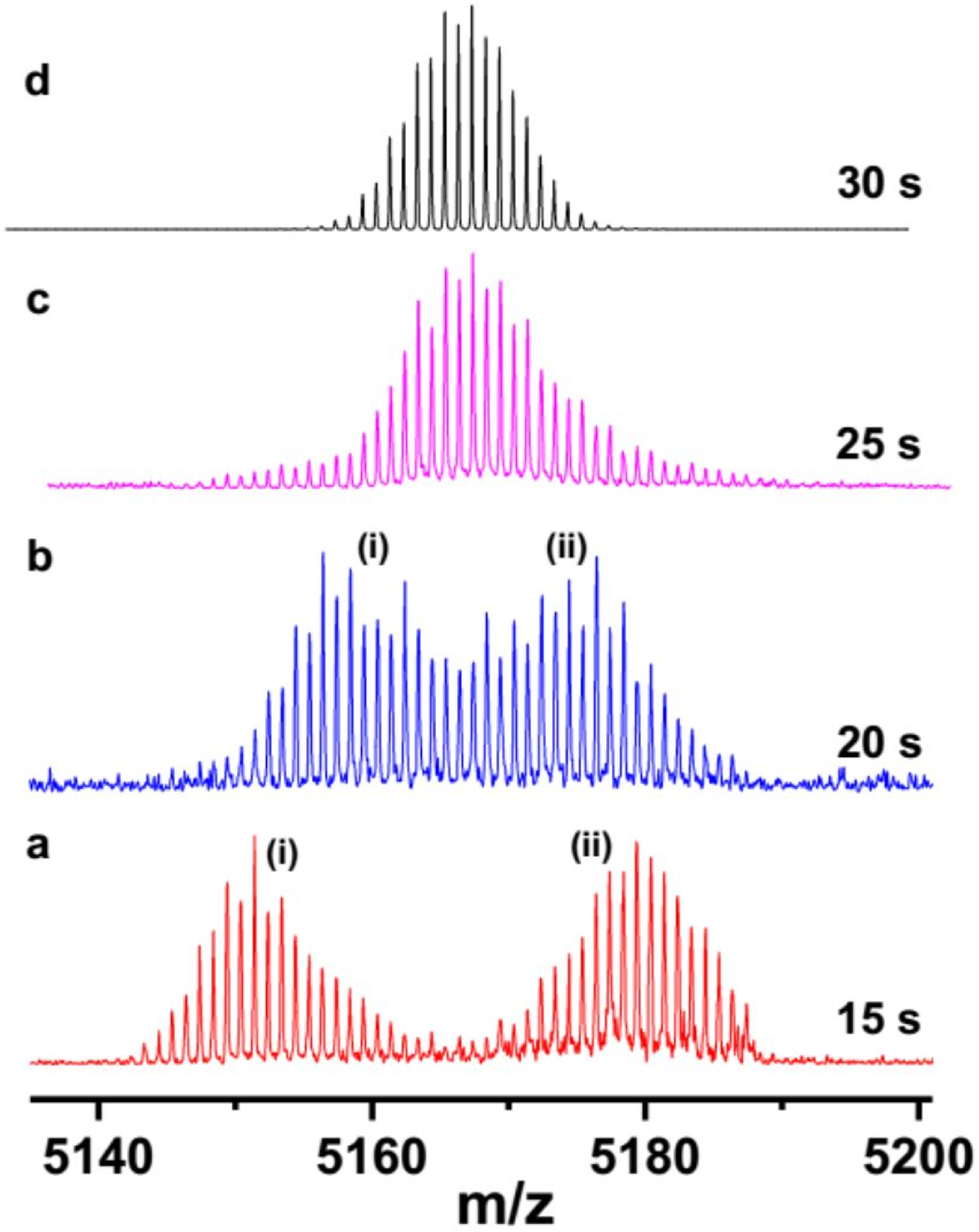
Kinetics of the exchange (monitored on the Ag25 side
)



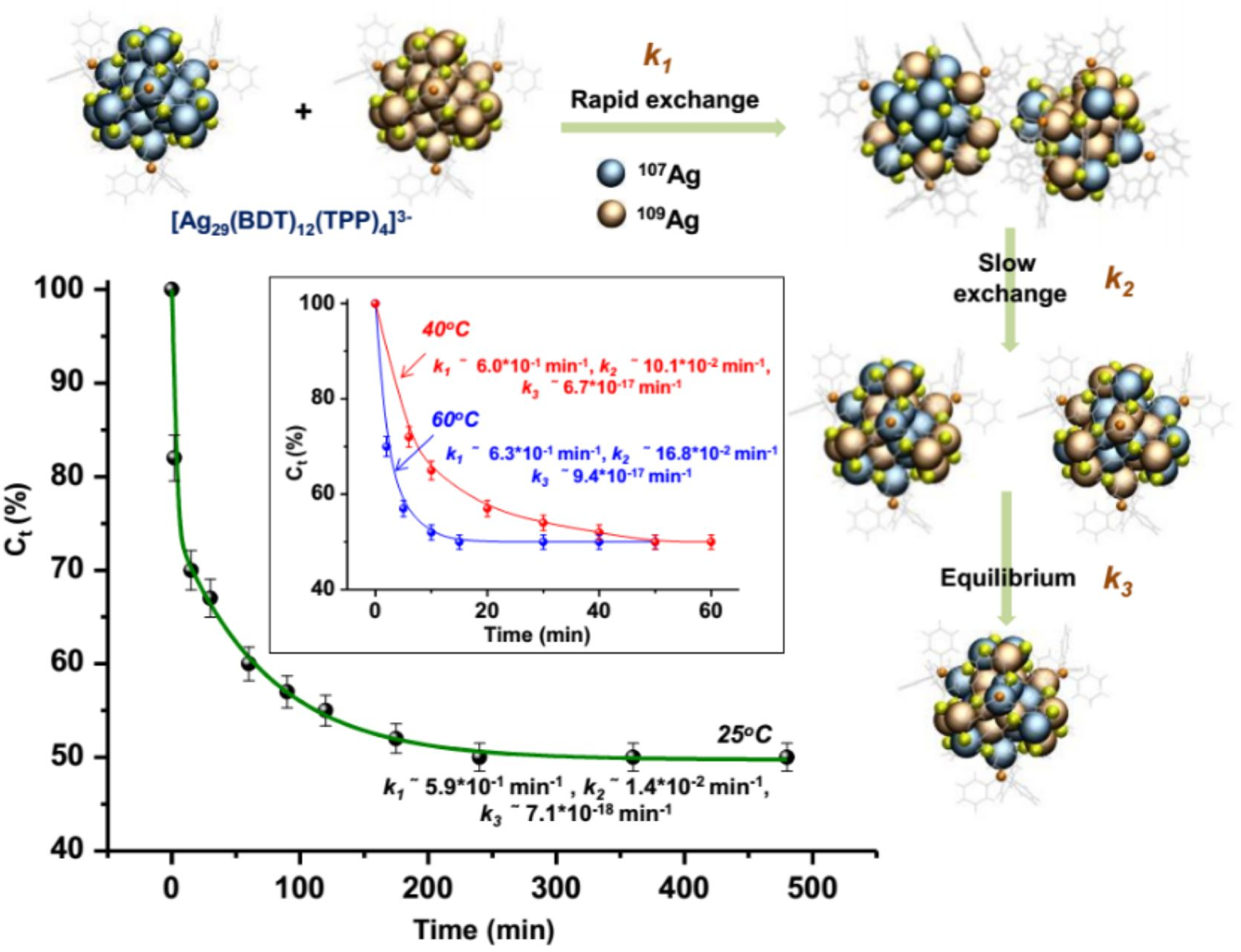
ESI MS of **A)** 107Ag25(DMBT)18 and **B)**109Ag25(DMBT)18. Insets shows the respective isotope patte
rns.



A
(a)
[$^{107}Ag_{25}(DMBT)_{18}]^-$
[$^{109}Ag_{25}(DMBT)_{18}]^-$
(b)
^{107}Ag
^{109}Ag
B
x:y=1:1
[$^{107/109}Ag_{25}(DMBT)_{18}]^-$
(^{107}Ag:^{109}Ag=x:y)
[$^{107}Ag_{25}(DMBT)_{18}]^-$
+
[$^{109}Ag_{25}(DMBT)_{18}]^-$
(x:y)
5140
5160
5180
5200
m/z



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

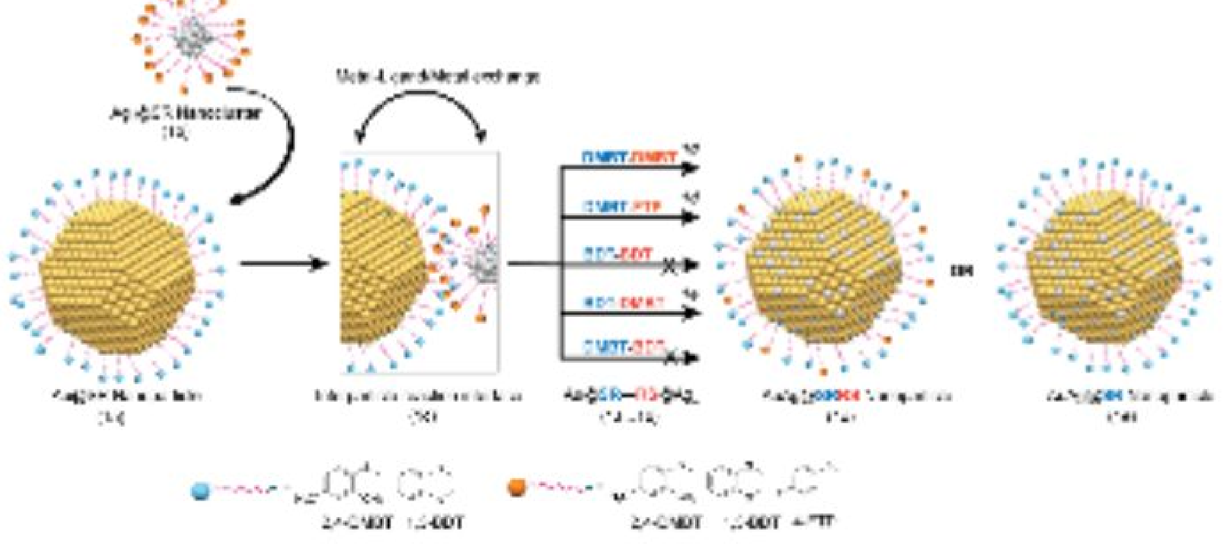


k1
Rapid exchange
107Ag
109Ag
[Ag29(BDT)12(TPP)4]3-
Slow exchange
k2
Equilibrium
k3
Ct (%)
Time (min)
25oC
k1 ~ 5.9*10-1 min-1 , k2 ~ 1.4*10-2 min-1,
k3 ~ 7.1*10-18 min-1
40oC
k1 ~ 6.0*10-1 min-1, k2 ~ 10.1*10-2 min-1,
k3 ~ 6.7*10-17 min-1
60oC
k1 ~ 6.3*10-1 min-1, k2 ~ 16.8*10-2 min-1
k3 ~ 9.4*10-17 min-1

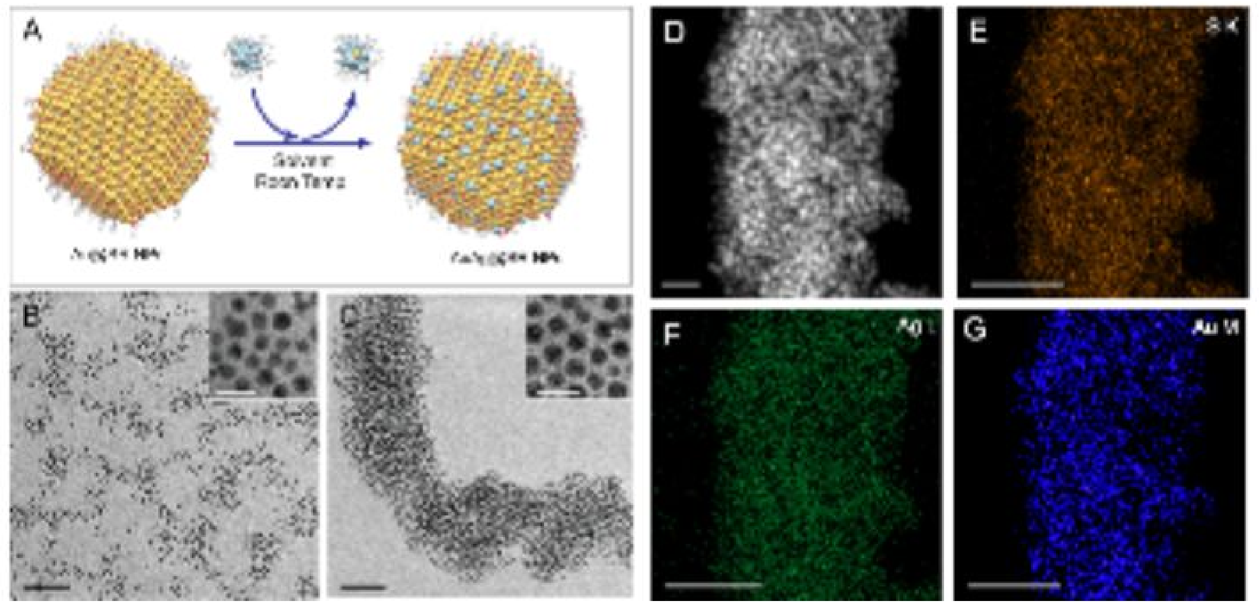
Can clusters react with nanoparticles ?

Ag25 with Au nanoparticles

1

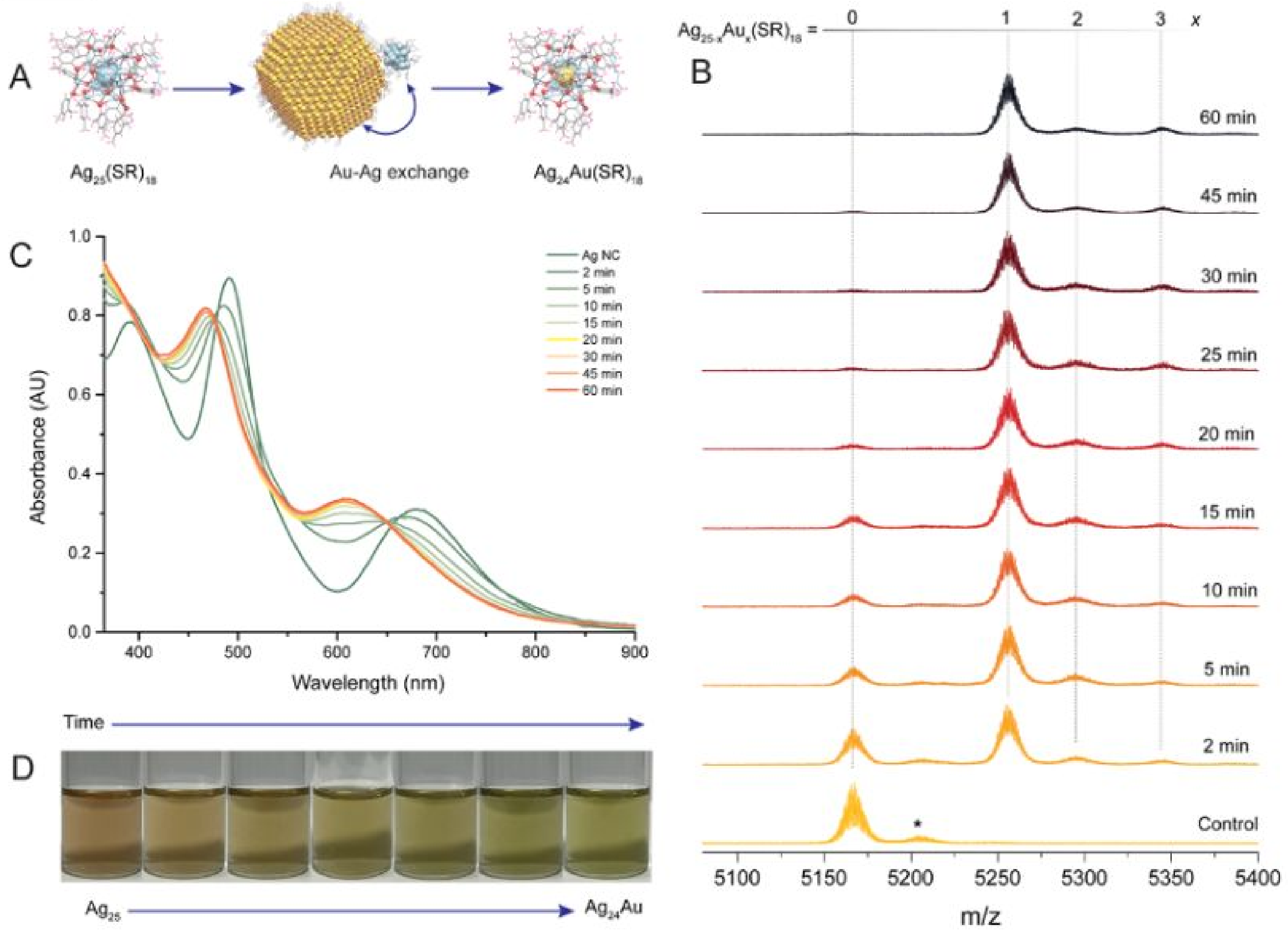


2



Scale bars: 50 nm (B-G) and 10 nm (insets of B and C).

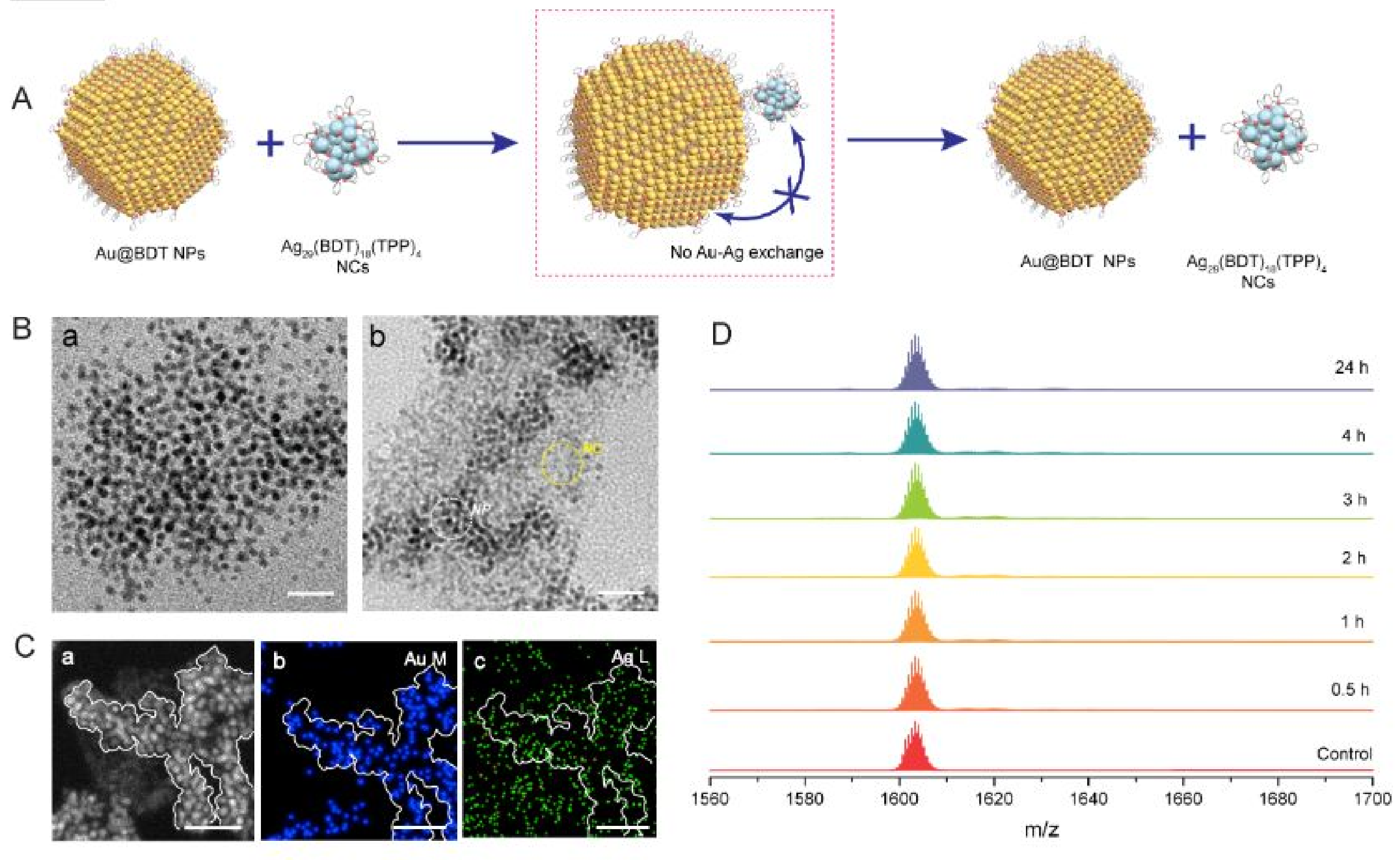
3



Paulami Bose, et al. *Chem. Mat.* 2024

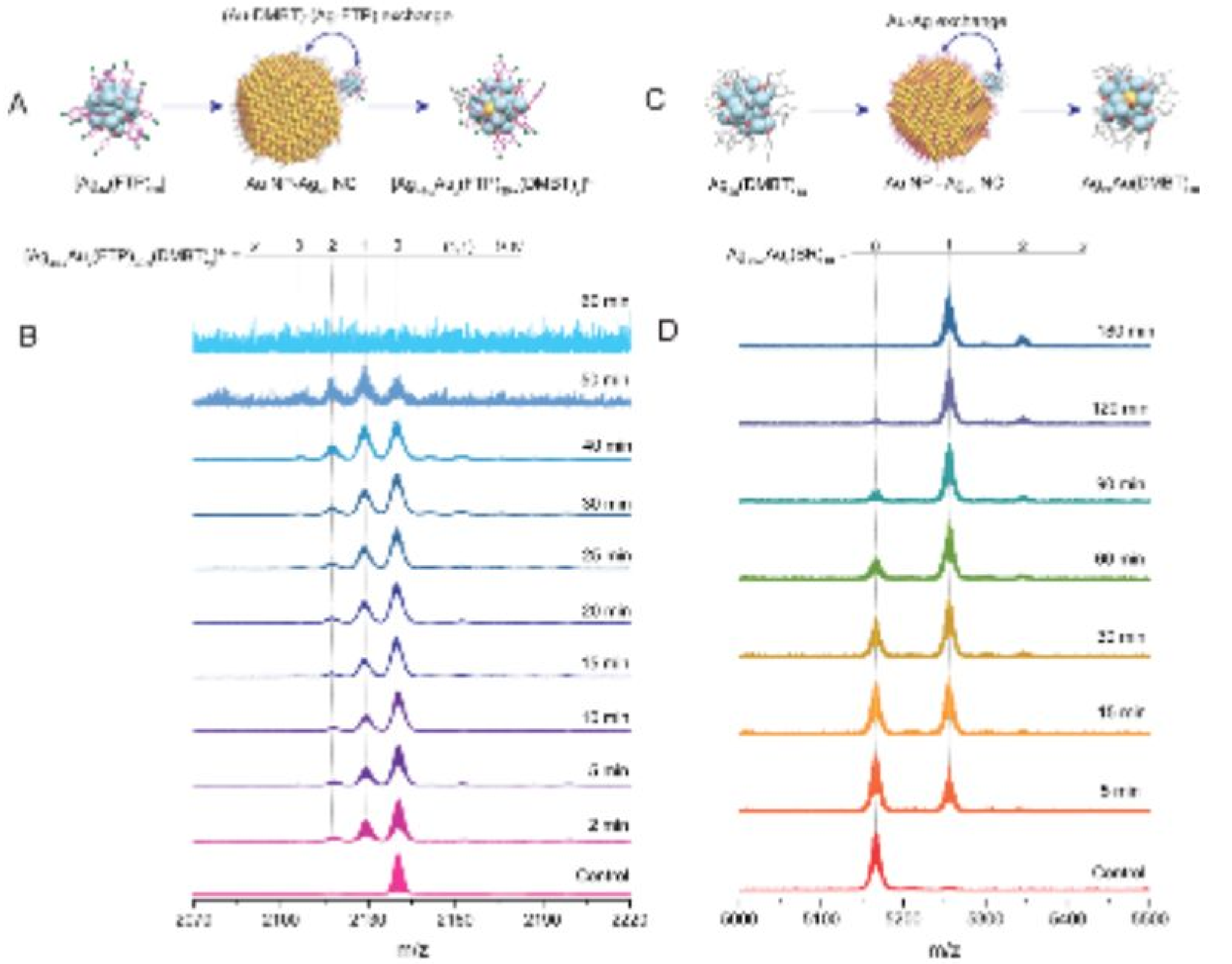
Interface controls the reaction

4



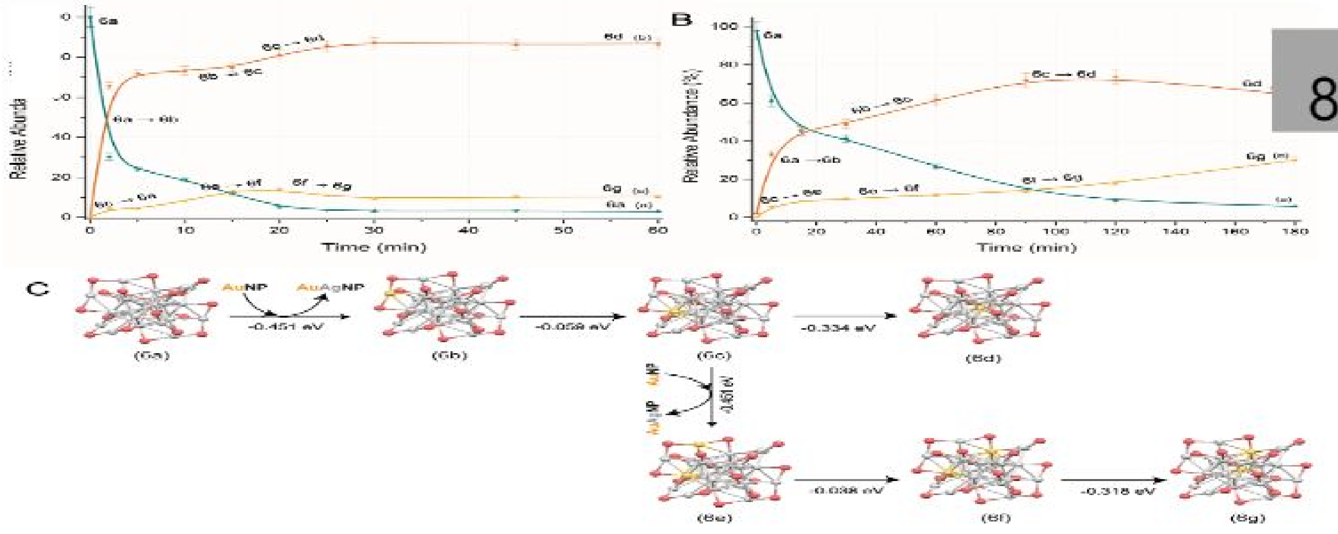
Scale bars: 20 nm

5



Computational insights

6



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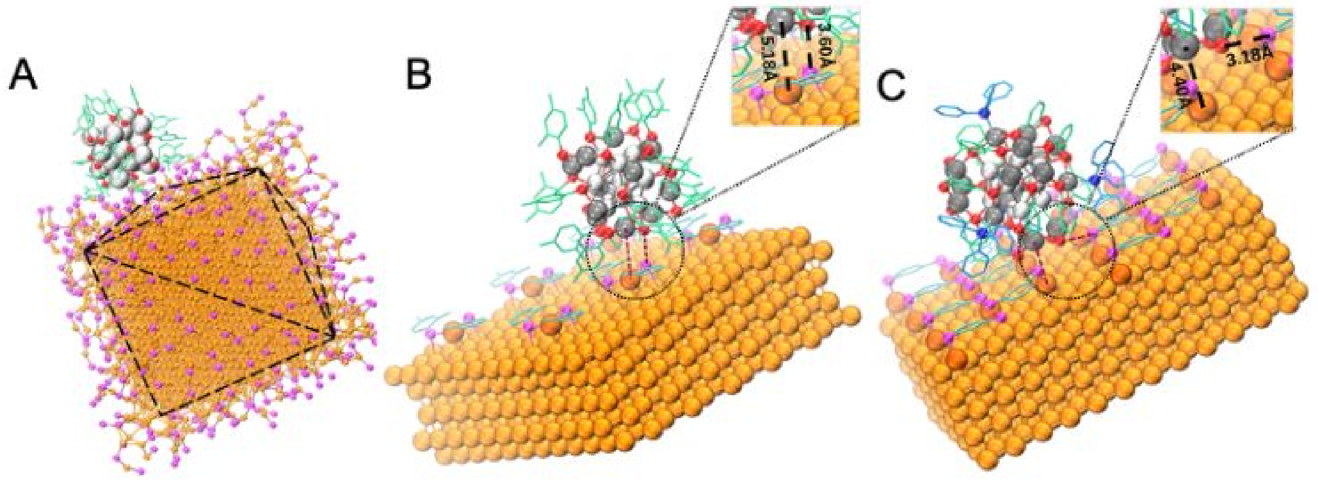

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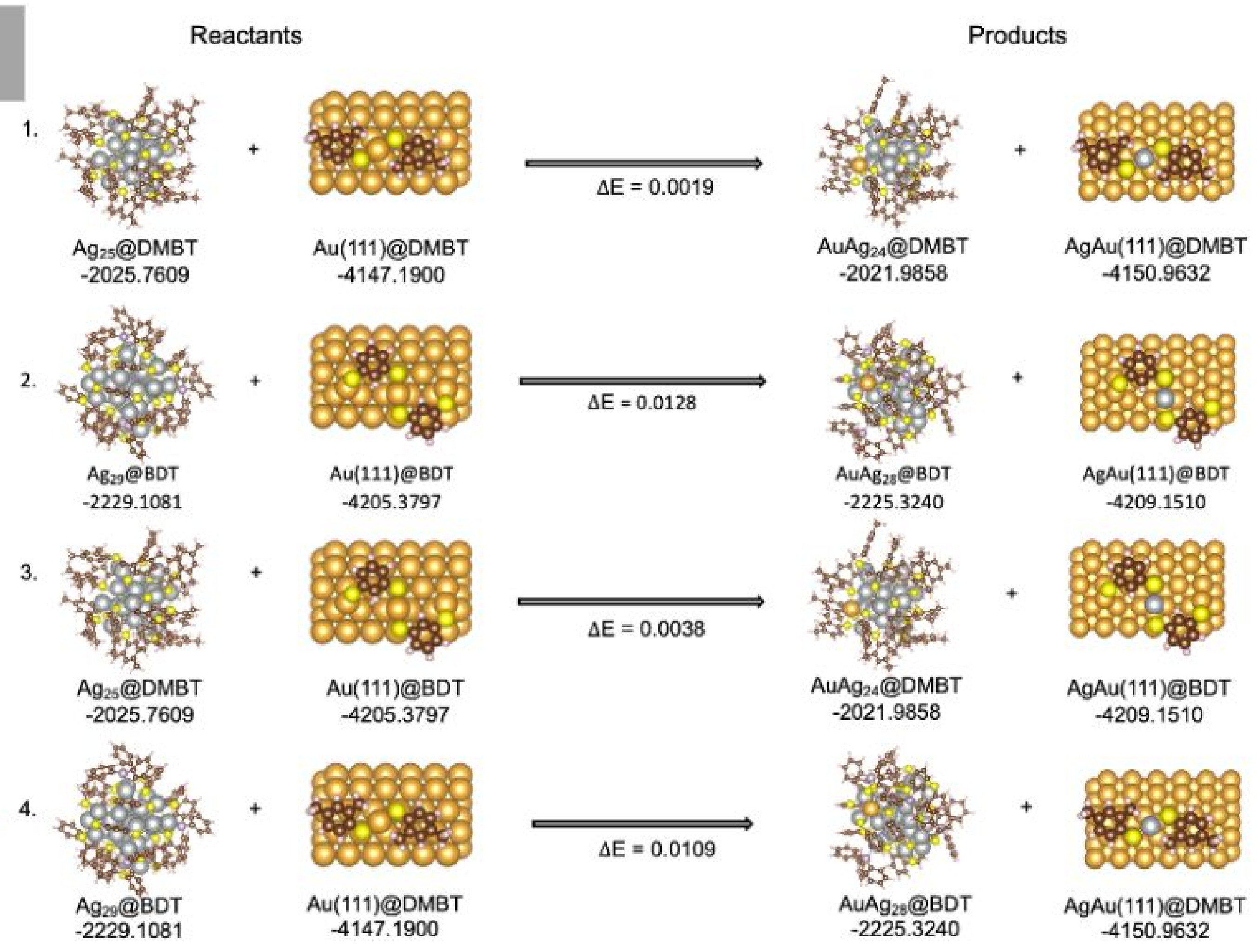


Reactions and new materia ls

Reactions leading to co-crystals

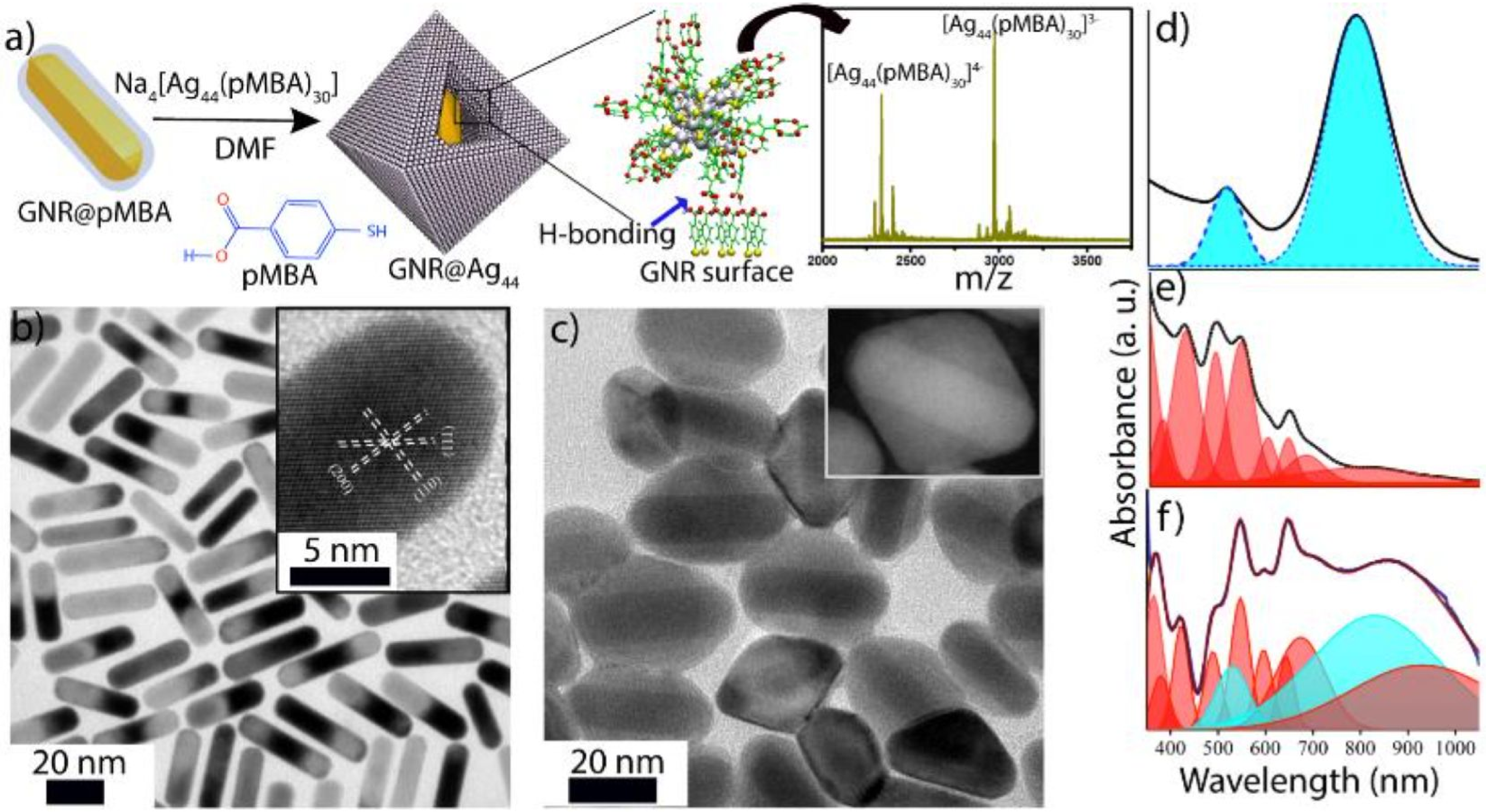
Supramolecular chemistry

Papri Chakraborty, et,. al. *ACS Nano* 2018

Figure 1. A) (a) Full range ESI MS, **(b)** experimental and calculated isotope patterns and **(c)** DFT optimized structure of $[Ag_{29}(BDT)_{12}]^{3-}$ cluster. **B) (a)** ESI MS of $[Ag_{29}(BDT)_{12}(C_{60})_n]^{3-}$ (n=1-4) complexes, **(b)** experimental and calculated isotope patterns of $[Ag_{29}(BDT)_{12}(C_{60})_4]^{3-}$ and **(c)** schematic of the possible structure of $[Ag_{29}(BDT)_{12}(C_{60})_4]^{3-}$.

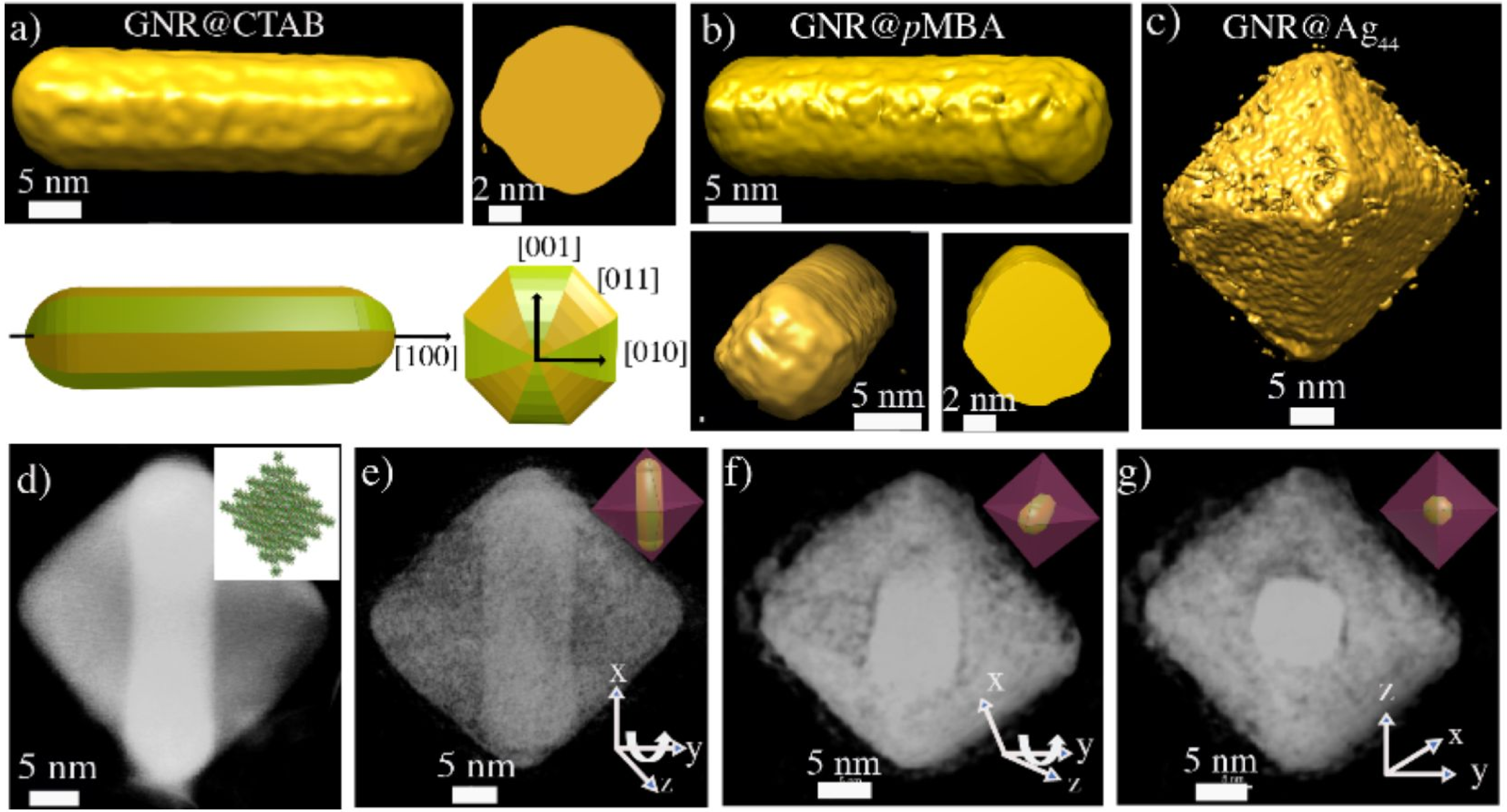
Assemblies and superstructure
s

Atomically precise nanocluster assemblies encapsulating plasmonic gold nanorods

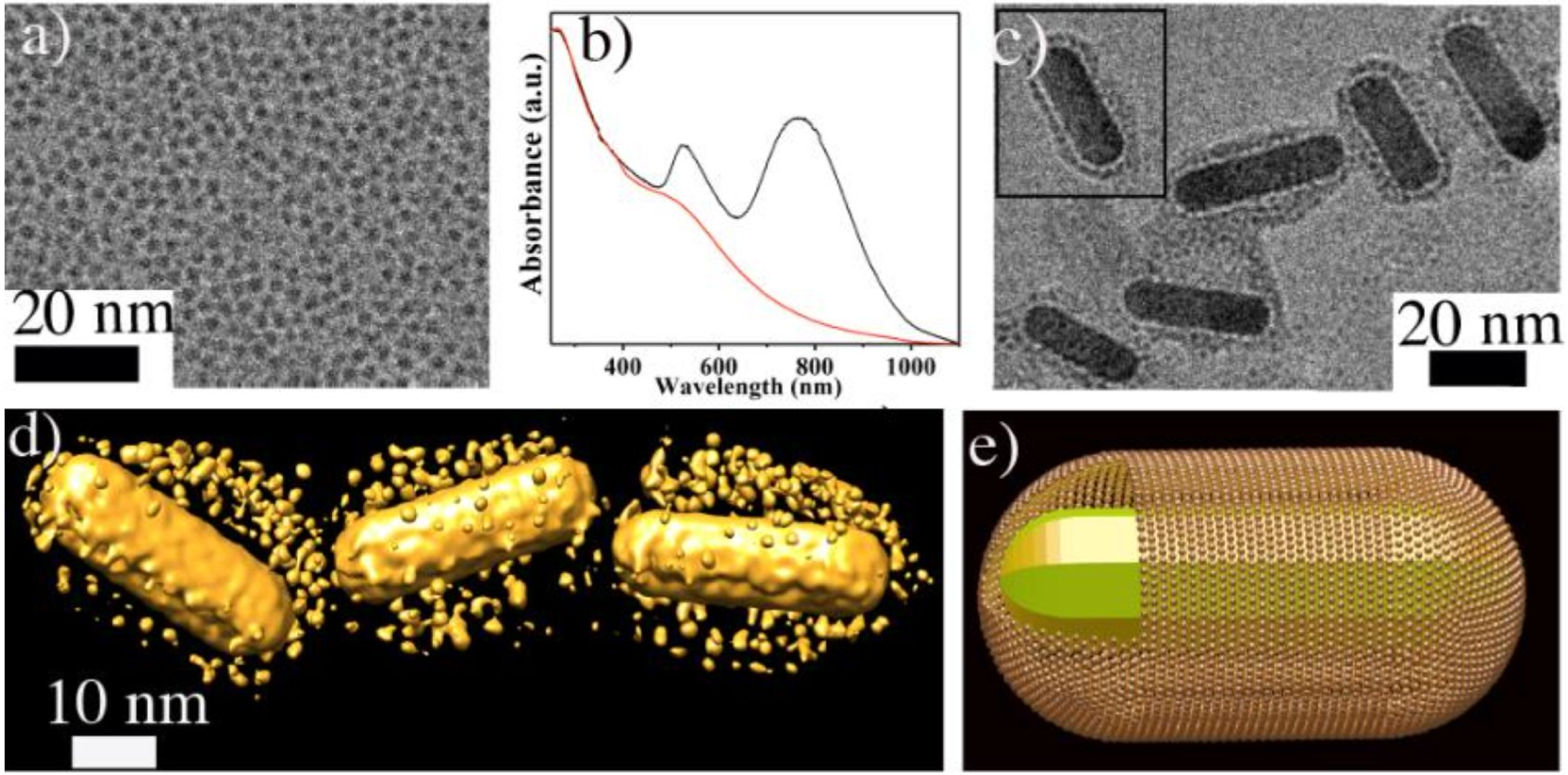


Chakraborty, A. et al., *Angew. Chem. Int. Ed.* **2018,** *57*, 6522–6526.

3D morphological analysis



Works for Au250(*p*MBA)n and aqueous solvent



Co-crystals

Ag40 and Ag46 with the same shell

M. Bodiuzzaman, et. al. *Angew. Chem. Int. Ed.* **2018**

Where are they taking us t
o?

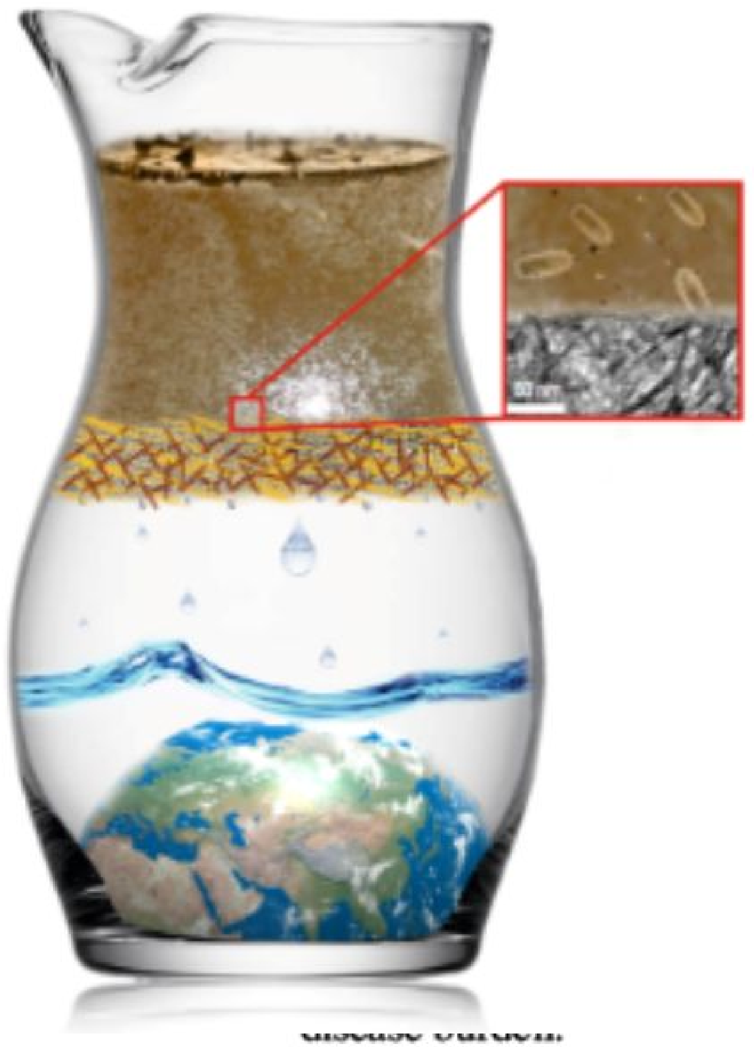
PNAS PNAS PNAS PNAS

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 abc
affordable, all-inclusive drinking water
without electricity. The critical probler
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

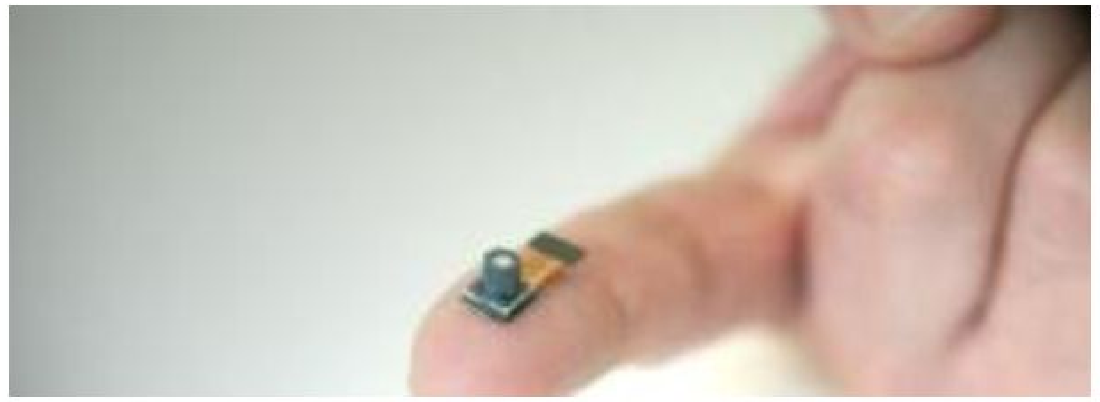
vailable; and (*c*) continued retention
matrix is difficult.
ate a unique family of nanocrystalline
n granular composite materials pre-
ature through an aqueous route. The
mposition is attributed to abundant -O-
on chitosan, which help in the crys-
oxide and also ensure strong covalent
surface to the 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
al antimicrobial activity in drinking
osites have been developed that can
its in water. We demonstrate an af-
device based on such composites de-
nd 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) 8459-846
4.

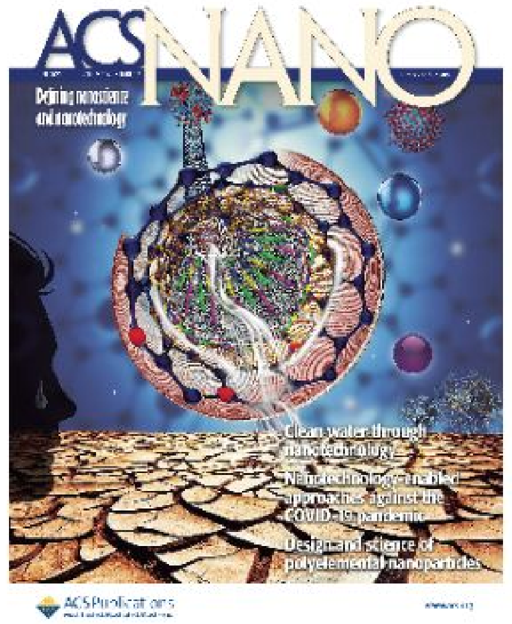

We developed environmentally friendly water positive nanoscale materials for affordable, sustainable and rapid removal of arsenic from drinking water.
There are over 1700 community installations across the country, serving 1.3 million people with arsenic and iron-free water every day.

Sensors and new opportunities



Water quality measurement – In the pipe line

Smart water purifiers and big data



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

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

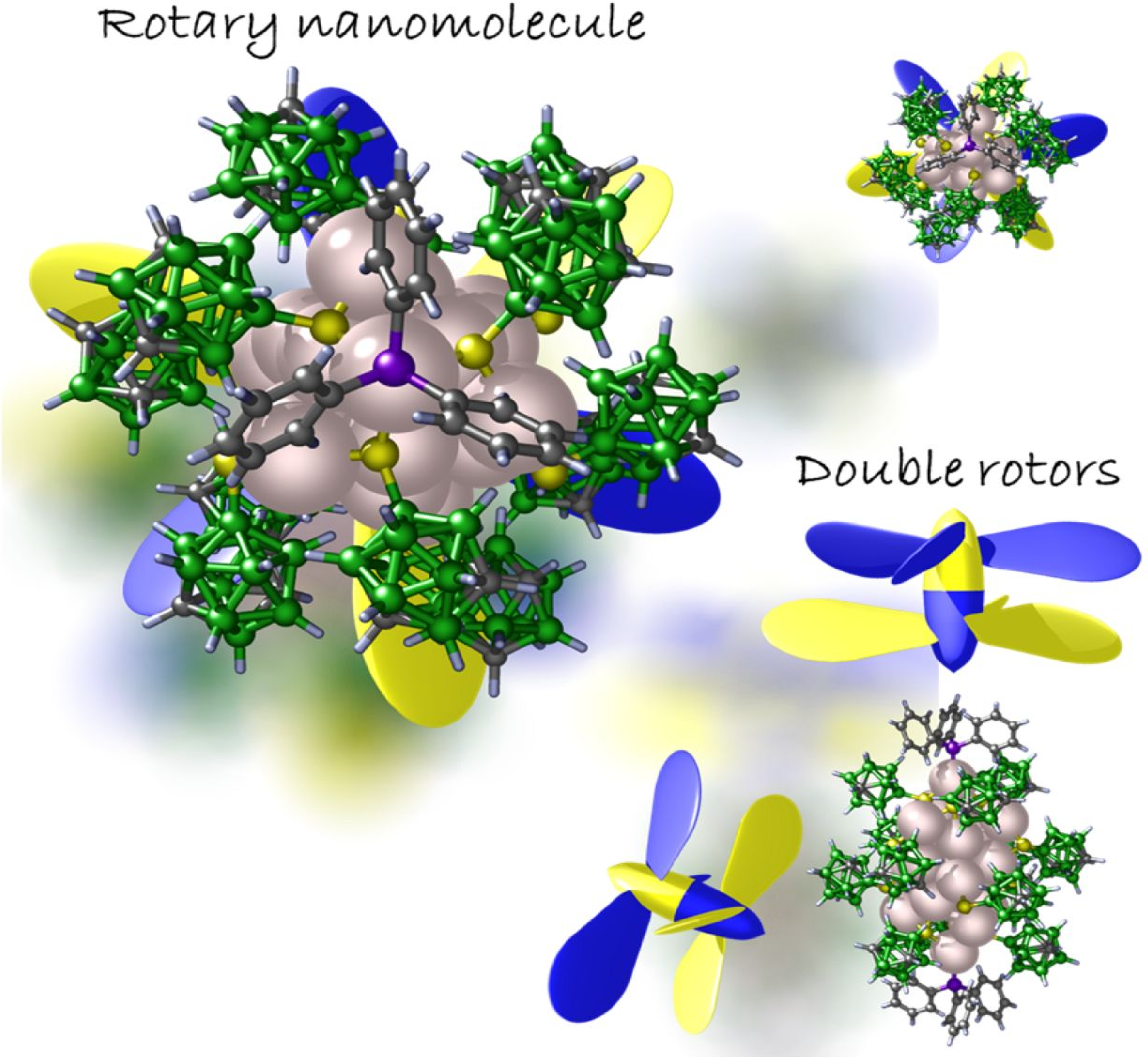
Anu George et al. *ACS Applied Materials & Interfaces*, 2012.

Approaching detection limits of tens of Hg2+

Atanu Ghosh et al. Anal. Chem. 2014

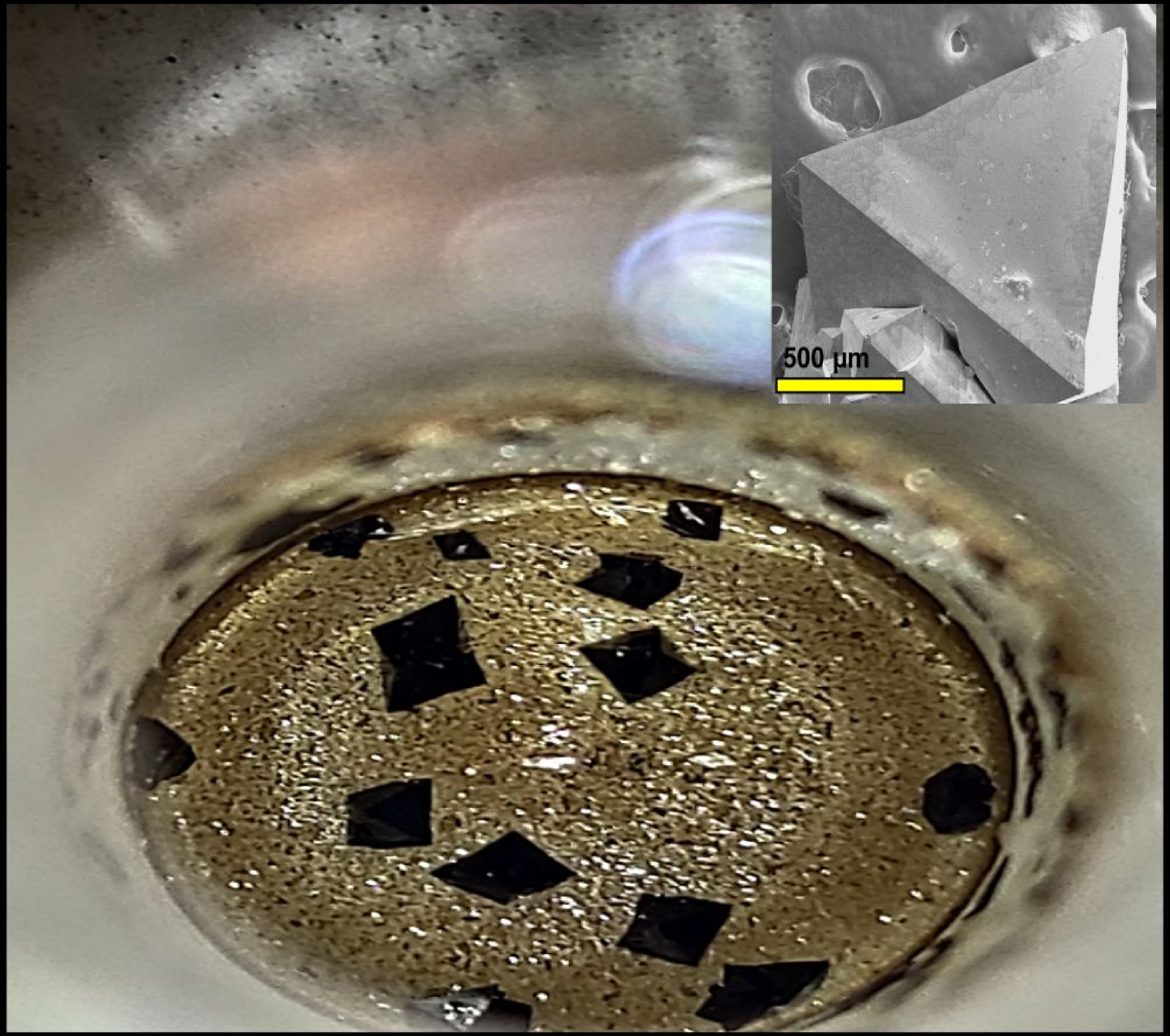
Mercury quenching experiment using nanofiber

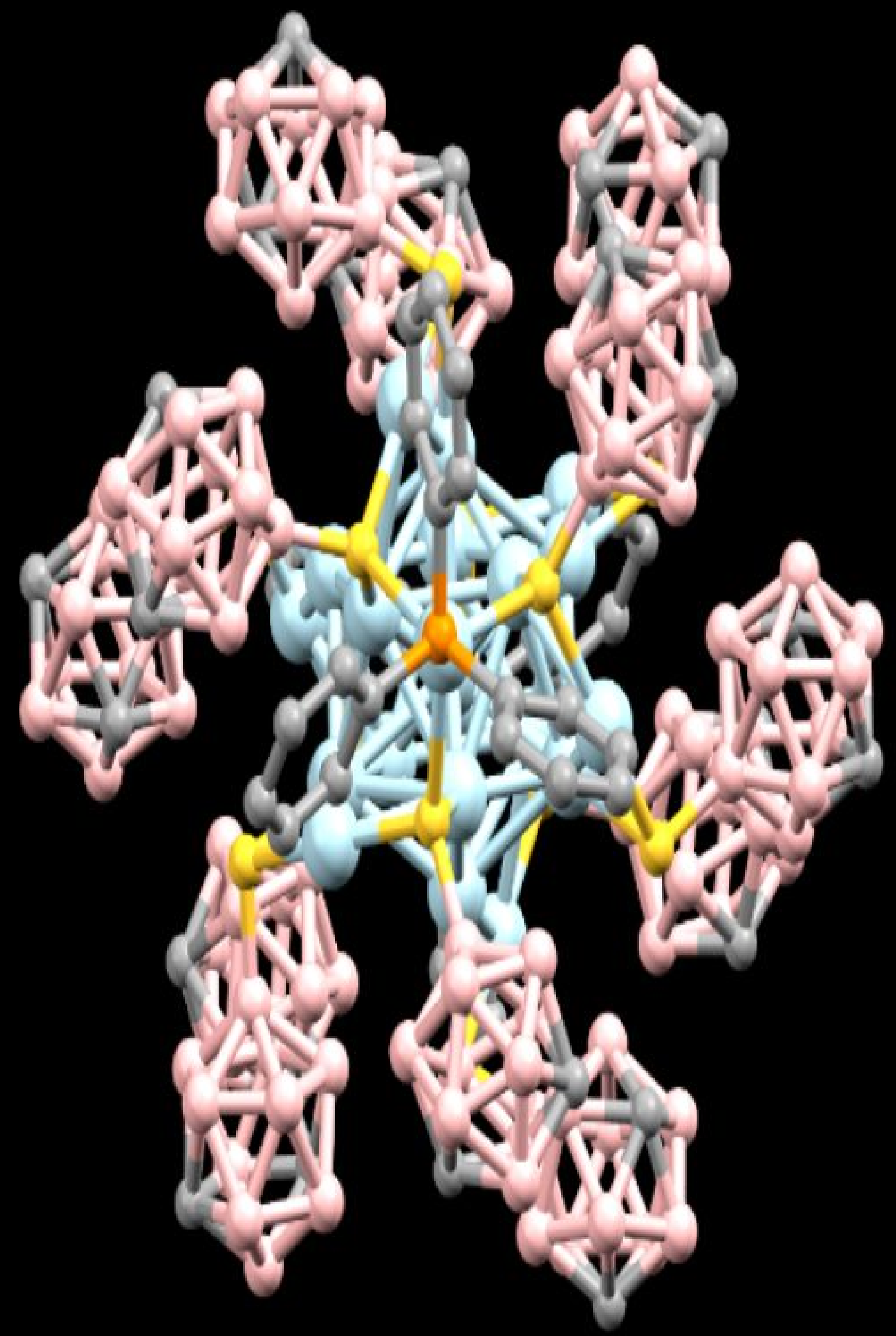
Carborane-thiol protected silver nanomolecule



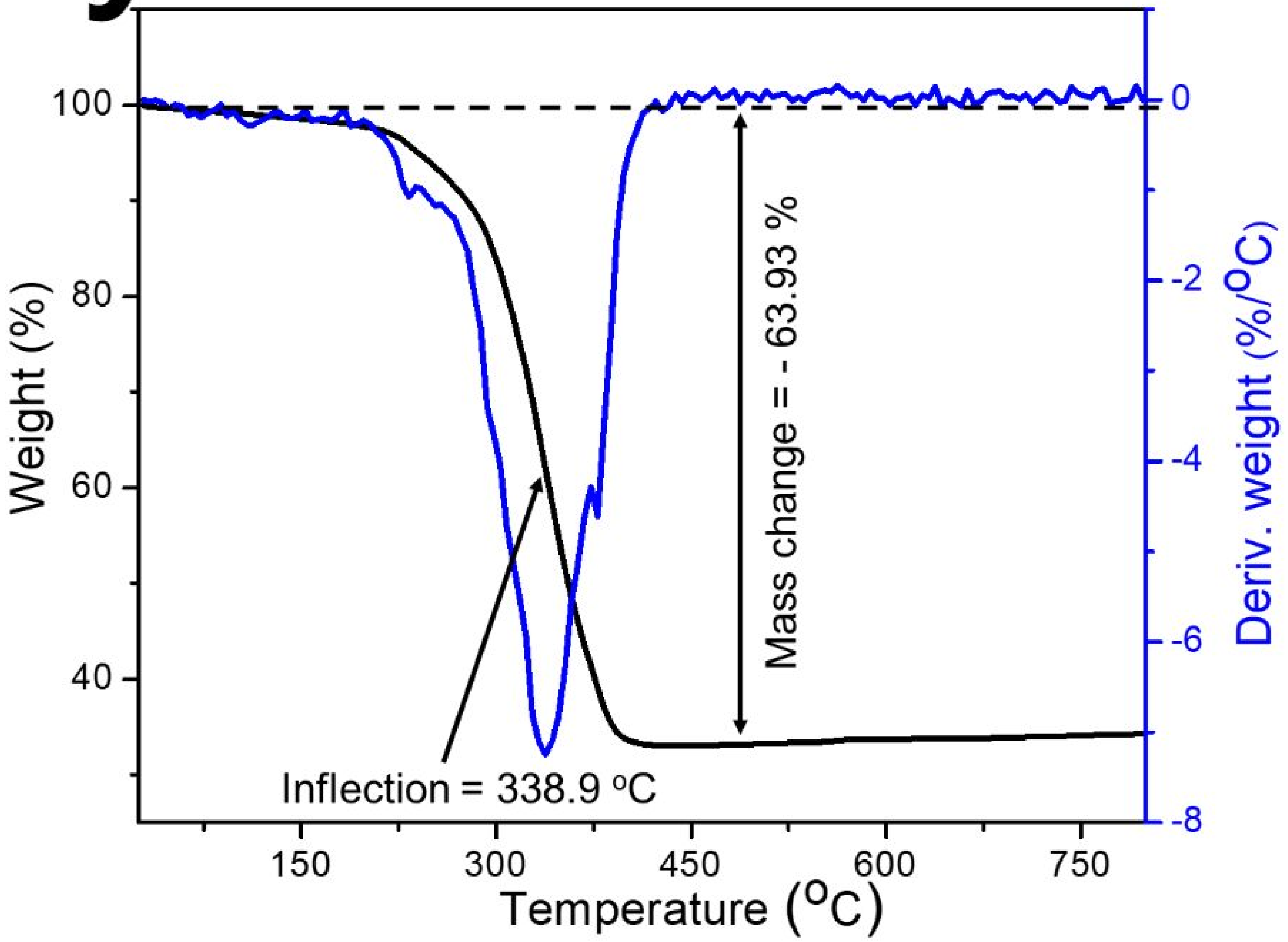
With Tomas Base

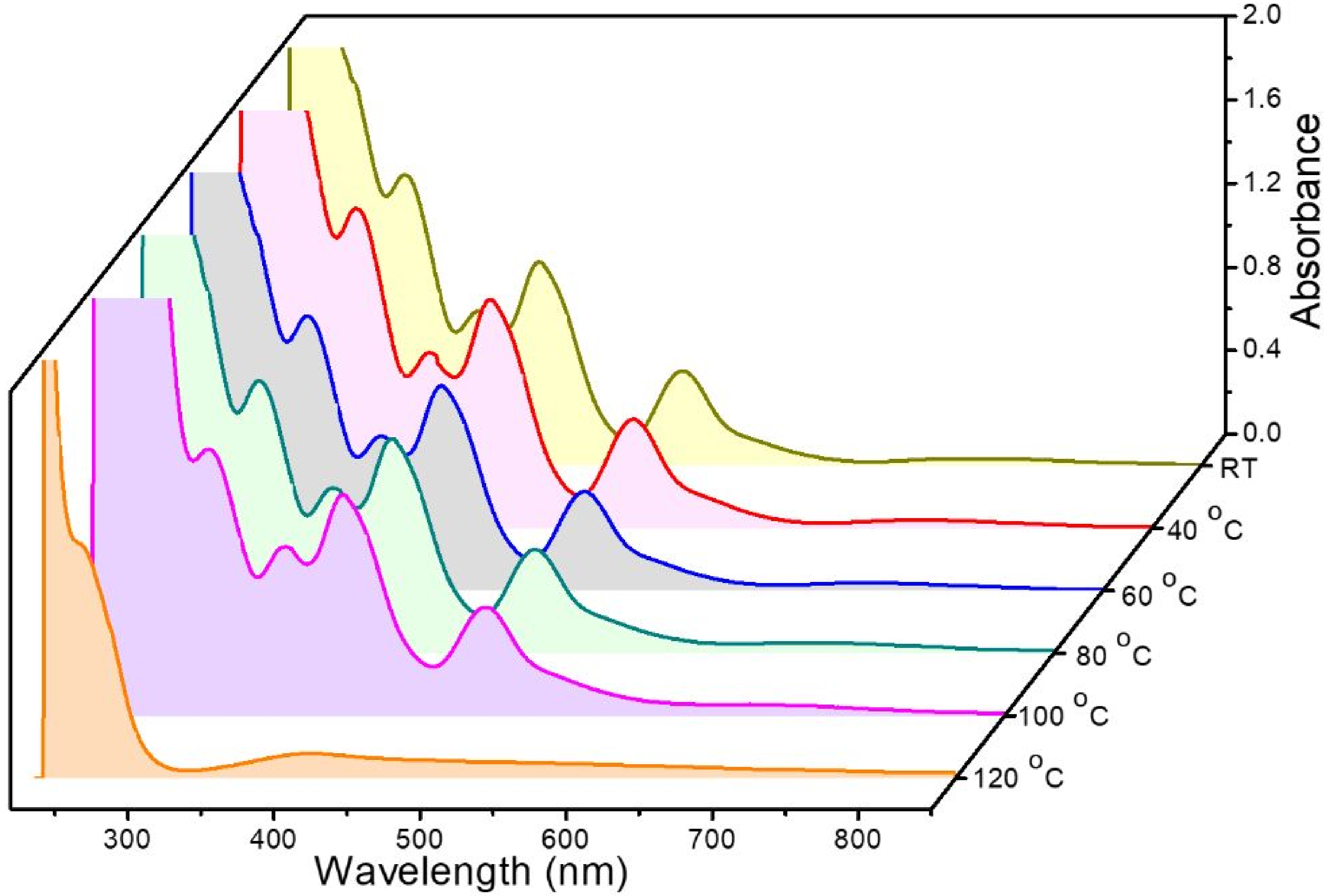
Jana *et. al*, Inorganic Chemistry (2022)


500 µm



Thermal stability

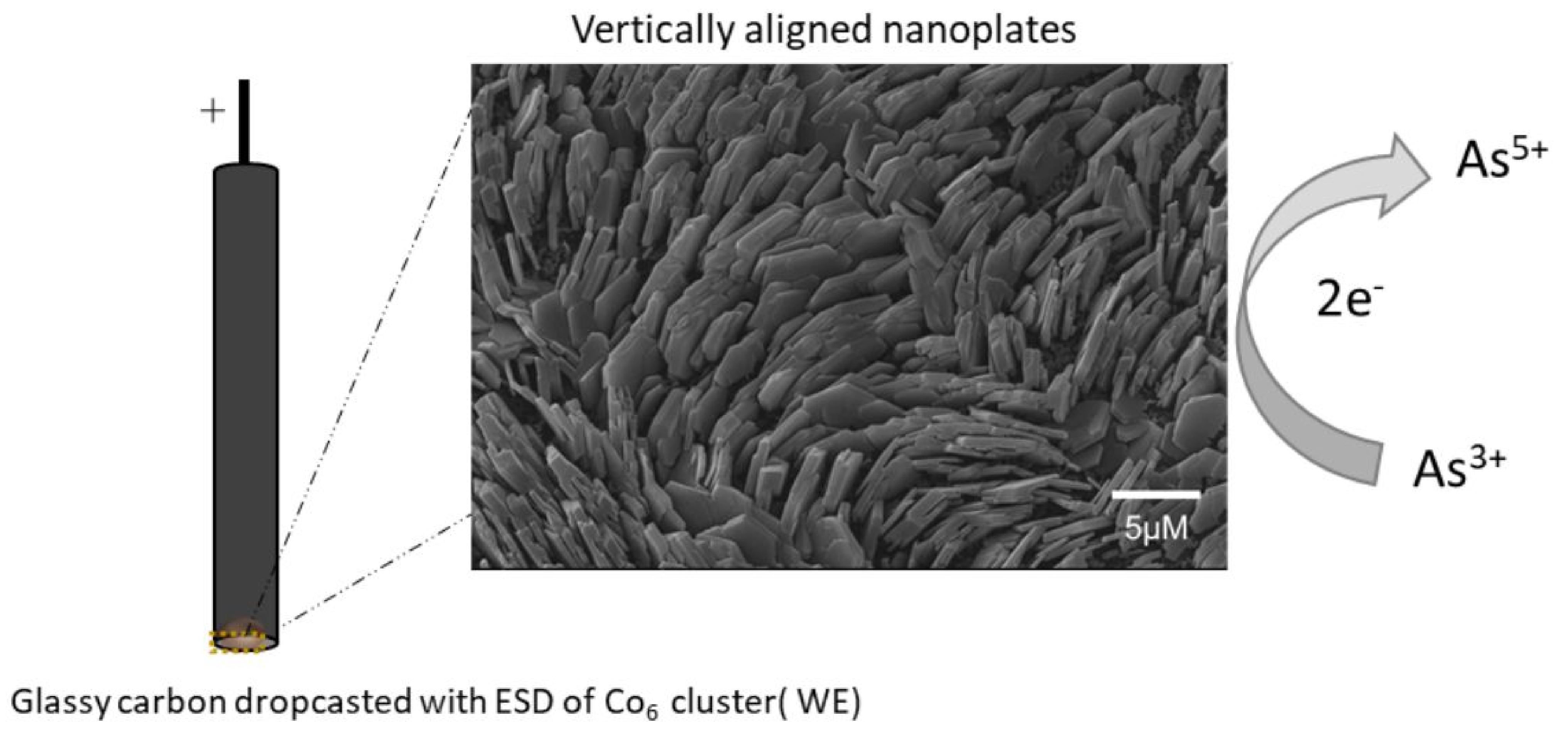


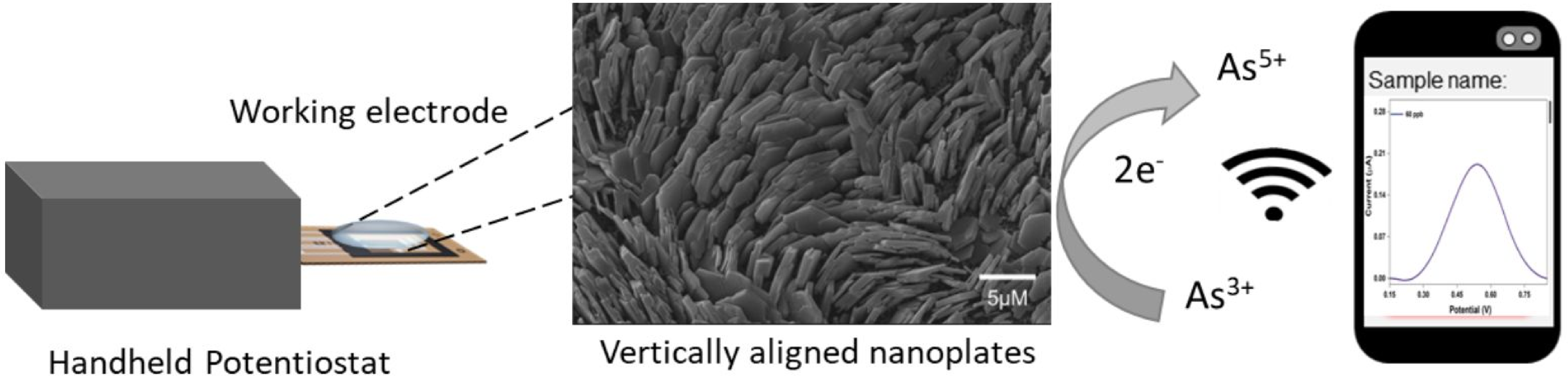


New electrodes - Aligned nanoplates of Co6S 8

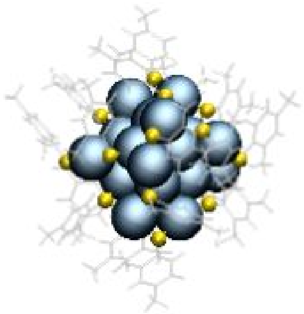
1,2-bis(diphenylphosphino)ethane (DPPE)

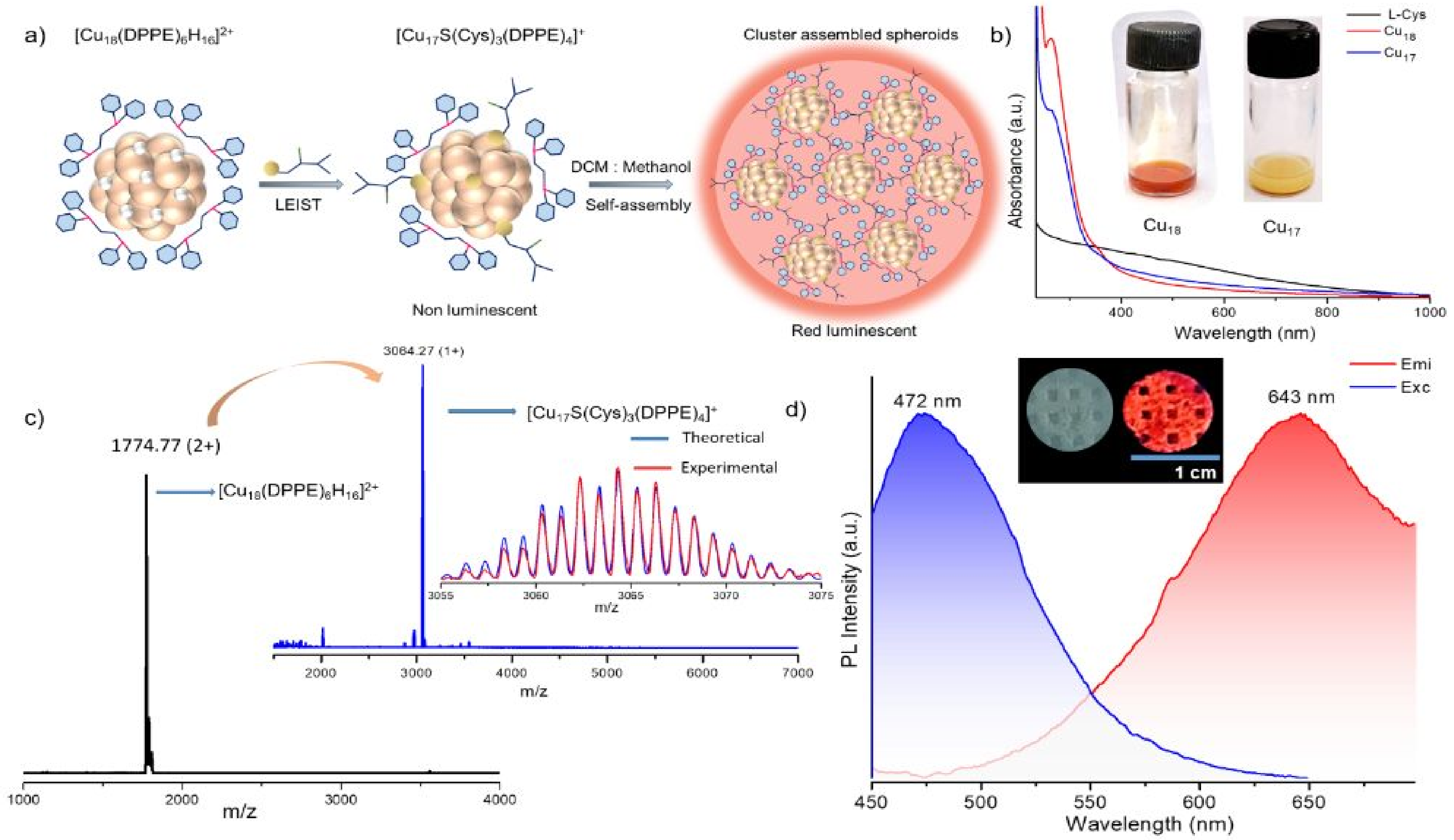
Working electrode





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



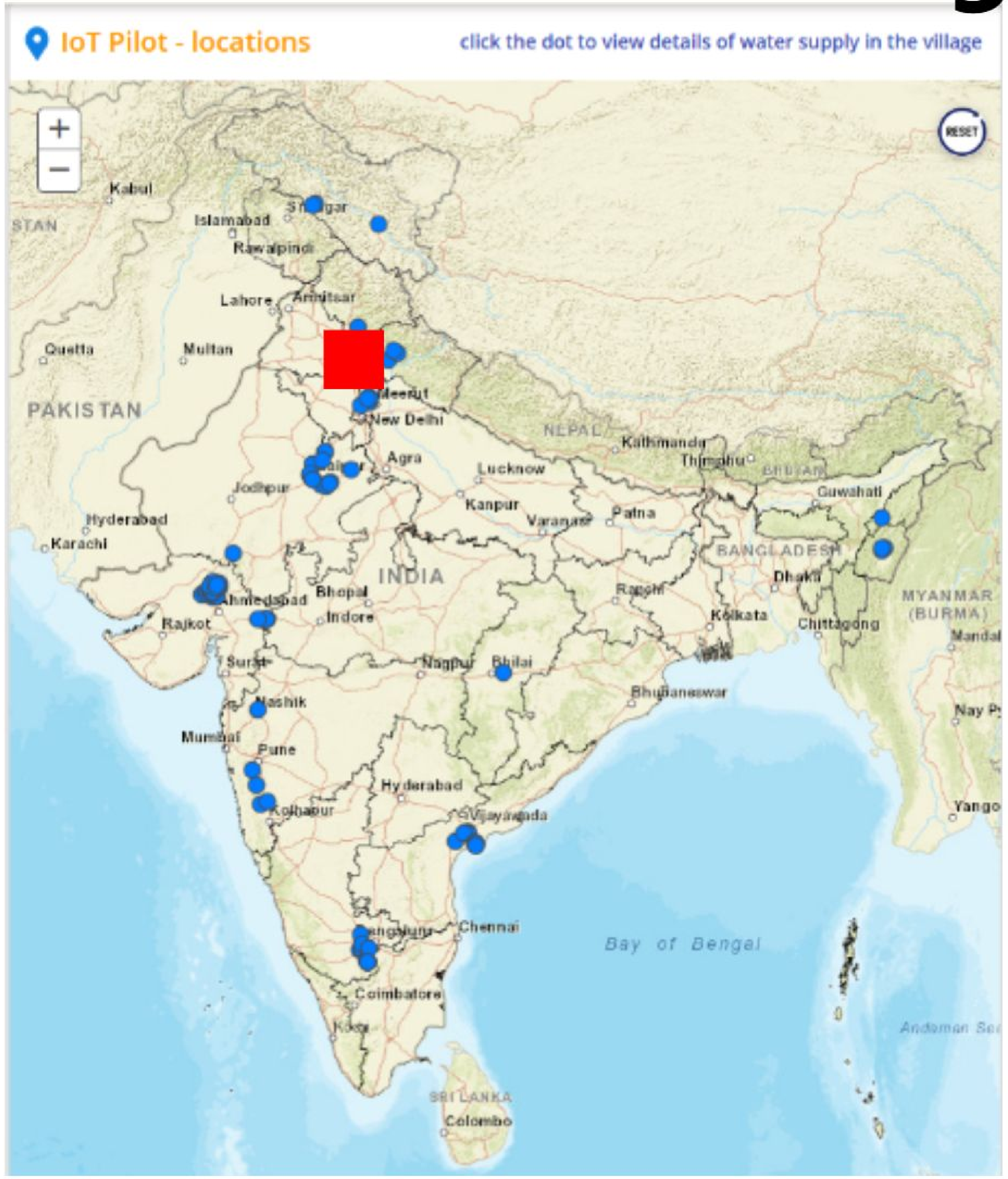


J. S. Kumar, *ES&T Lett.* 2024, 11, 8, 831–837.

Arsenic poisoning across the worl d

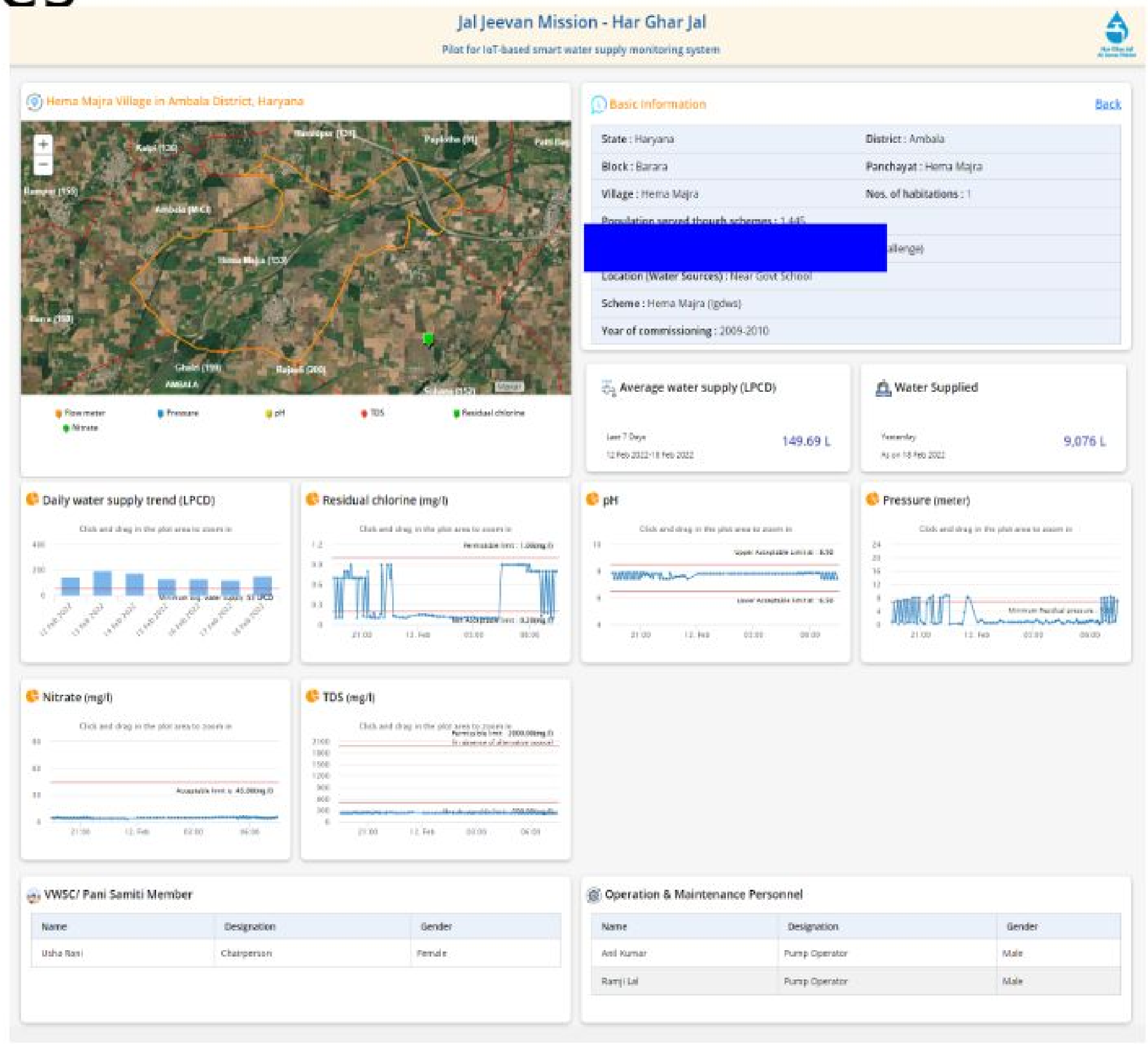
E. Shaji, M. Santosh, K. V. Sarath, Pranav Prakash, V. Deepch and B. V. Divya, Geoscience Frontiers, 12 (2021) 10107 9.

India’s water is being monitored



IITM/IISc

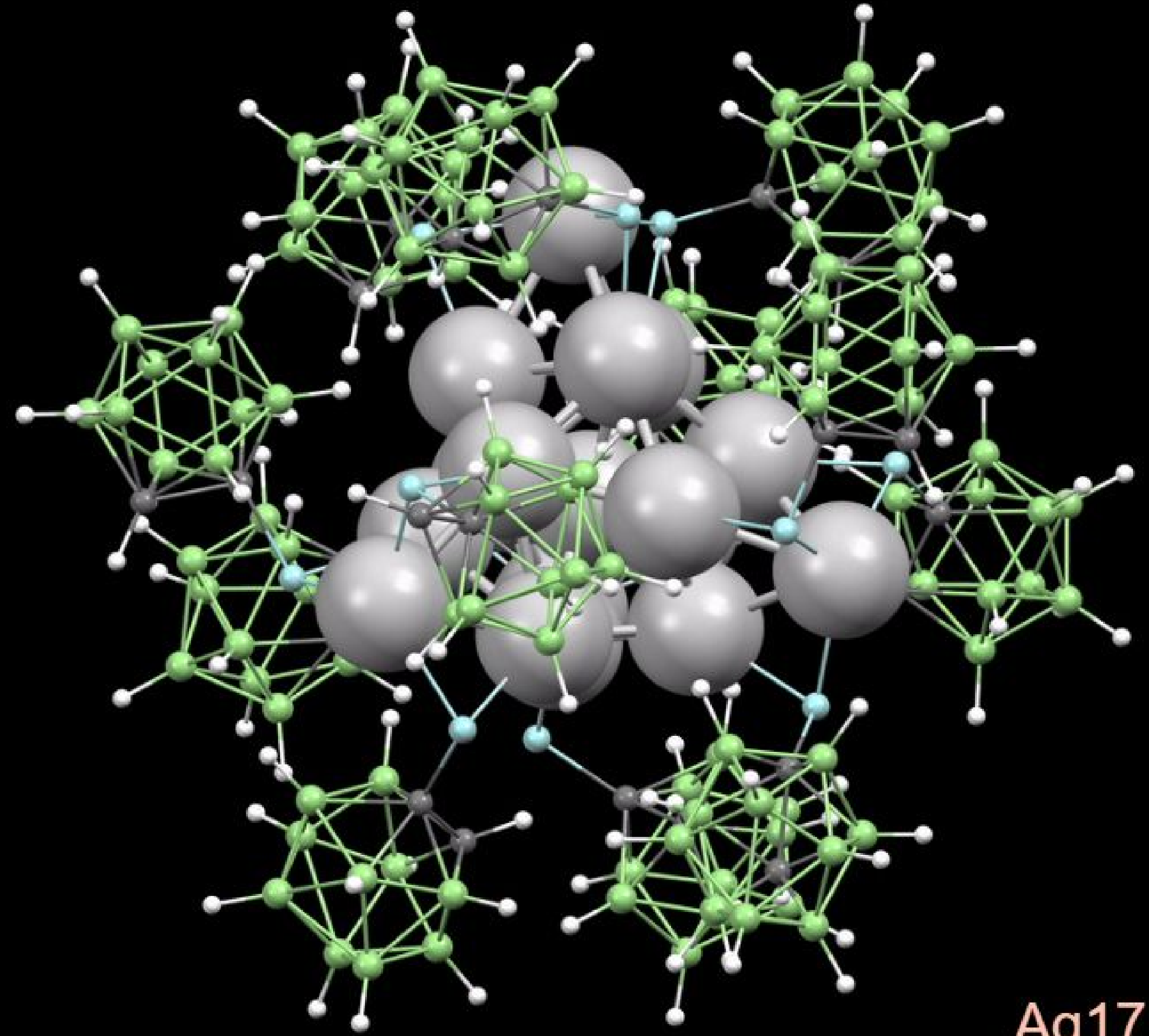
Installations made by four companies



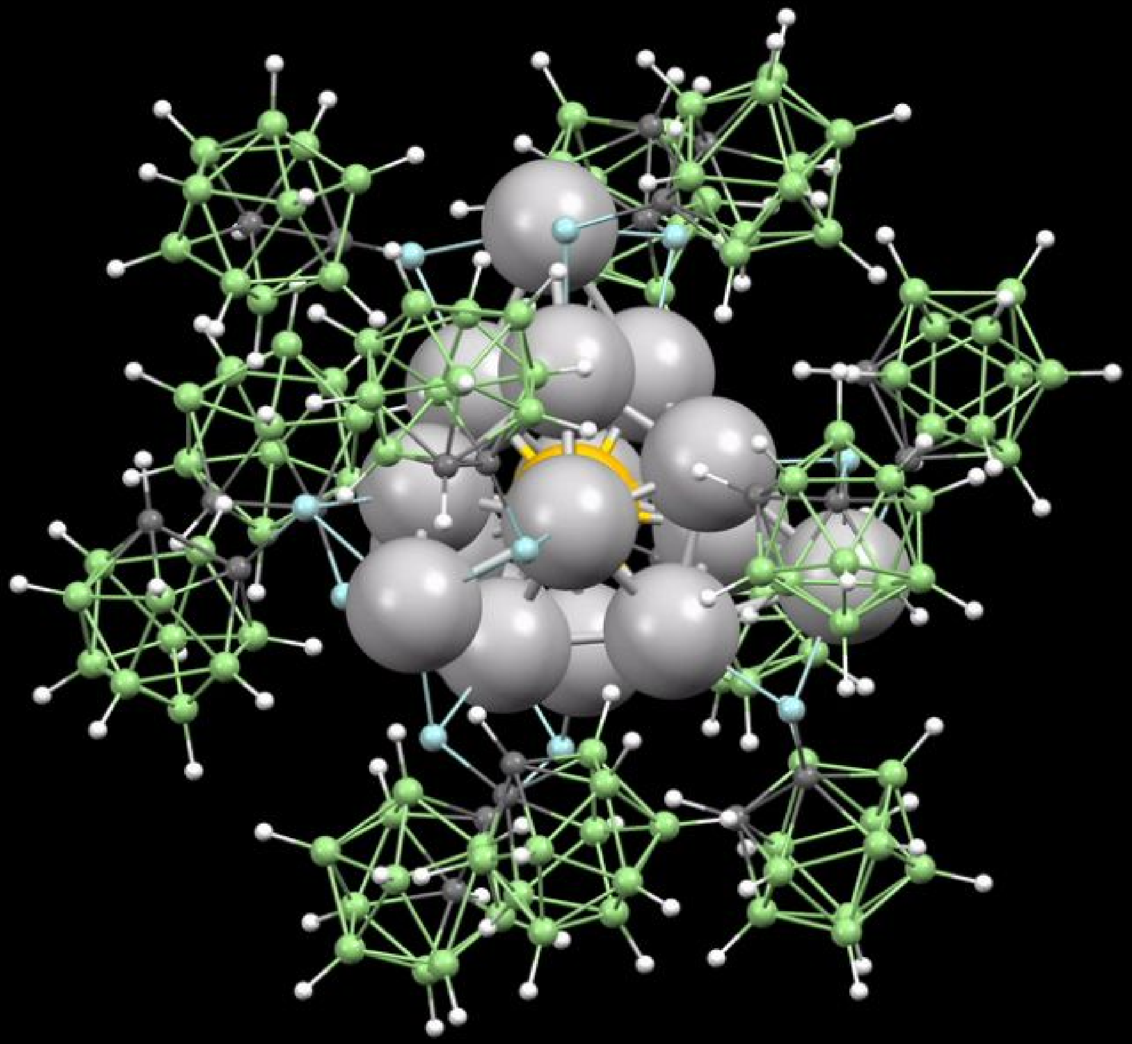
Ag17 AuAg16 Ag13Cu4 AuAg12Cu
4

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

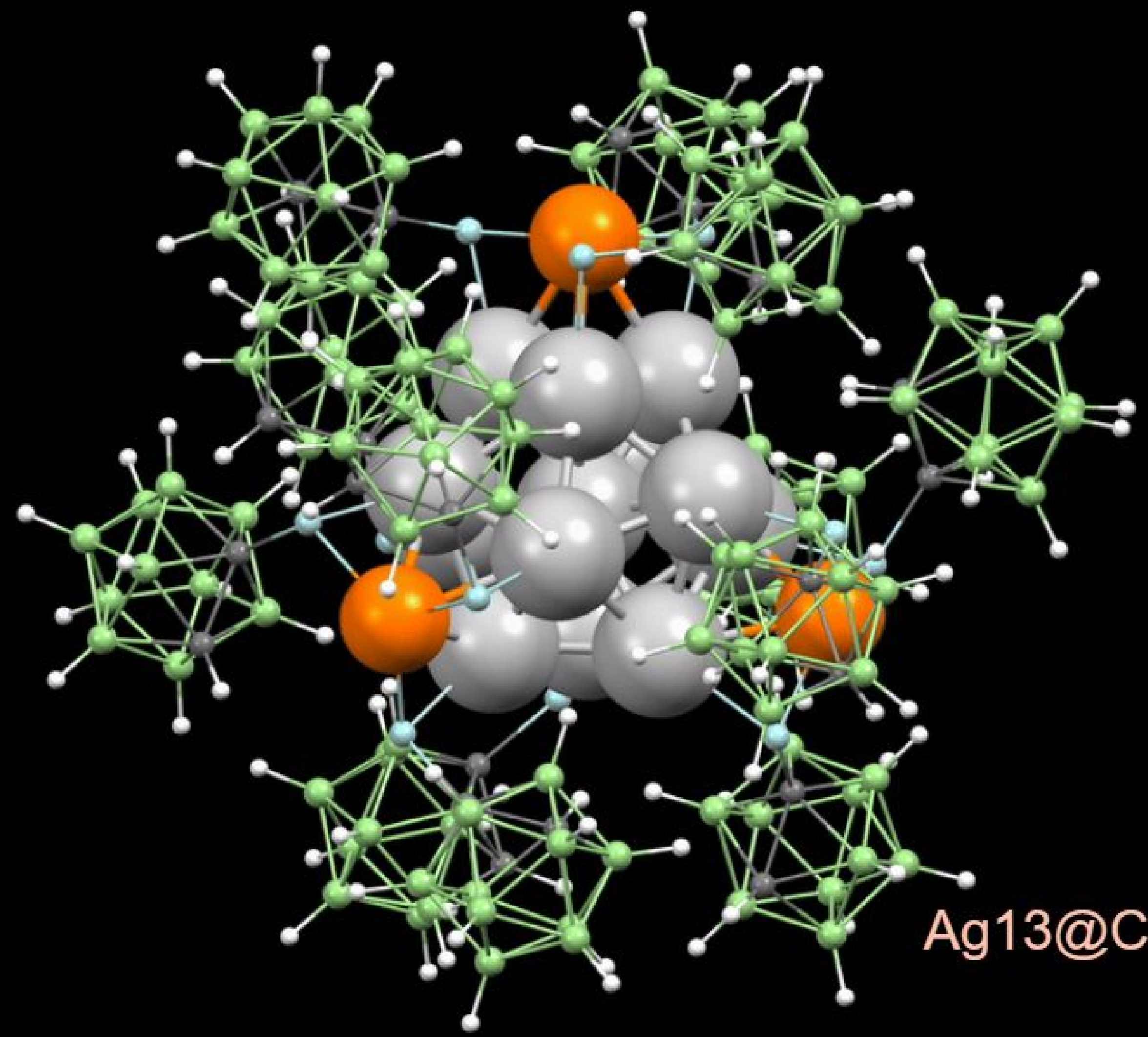
Structure of M17 Nanoclusters



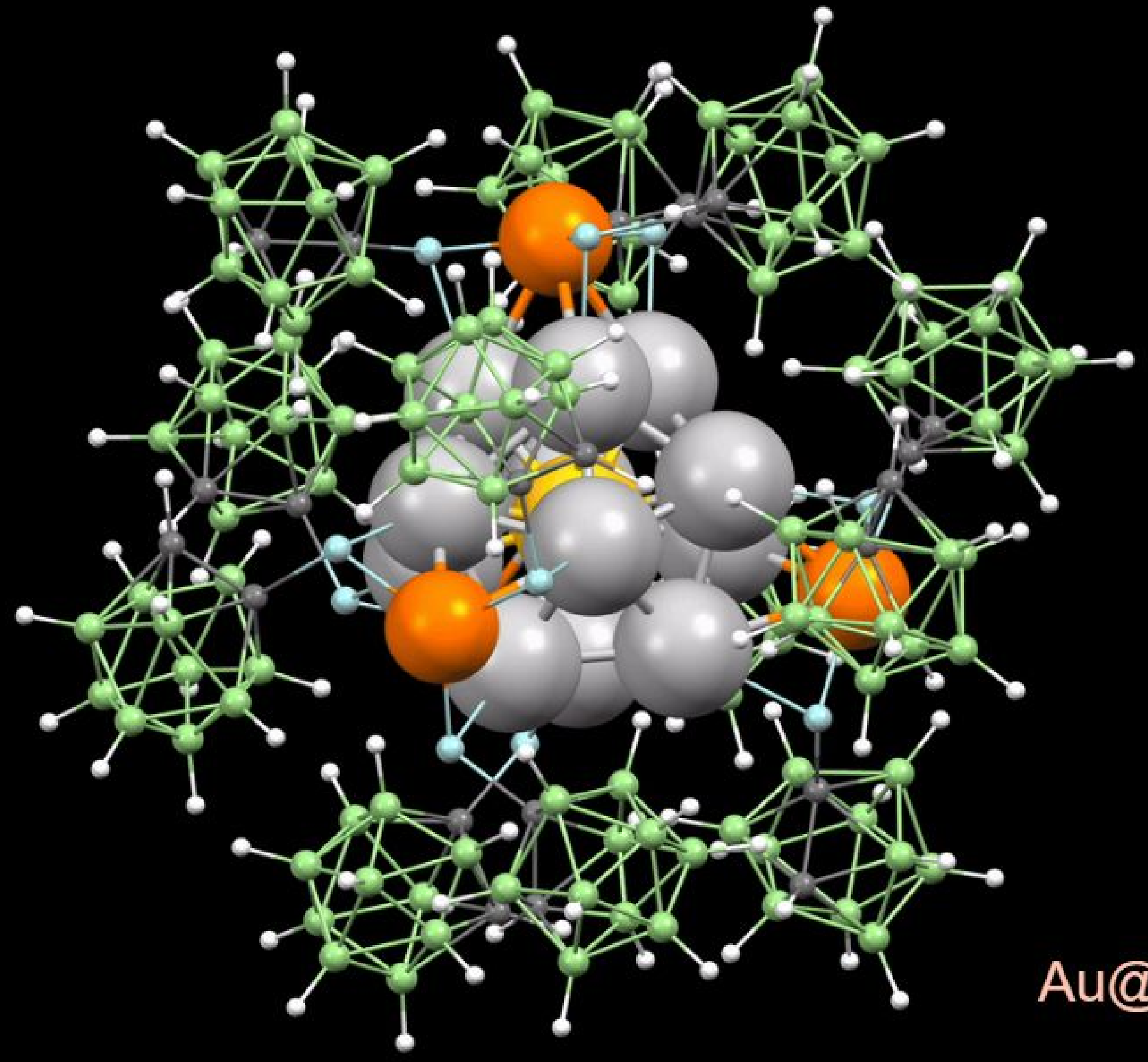
Ag17



Au@Ag16

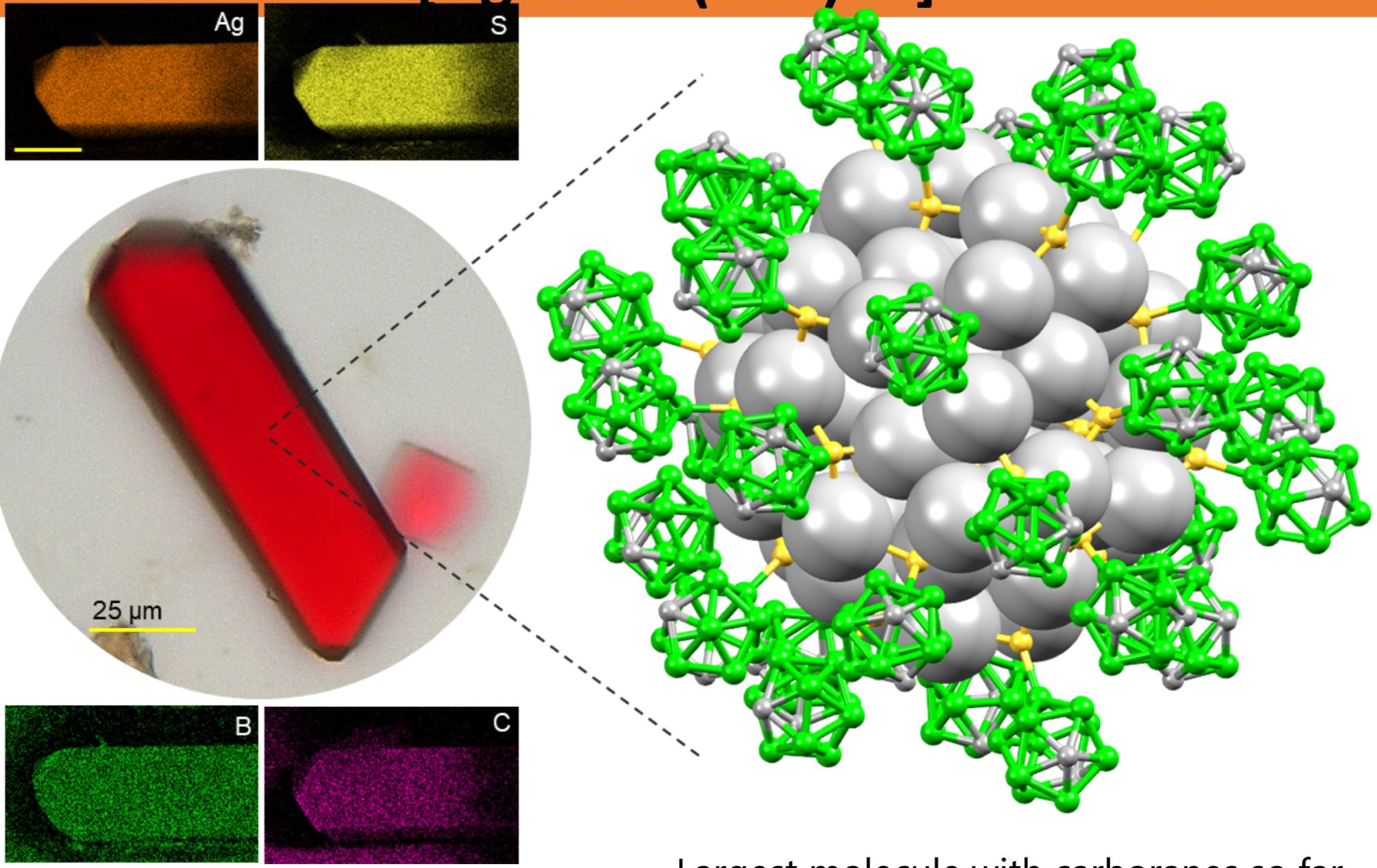


Ag13@Cu4



Au@Ag12@Cu4

[Ag62S12(CBT)32] Nanoclus

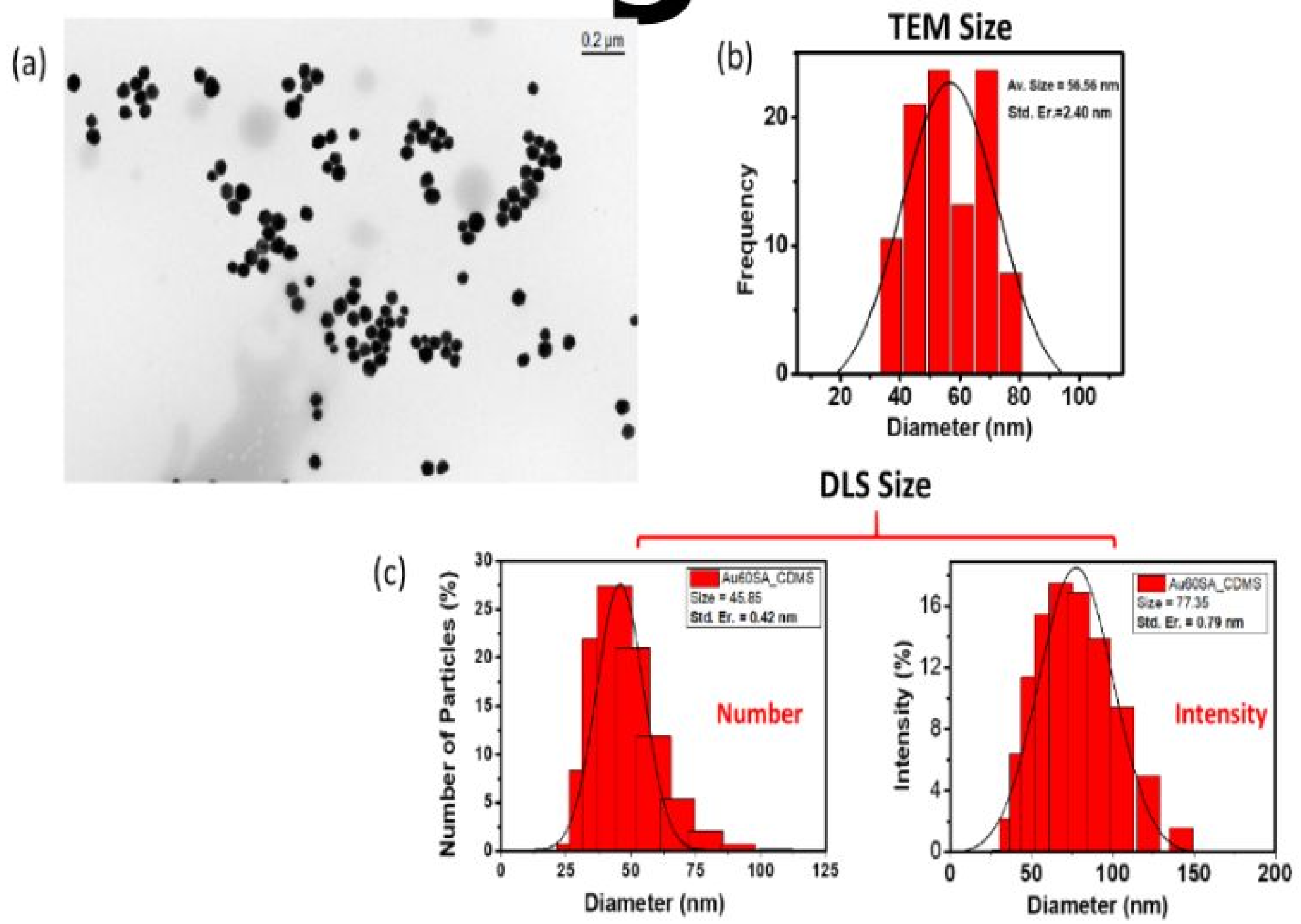


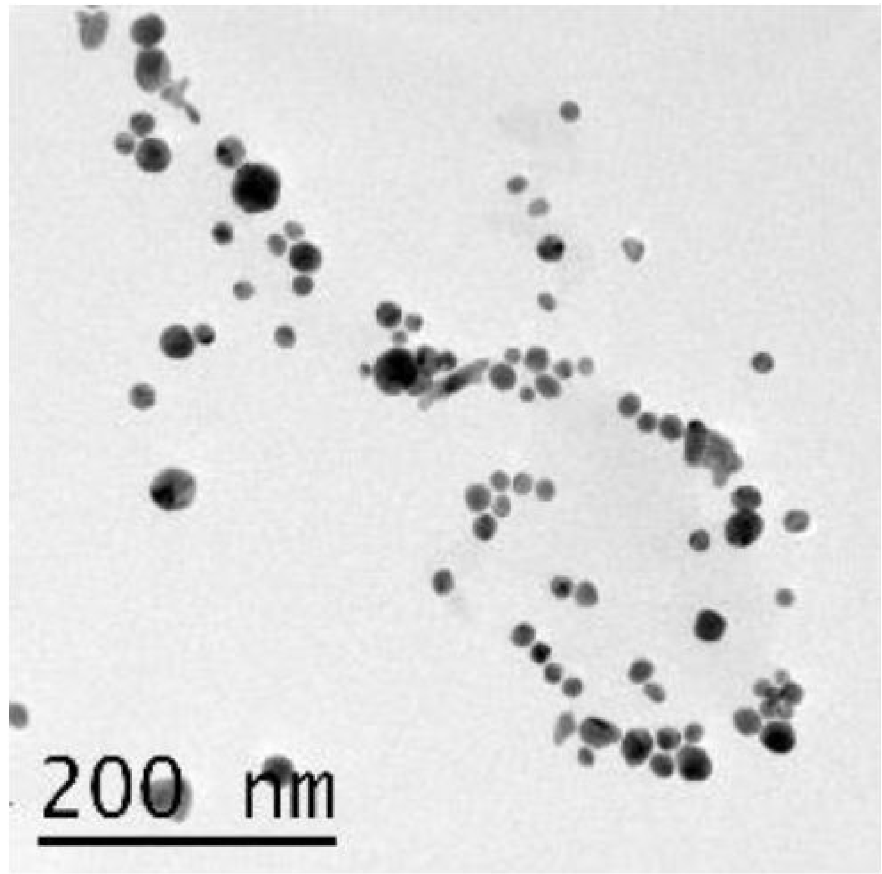
Largest molecule with carboranes so far…

…

Jana *et al.*, ACS Nano (2025), in revision

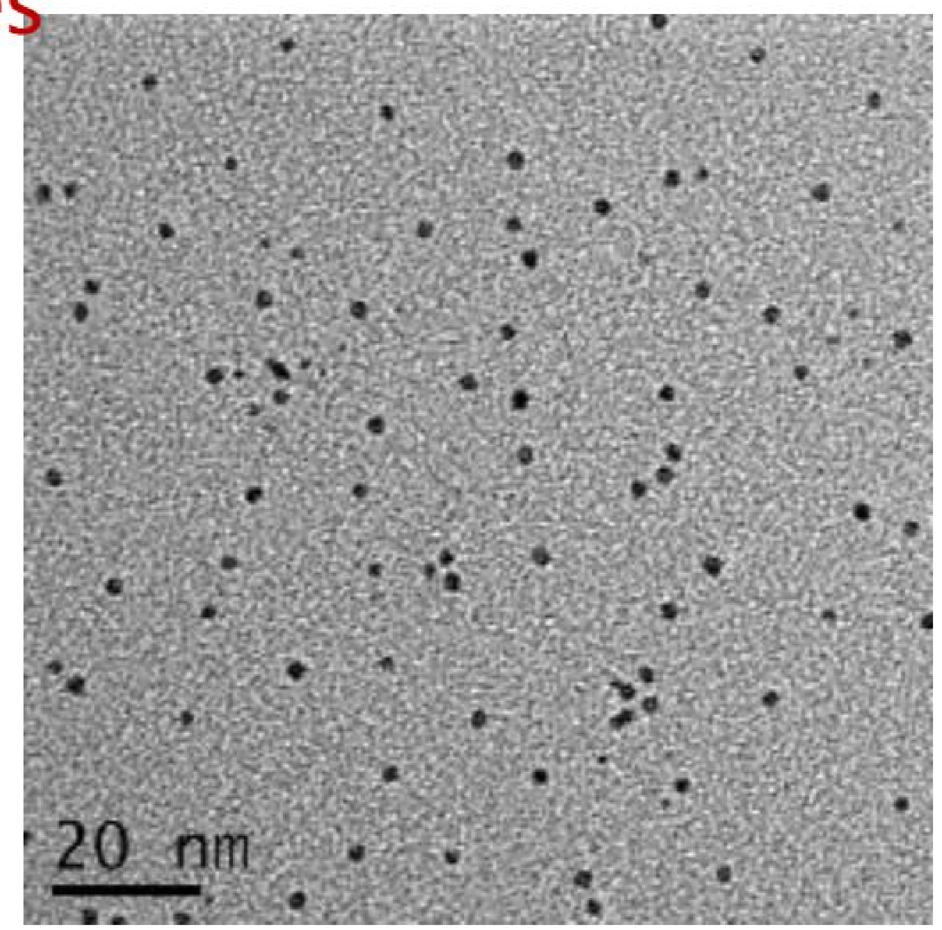
Larger clusters - TE

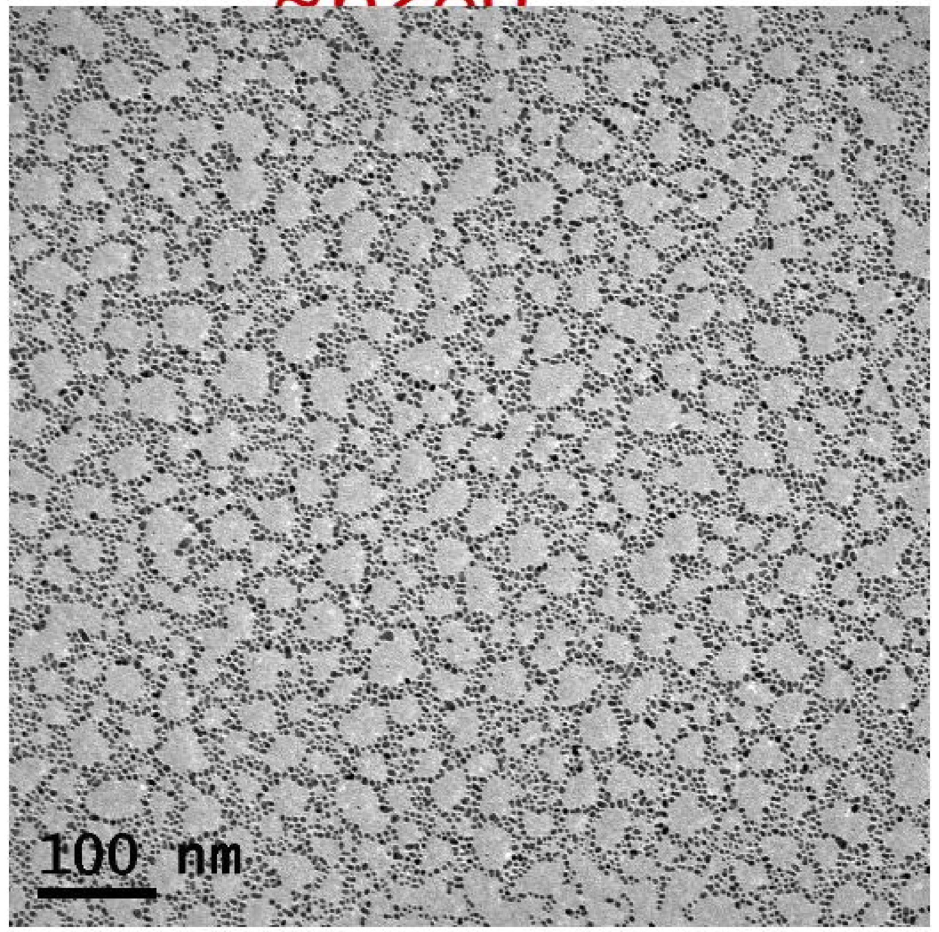


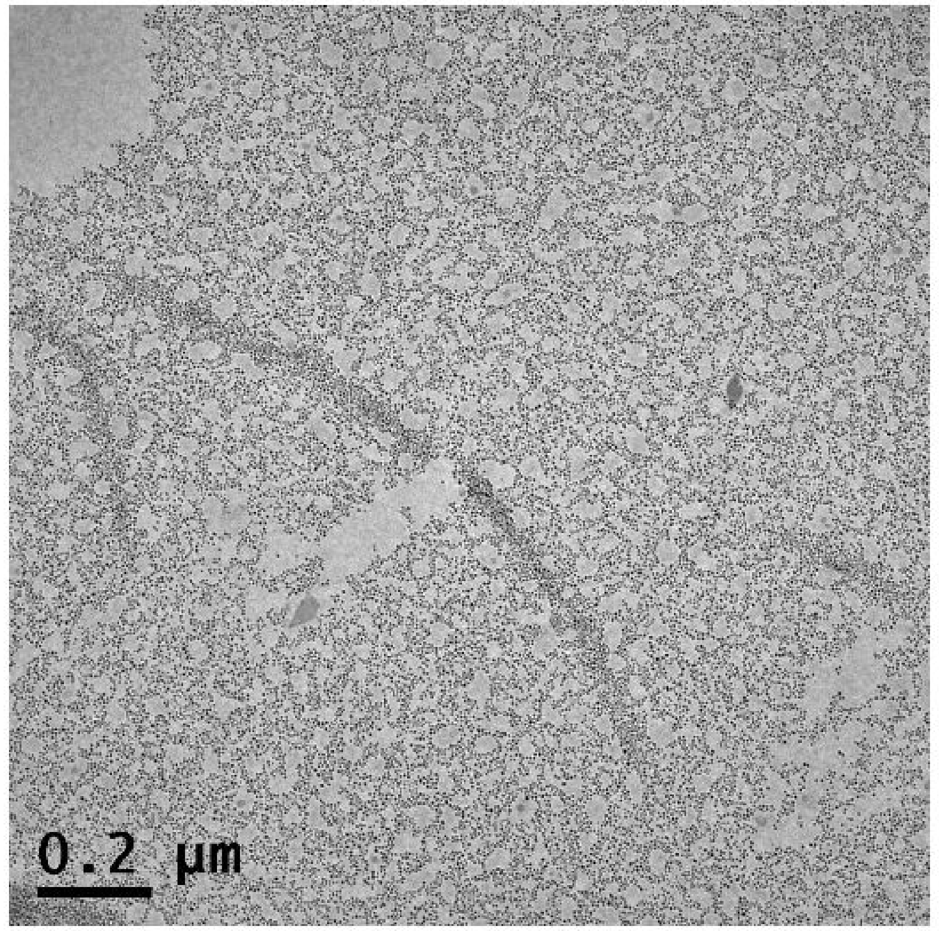


60 nm sized Au-citrate nanopartic les

Au~246000(MUTAB) ~6280







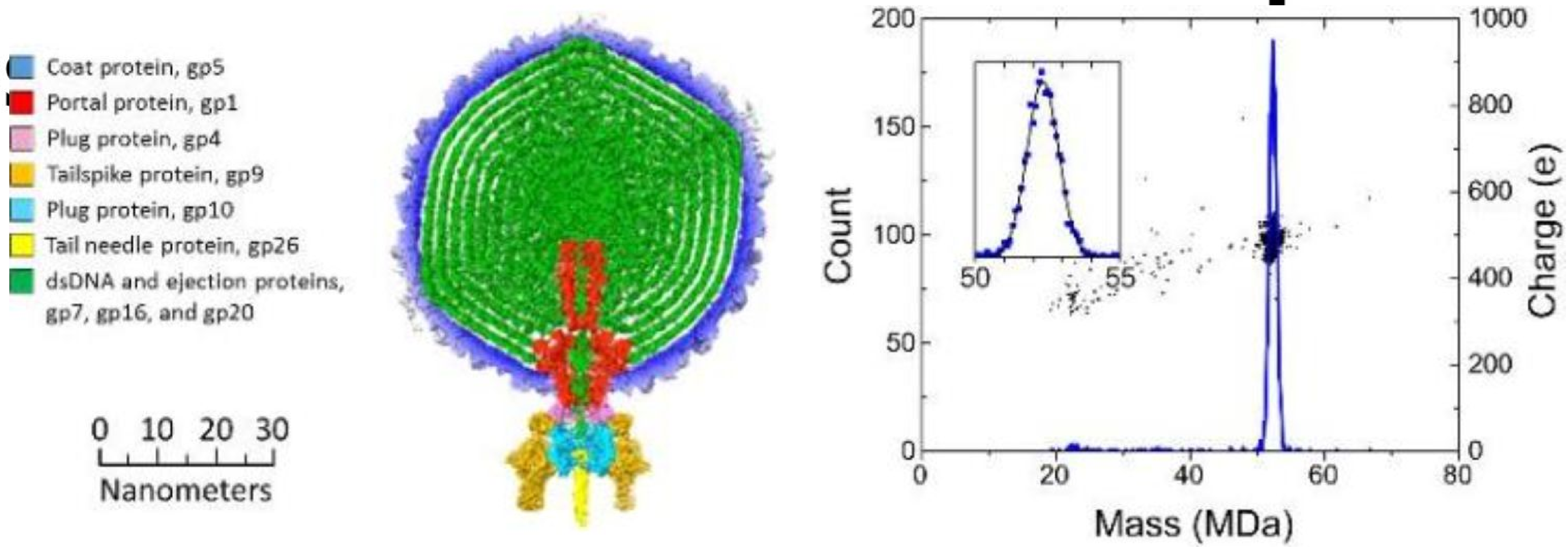
Au279(TBBT)84

Au144(PET)60

Au25(PET)18

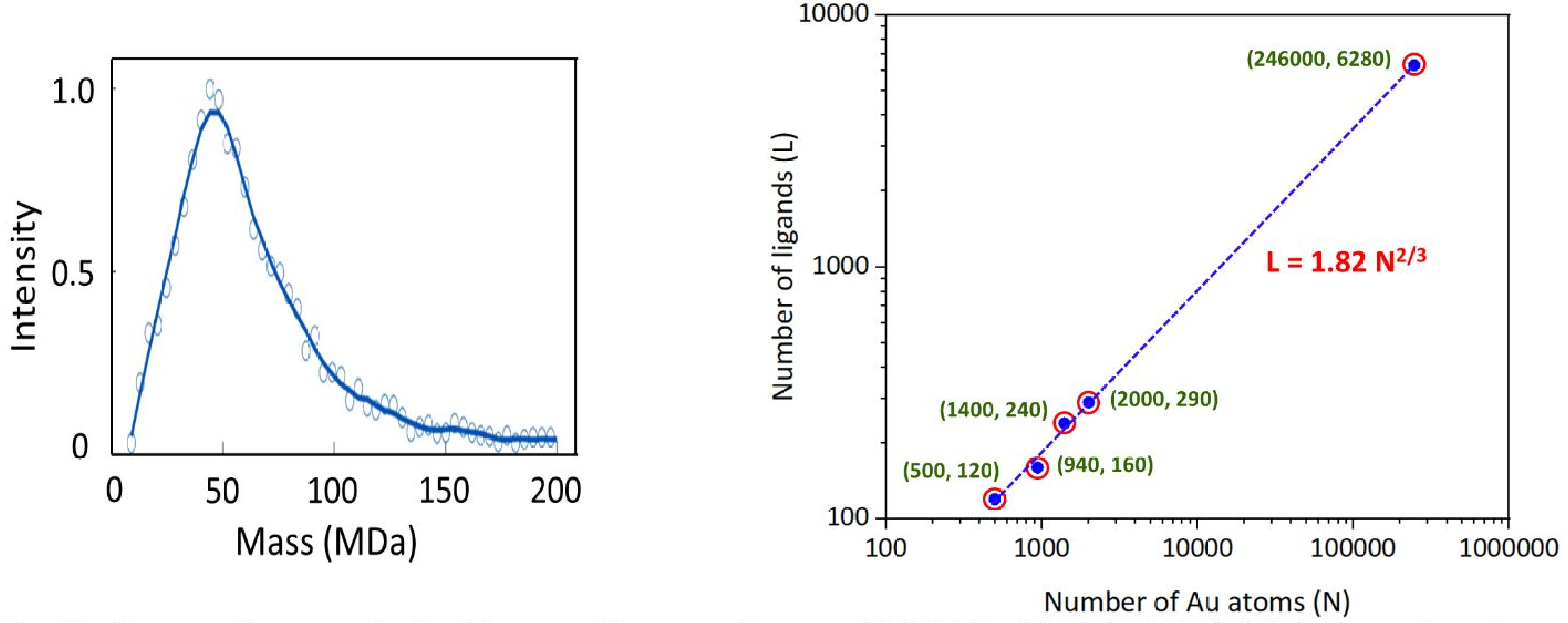
CDMS of viruses and nanoparticles

(a)



Keifer, D. Z.; Motwani, T.; Teschke, C. M.; Jarrold, M. F. Measurement of the Accurate Mass of a 50 MDa Infectious Virus. *Rapid Commun. Mass Spectrom.* **2016**, *30* (17), 1957–1962.

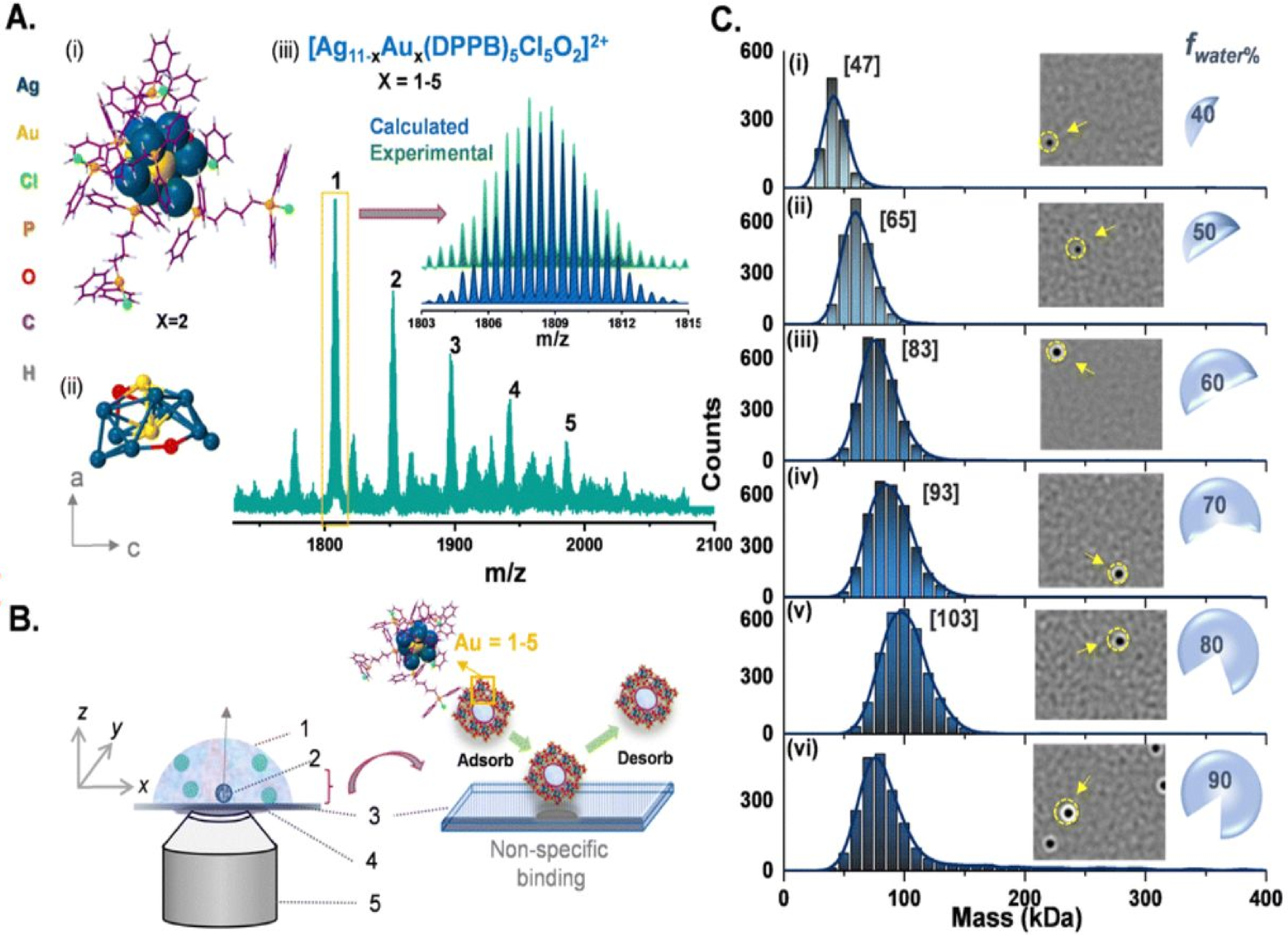
(b)



B. S. Sooraj, et. al. J. Phys. Chem. Lett. (2025) (DOI: 10.1021/acs.jpclett.5c0107

Mass Photometry

Mass Range: 30 kDa to 5 MDa

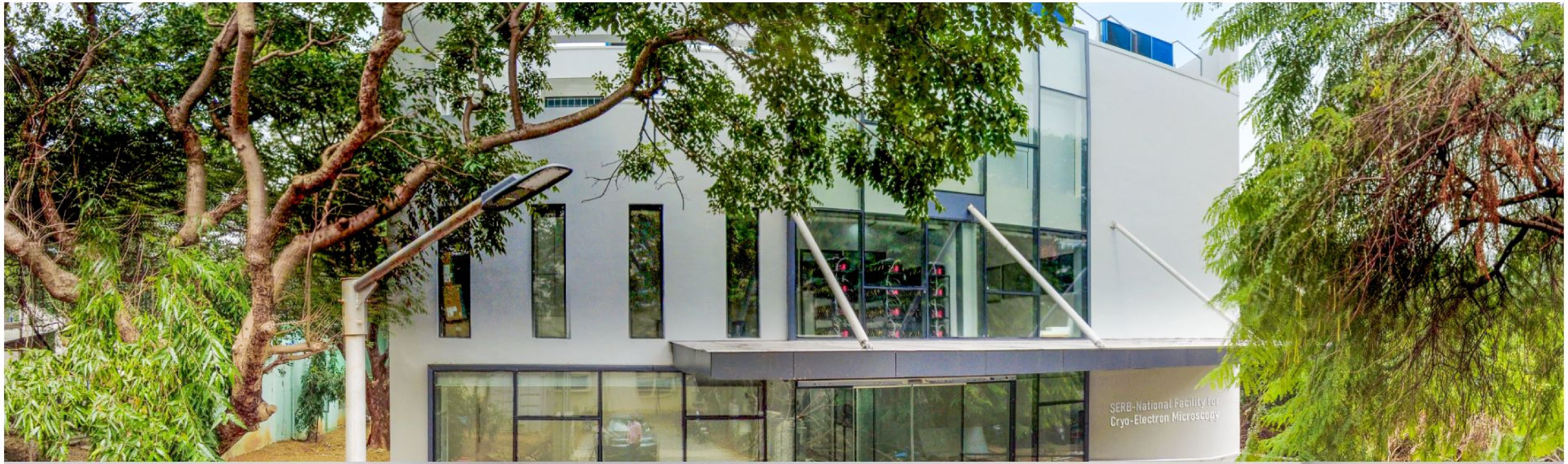


J. Roy, et. al., *Chem. Commun.*, 2024,60, 6655-6658

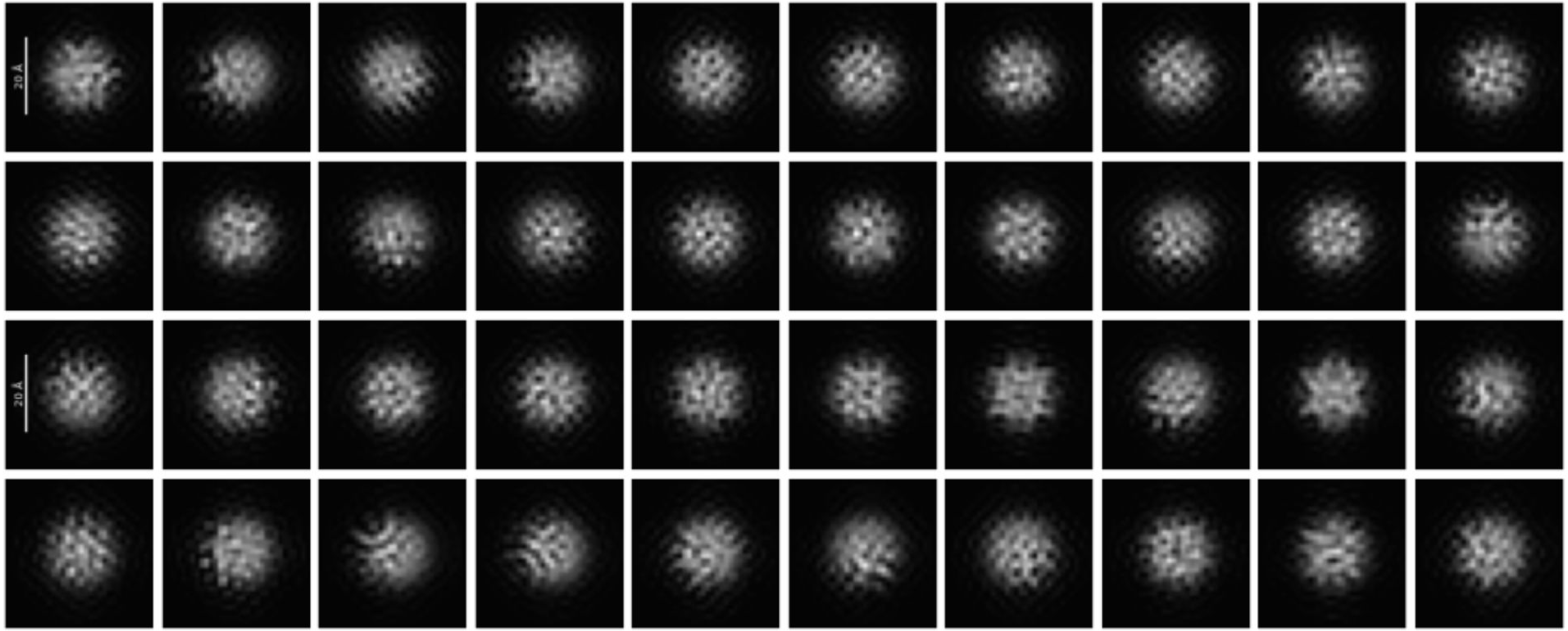
[redacted]

Structural Transitions and Micro-ED

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


SERB-National Facility for
Cryo-Electron Microscopy


thermoscientific
ThermoFisher
SCIENTIFIC



B. S. Sooraj, et. al. Unpublishe
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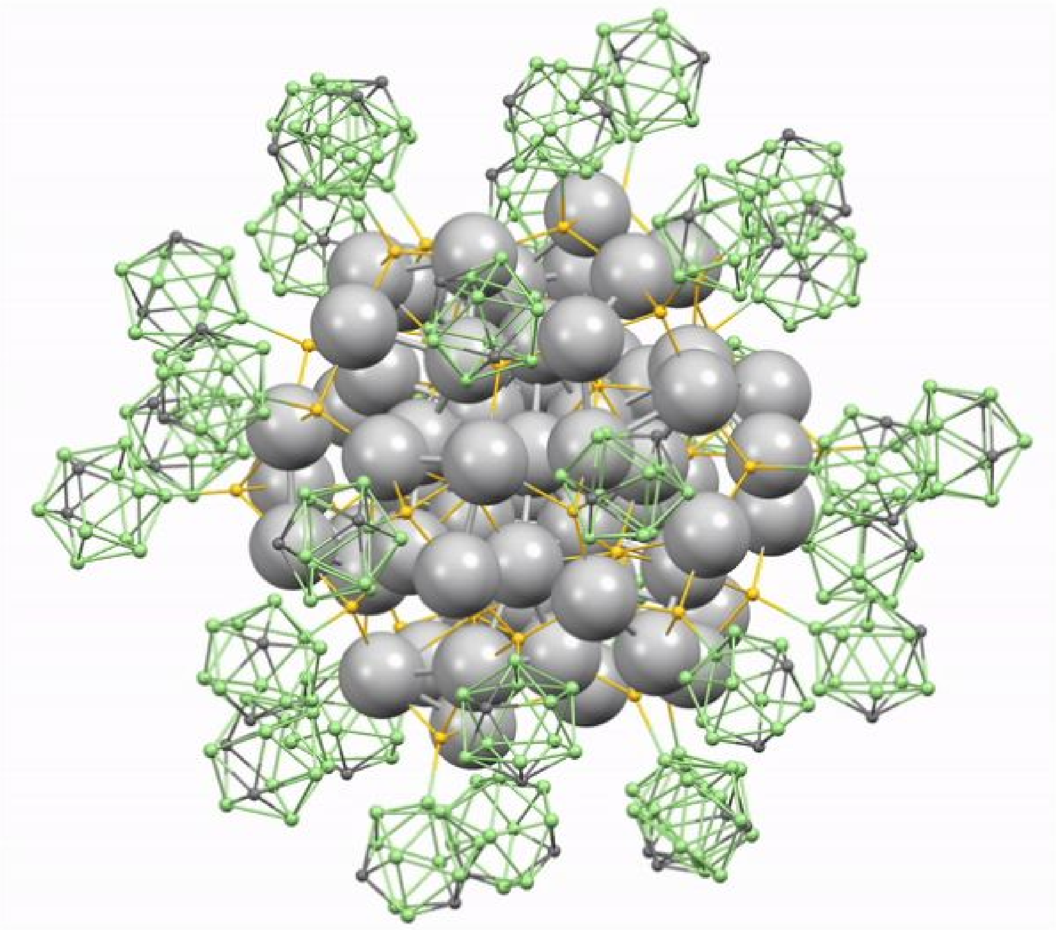
Summary

- Atomically precise clusters are a category of new materials
- They are molecules – properties, nomenclature,…
- Clusters are thermally stable up to 400°C.
- They exhibit useful applications
- Atomic precision across the periodic table
- An era cluster-based materials is being born



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Robin Ras

Nonappa

Tomas Base

Manfred Kappes

Olli Ikkala

Horst Hahn

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Vivek Polshettiw

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

Funding: Department of Science and Technology, Government of India

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MS Theses: Ananthu Mahedranath, Ramesh Kumar Soni

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Many Outstanding Individuals

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https://preview.peopleswaterdata.org

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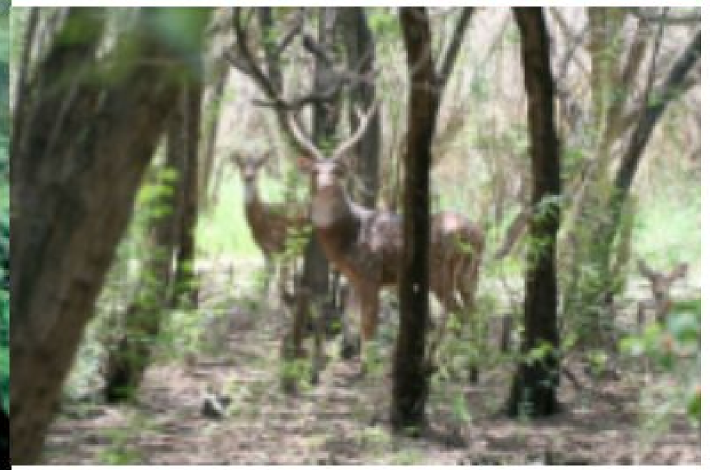

Associate Editor

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