



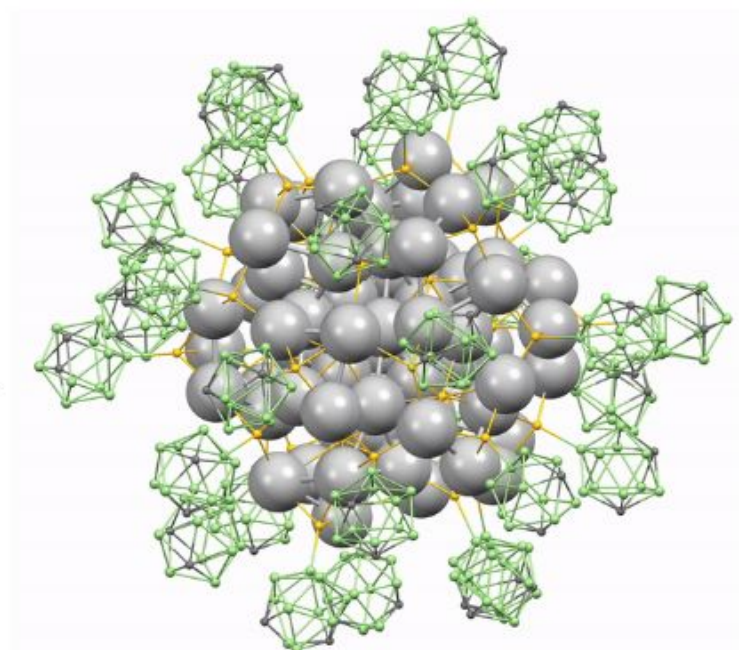
Since 1959

Transforming Water: Innovations in Materials, Droplets, and Ice

From scalable purification technologies to new discoveries in water and ice chemistry

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 EyeNetAqua Solutions
 DeepS



Thalappil Pradeep

Institute Professor, IIT Madras

pradeep@iitm.ac.in

http://Professor-in-charge '9



International Centre for Clean Water
 ter

<https://iccw.world>

Department of Chemistry, Purdue University, July 28, 2025





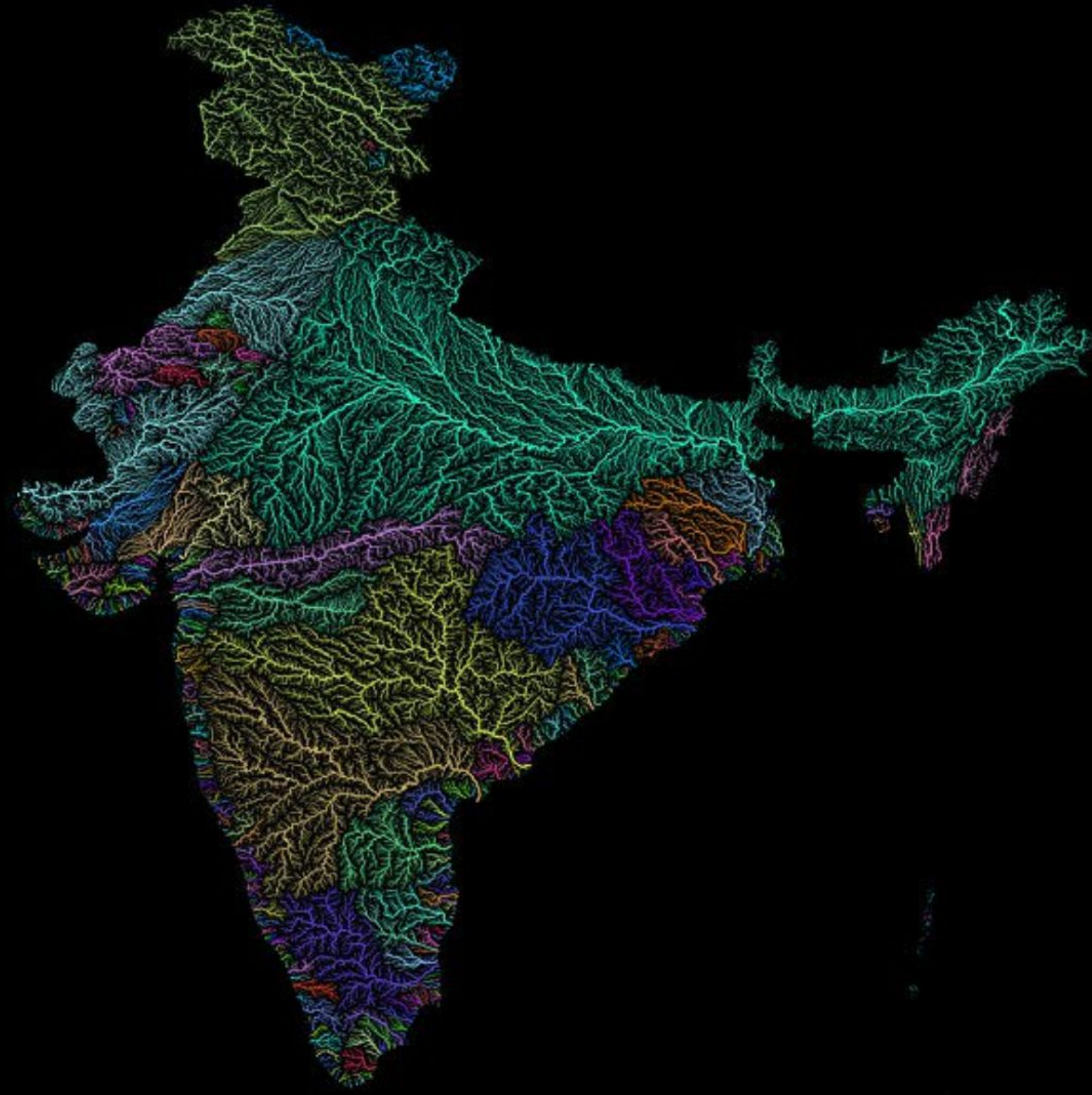








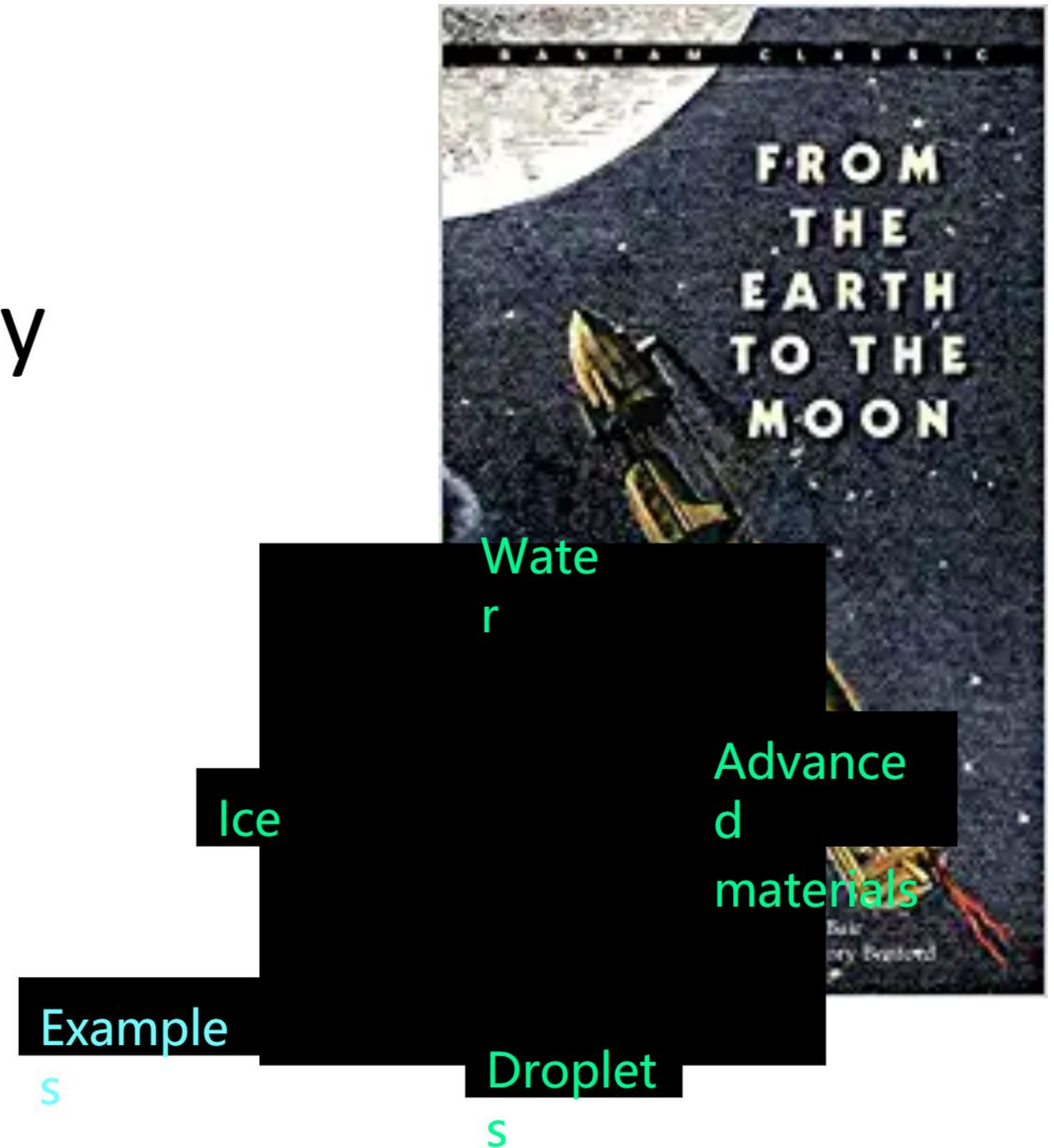
Using ChatGP
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© Robert Szucs/Grasshopper Geography

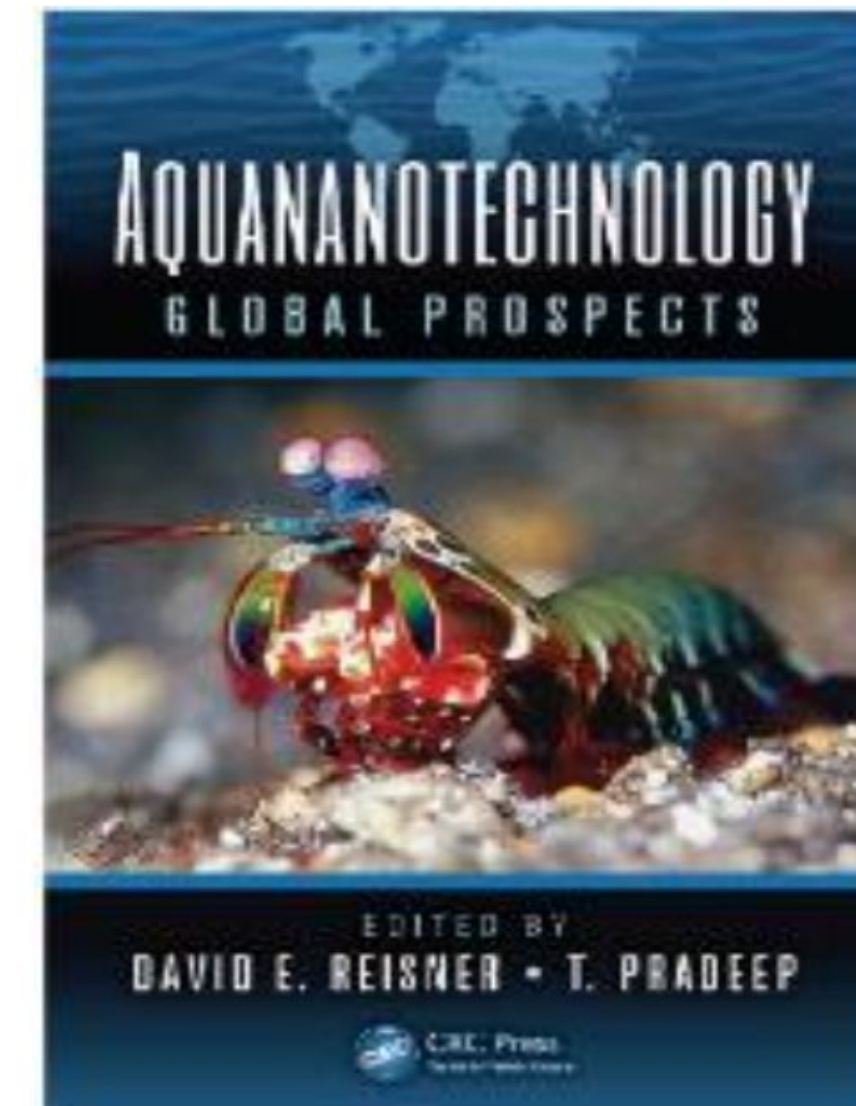
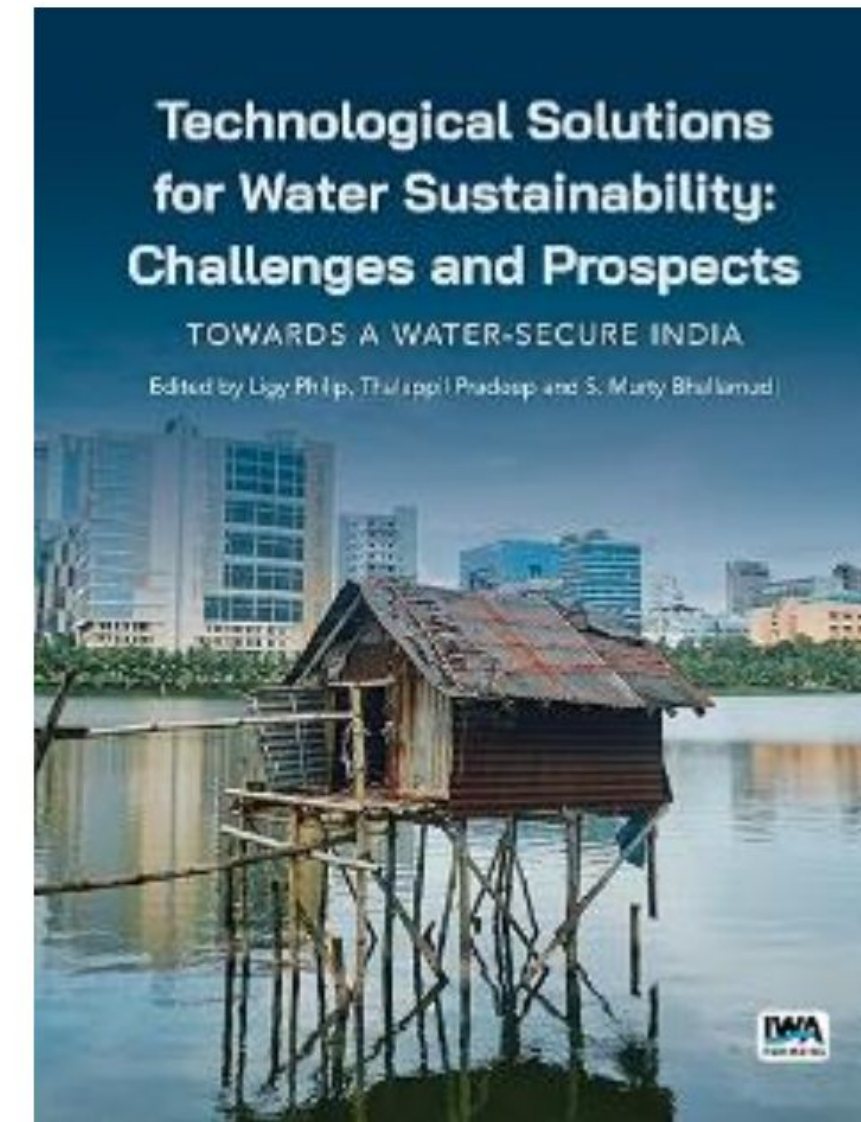
From S. Vishwanath

Our dreams become reality
with materials



Affordable clean water is a problem of advanced materials

New adsorbents
New sensors
New catalysts
Novel phenomena
New devices



Water purification, history

Future of water purification: An enigma with some pointers



Category-wise distribution of contaminants regulated by USEPA and future contaminants

Noble metal nanoparticles for water purification: A critical review, T. Pradeep and Anshup, Invited critical review, Thin Solid Films, 517 (2009) 6441-6478 (DOI: 10.1016/j.tsf.2009.03.195).

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. Jayachandrab 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,' Thirupathi Pradeep who led the team at IIT Chennai told Chemistry World. He and his student Suresh Kumar Hari 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 nanoparticles¹.

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 filter



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



Indian patent 200767

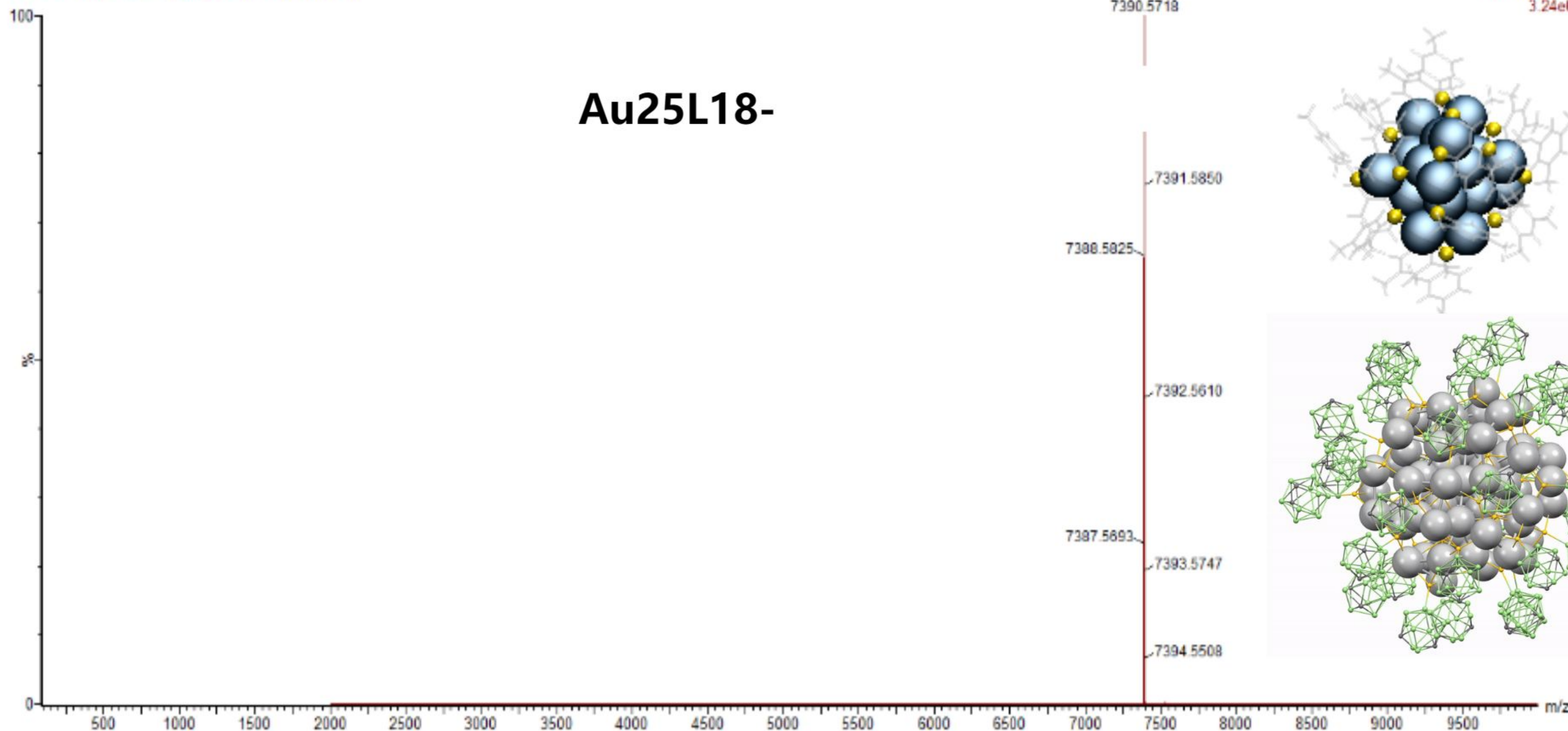
US 7,968,493

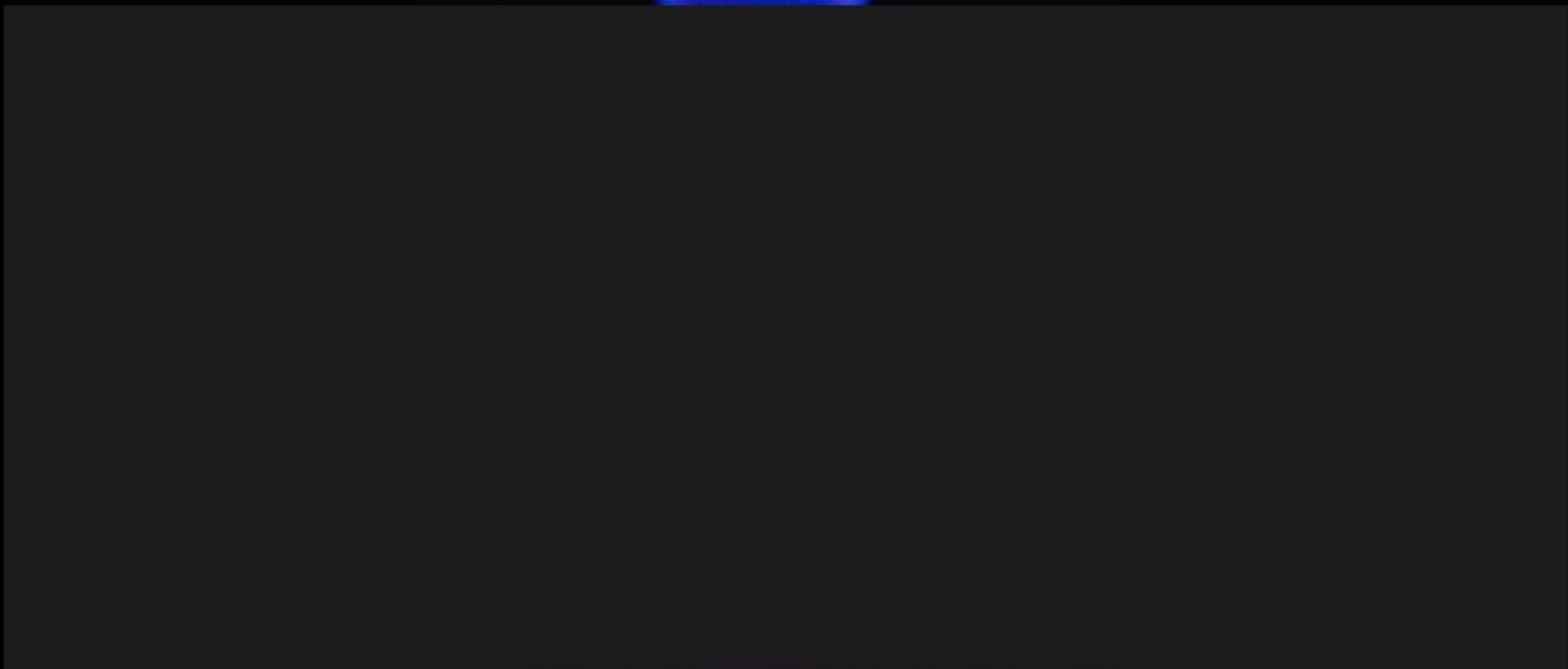
EP 17,15,947

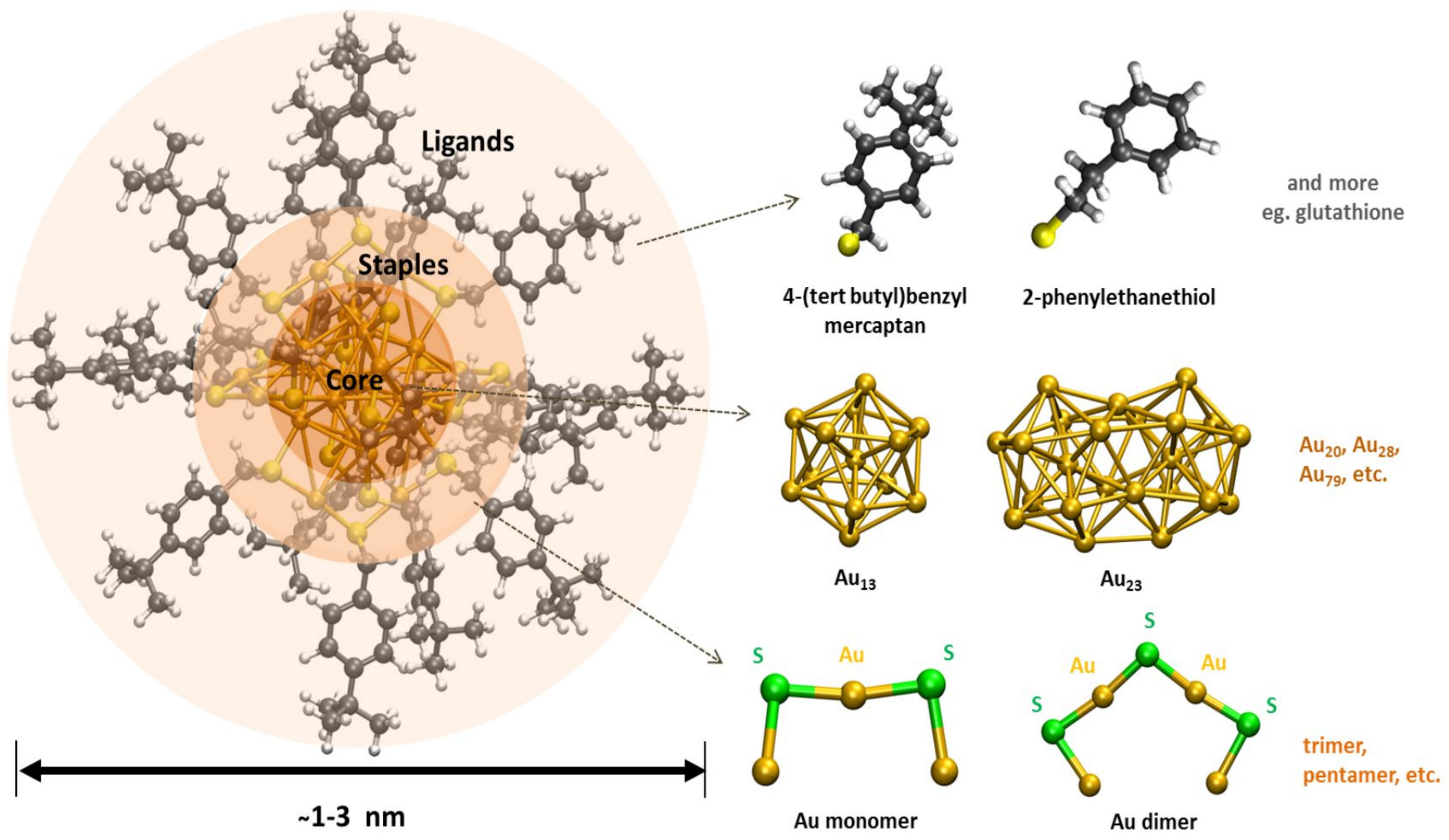
Product is marketed now by a Eureka Forbes Ltd

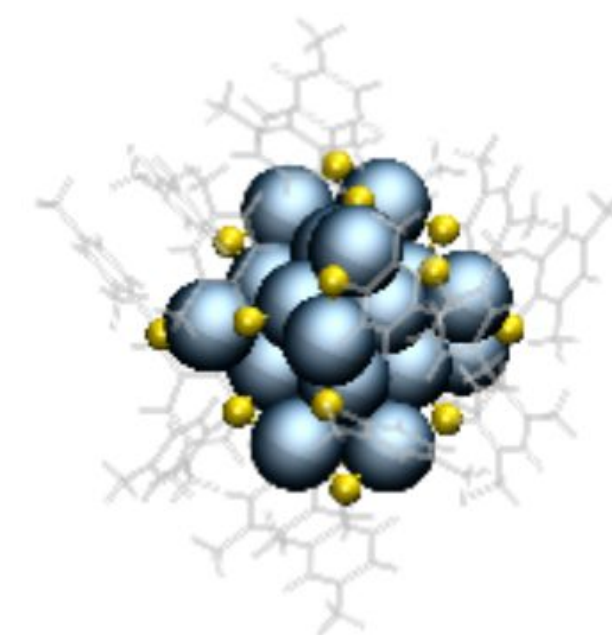
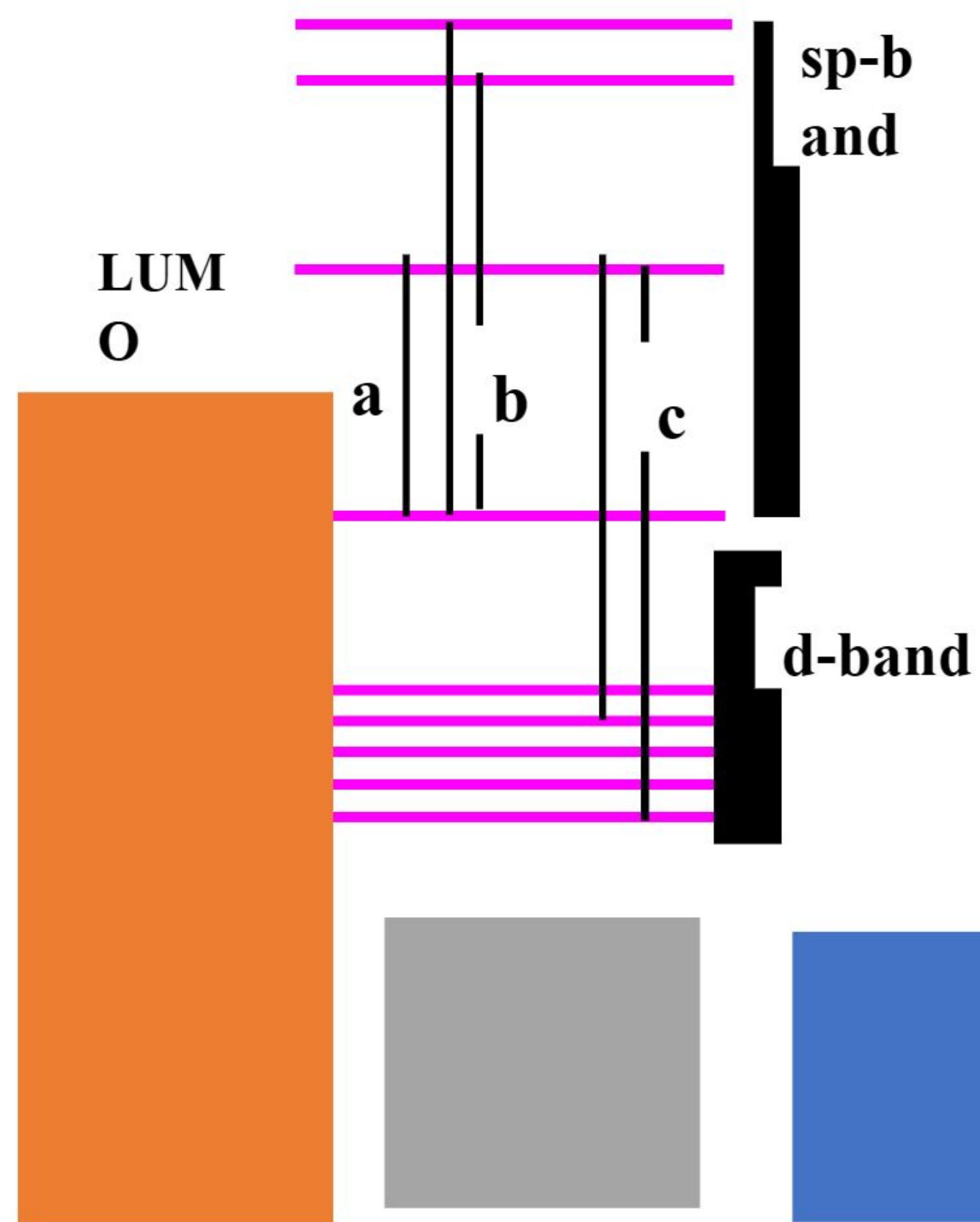
Nanomaterials are now atomically precise

AU25PET18_RES_NEG_MS_3 32 (0.558) Cm (5:80)









Jobin et. al. CPL, 2004

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

Evolution of noble metal clusters

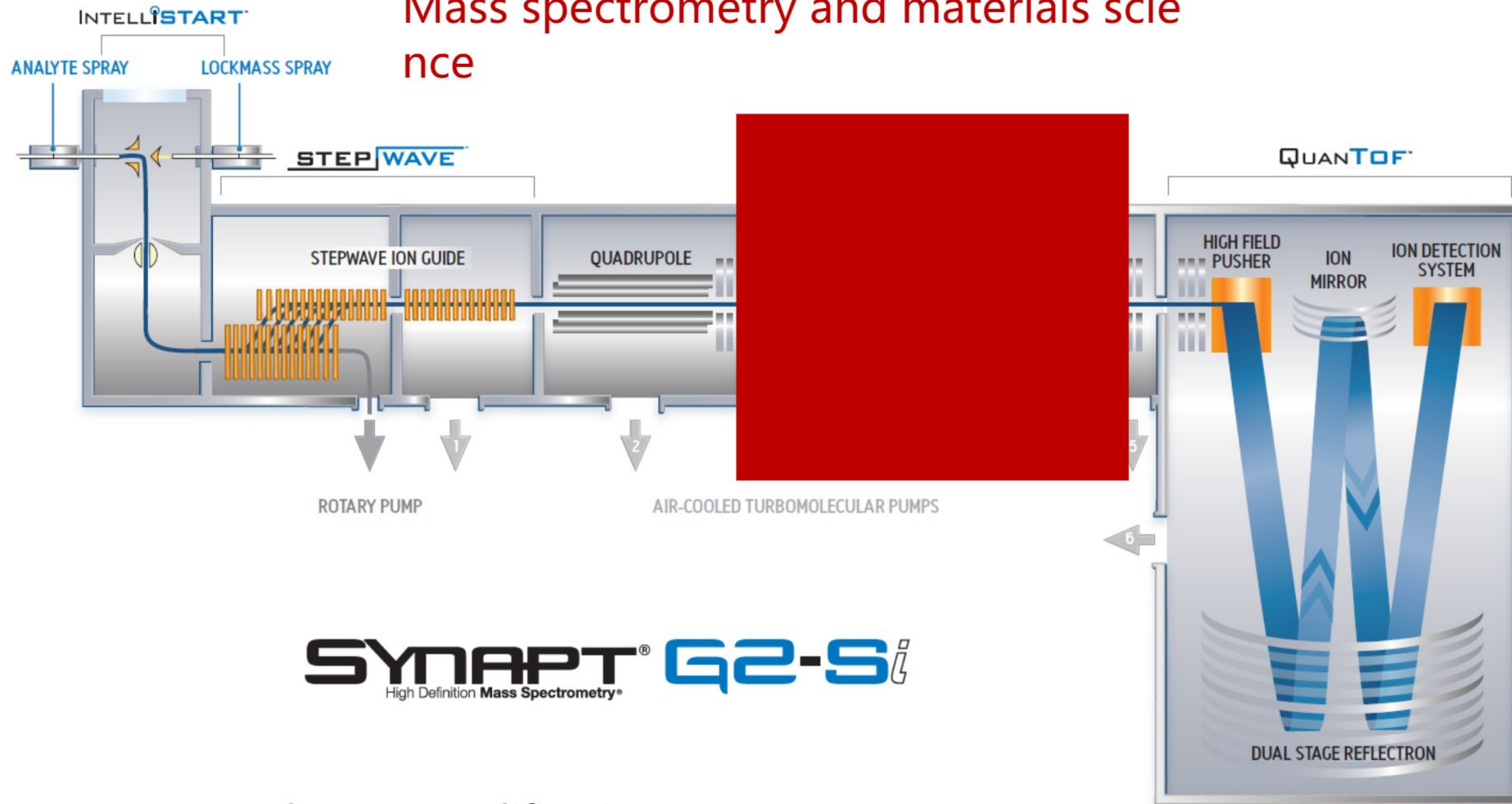
Citations: >210

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Also the pioneering work of R. W. Murray, Robert L. Whetten, Uzi Landman, Tatuya Tsukuda, Yuichi Negishi, Hannu Hakkinen,

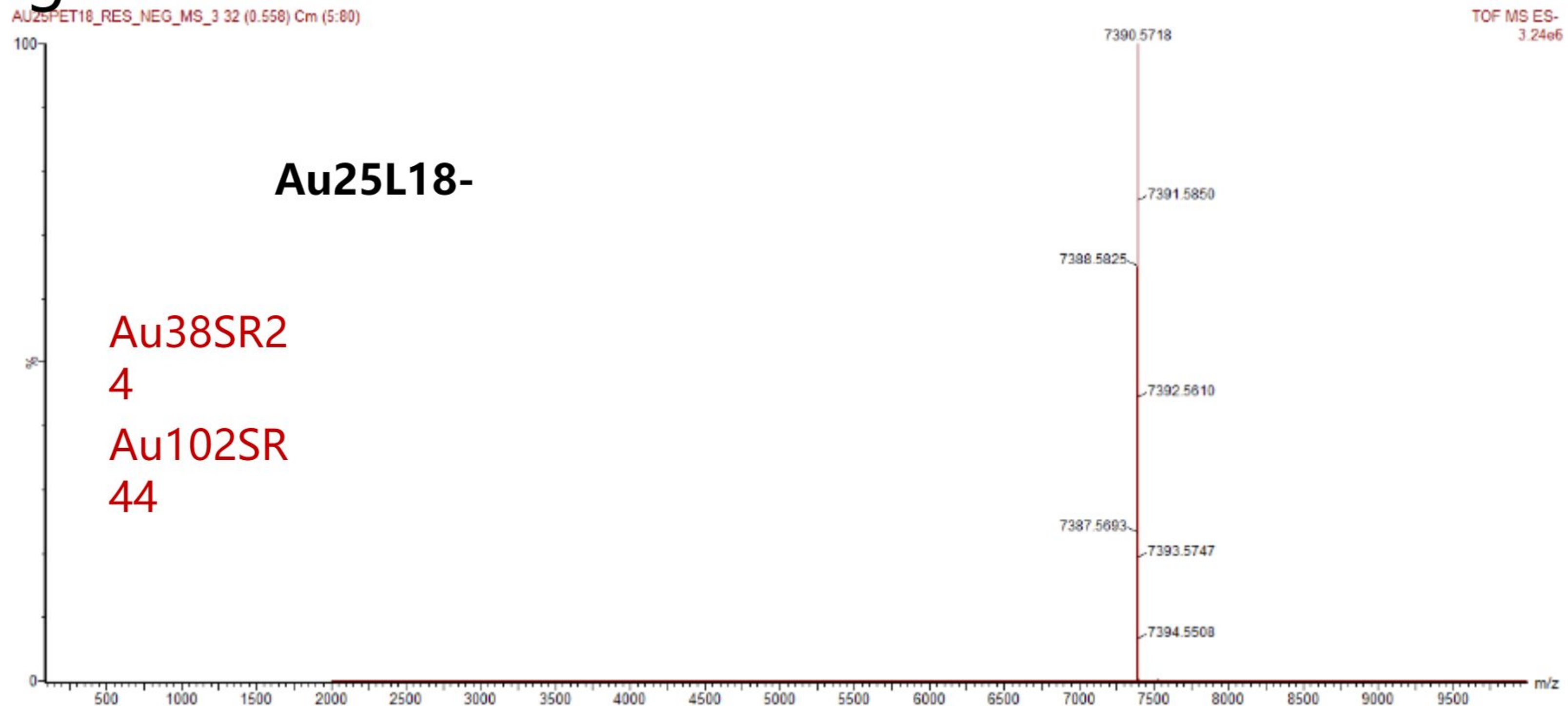
Rongchao Jin, Nanfeng Zheng, Terry Bigioni, Osman Bakr, Kornberg, Jianping Xie, C. M. Aikens, Thomas Buergi, Amala Dass, Ackerson, De-en Jiang, A. W. Castleman Jr., H. Schmidbauer, Robin Ras, Olli Ikkala

Mass spectrometry and materials science

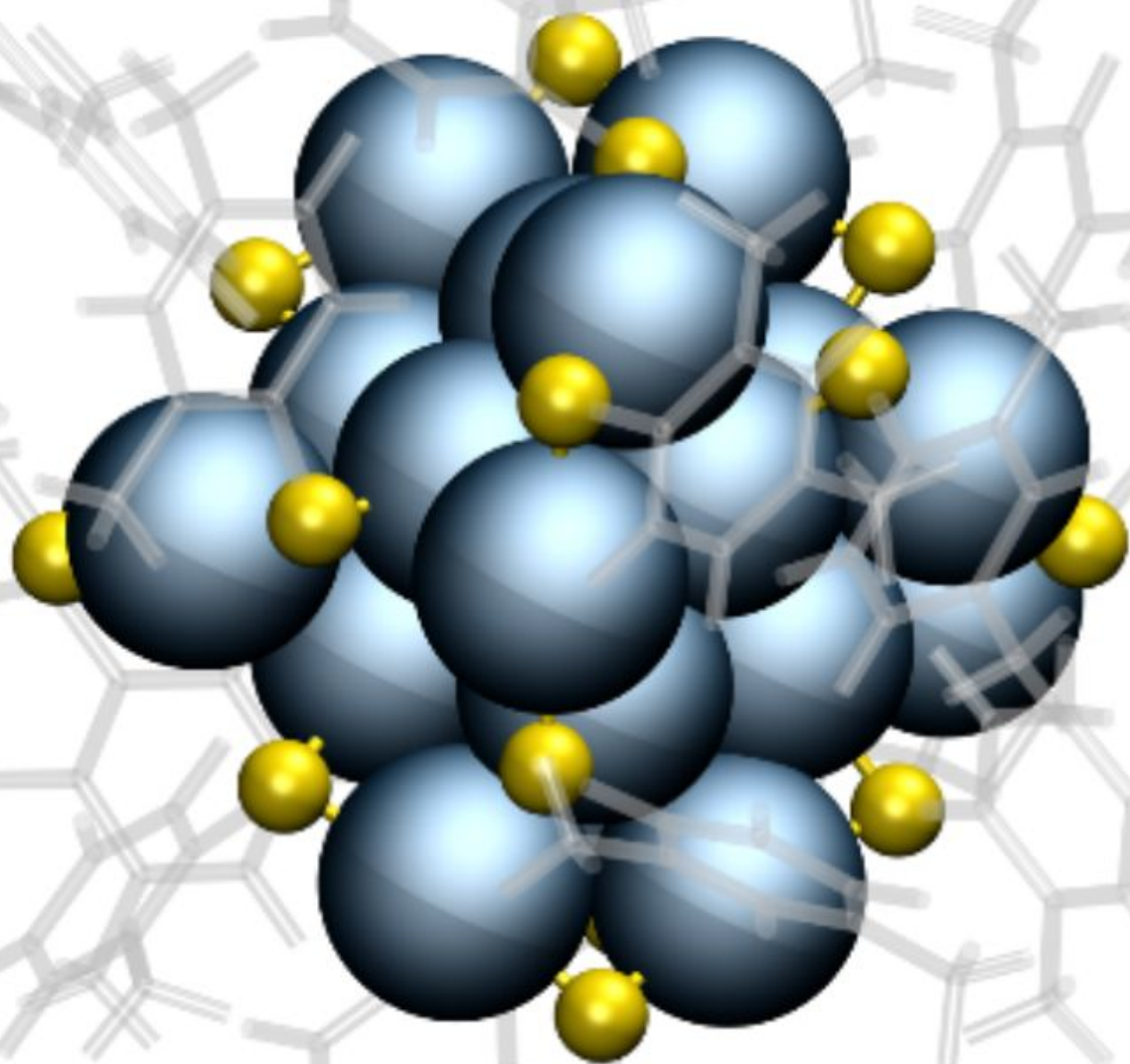


...and many modifications

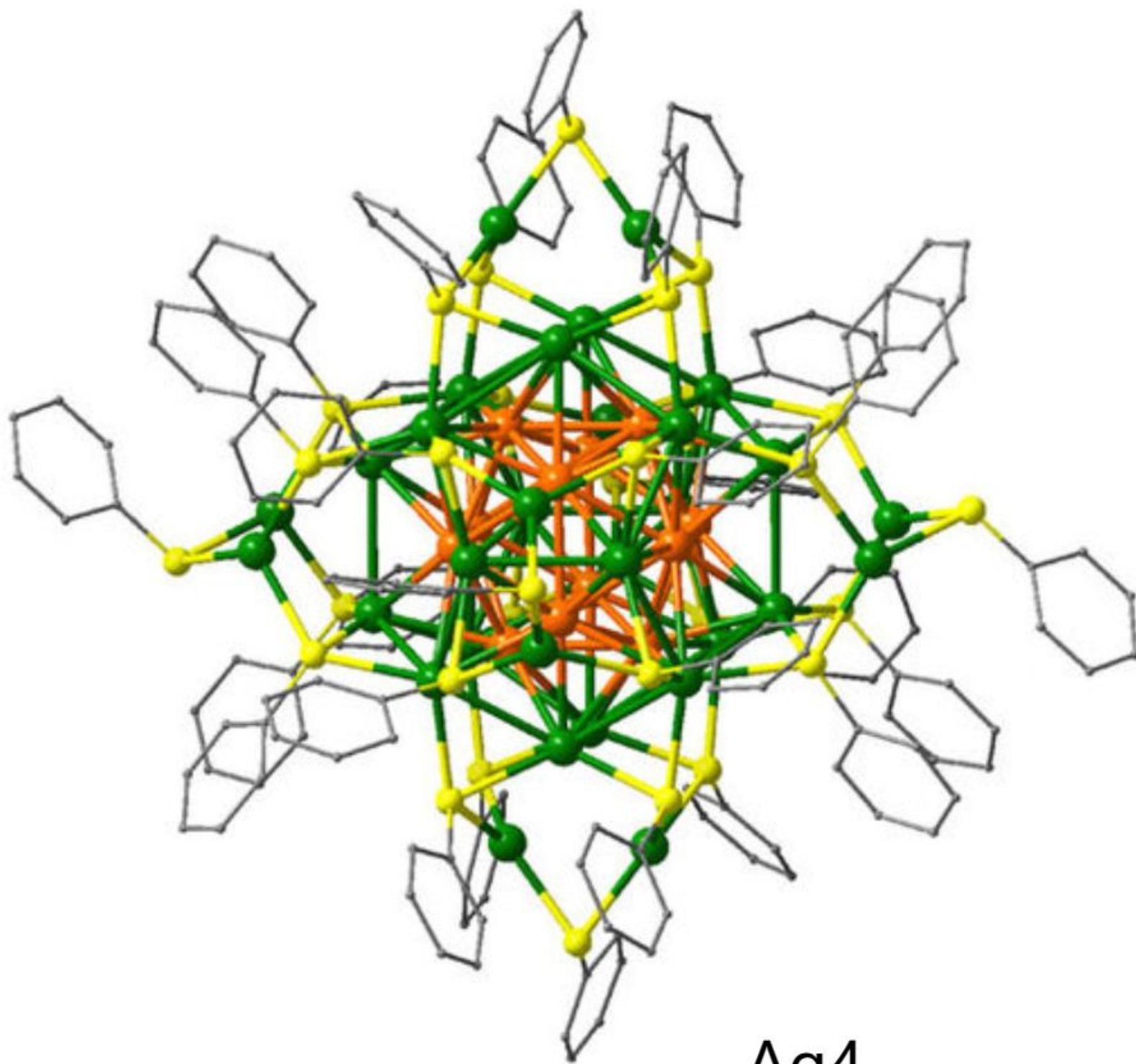
Molecular formula, Molecular weight



S



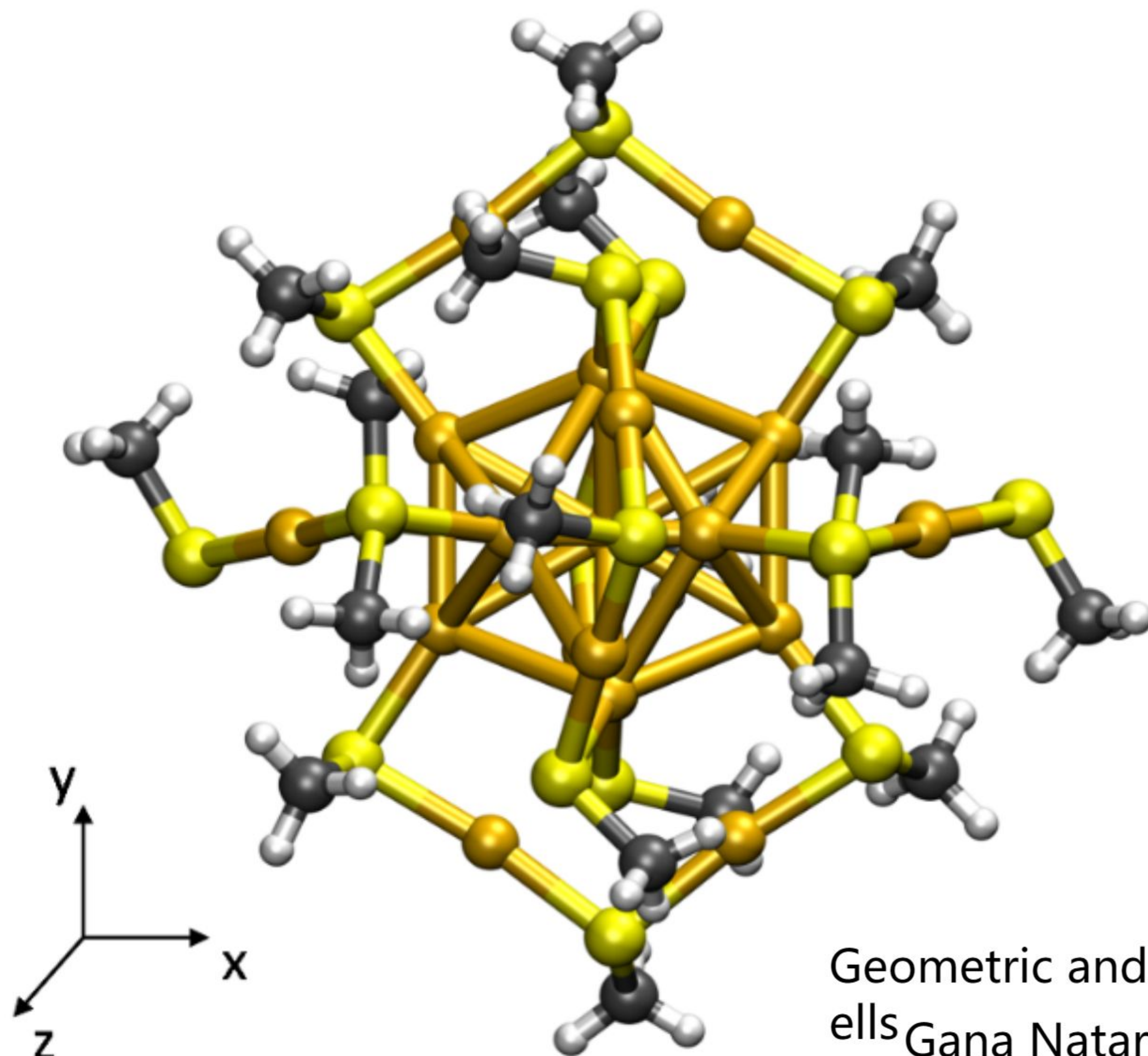
Au₂₅, Ag₂₅, A
g₂₉


$$\text{Ag}_4^4$$

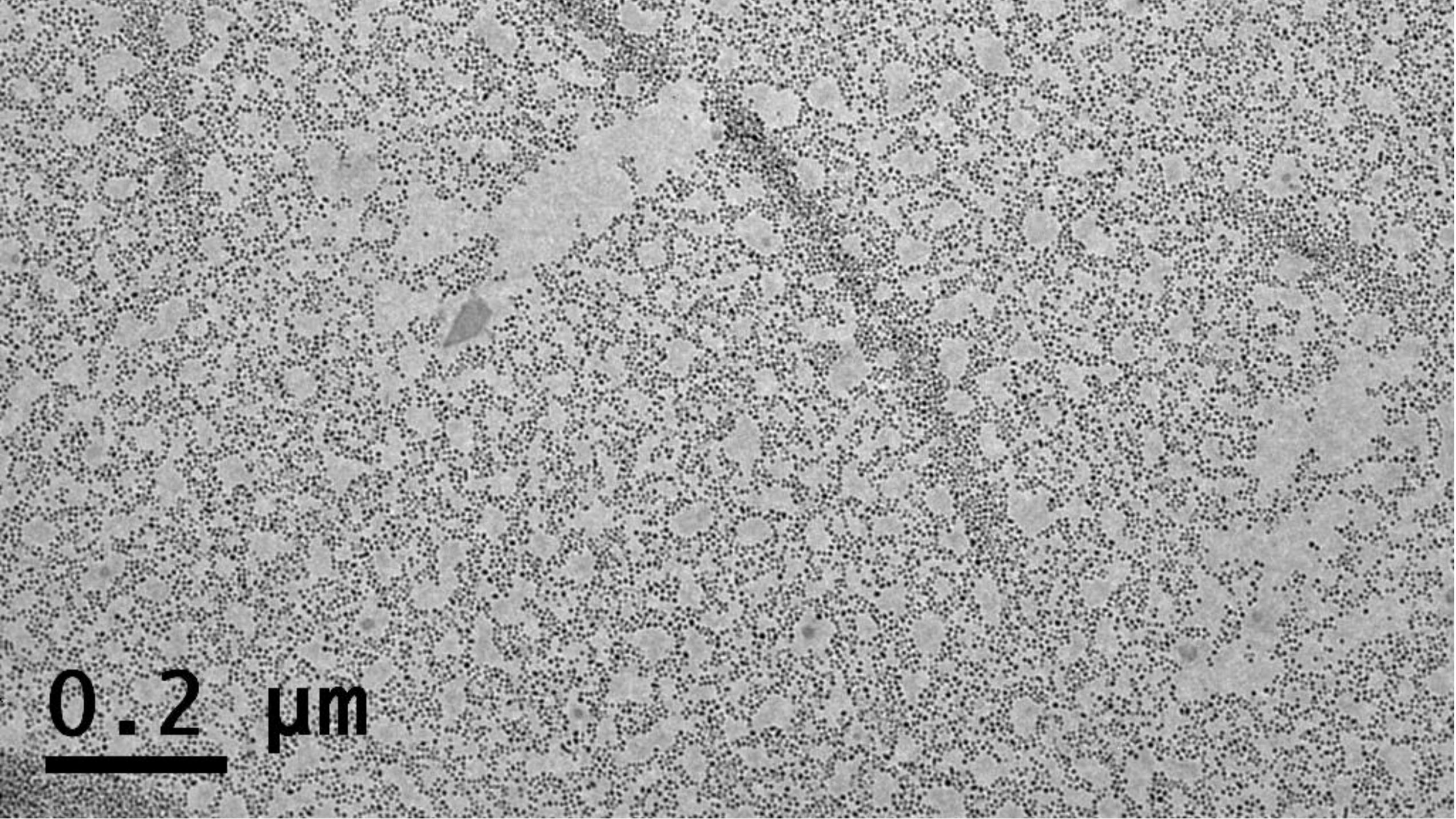
Nanfeng Zheng et al. *Nature Communications*, 2013

Terry Bigioni et al. *Nature* 2013

Molecular structure

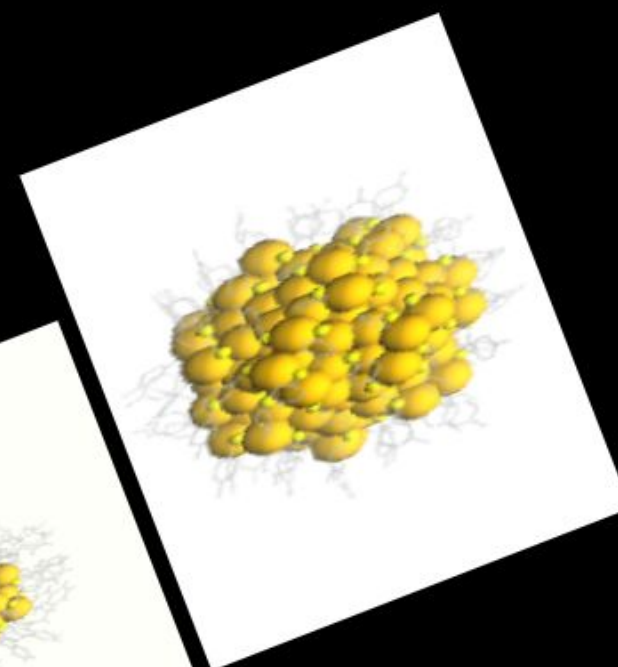
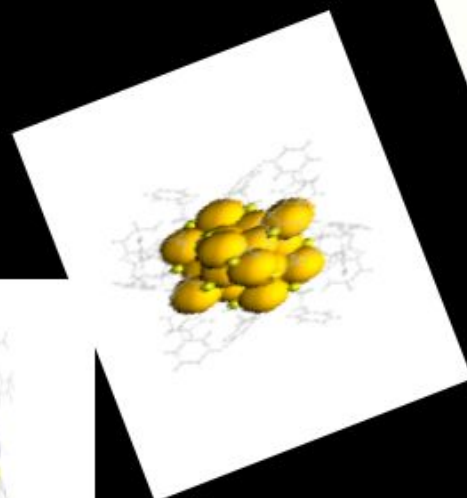
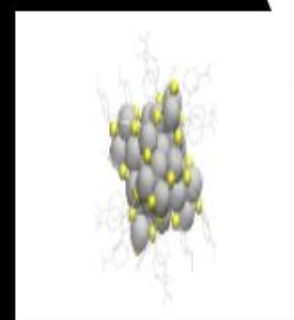


Geometric and electronic shells
Gana Nataraja
n



0.2 μm

Ag₂₉(BDT)₁₂₃⁻ Ag₂₅(DMBT)₁₈⁸⁻ Au₂₅(PET)₁₈⁻



HRMS of Au₂₅(PET)₁₈⁻

m/z

Molecular materials

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	$480. \times 10^{-12} \text{m}^2/\text{N}$
Coefficient of thermal expansion, 25°C	$256.32 \times 10^{-6} \text{K}^{-1}$
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

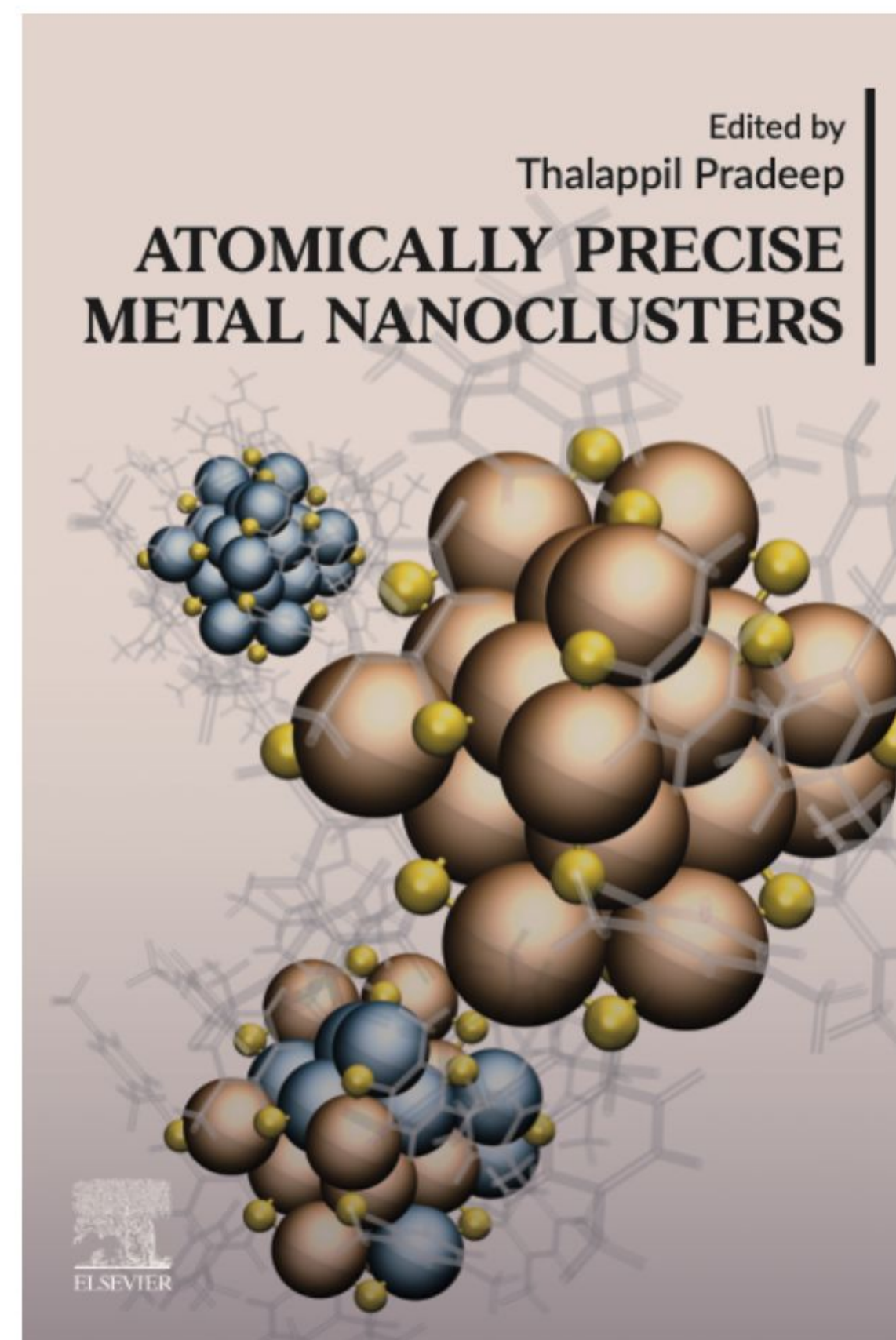
Physical properties

Electrical, magnetic

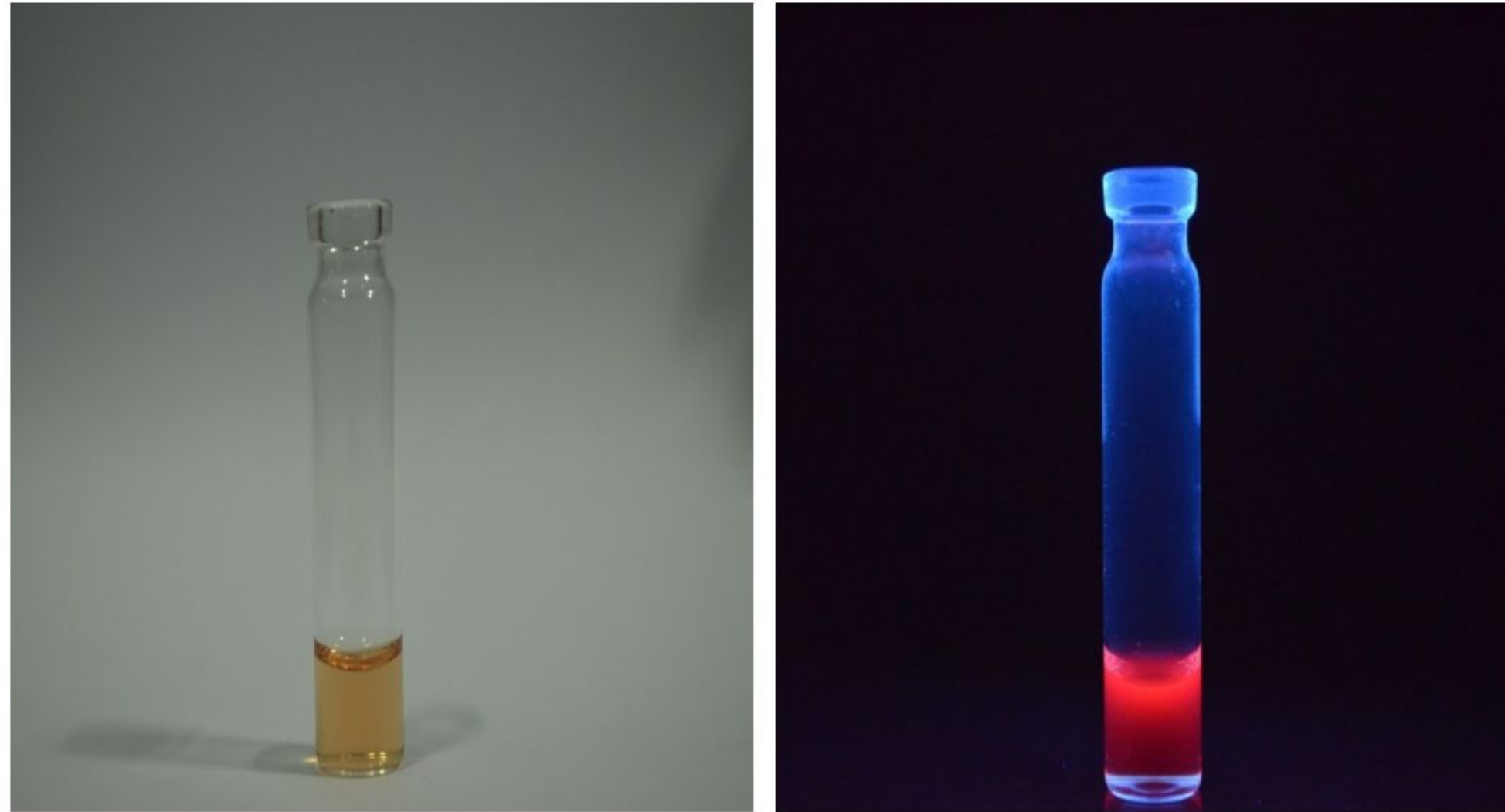
Mechanical properties

Electrochemical properties

Future?



Molecular reactions



Reactions on clusters

Reactions between clusters

Inter-cluster reactions



Article

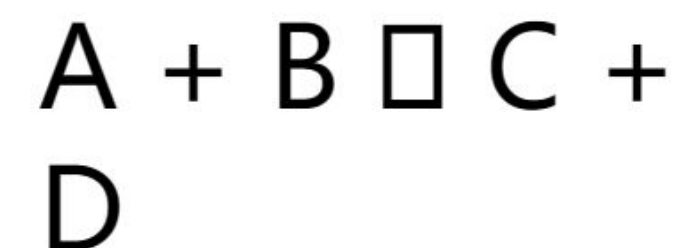
pubs.acs.org/JACS

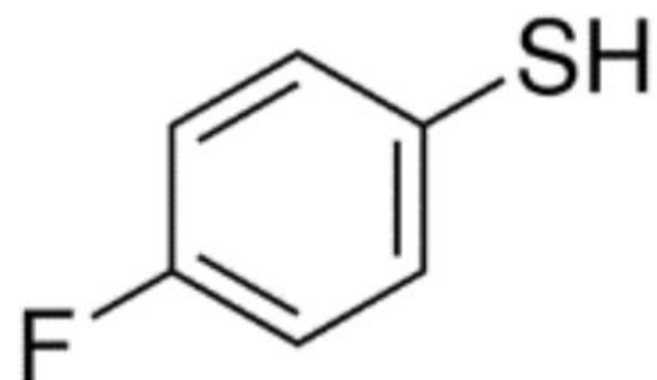
Intercluster Reactions between $\text{Au}_{25}(\text{SR})_{18}$ and $\text{Ag}_{44}(\text{SR})_{30}$

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





Energies for the substitution reaction of (A) Au in $\text{Ag}_{44}(\text{SR})_{30}$, (B) Ag in $\text{Au}_{25}(\text{SR})_{18}$ and (C) the overall reaction energies (in eV) as a function of their positions in product clusters, $\text{Au}_x\text{Ag}_{44-x}(\text{SR})_{30}$ and $\text{Au}_{25-x}\text{Ag}_x(\text{SR})_{18}$ for $x=1$

Ag₂₅-Au₂₅ experiments

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

DMBT

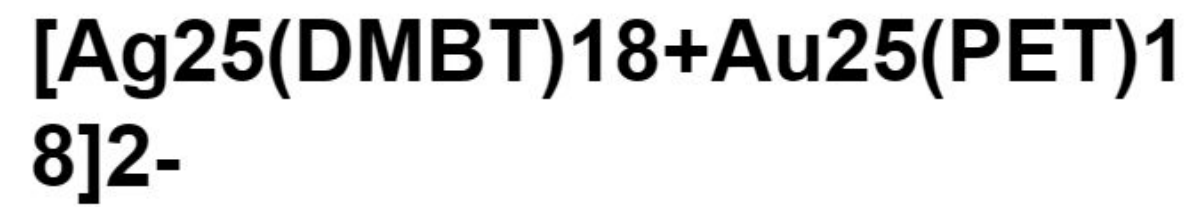
PE
T



DMBT

**PE
T**

**Ag₂₅(DMBT)
18**



**Au₂₅(PET)
18**

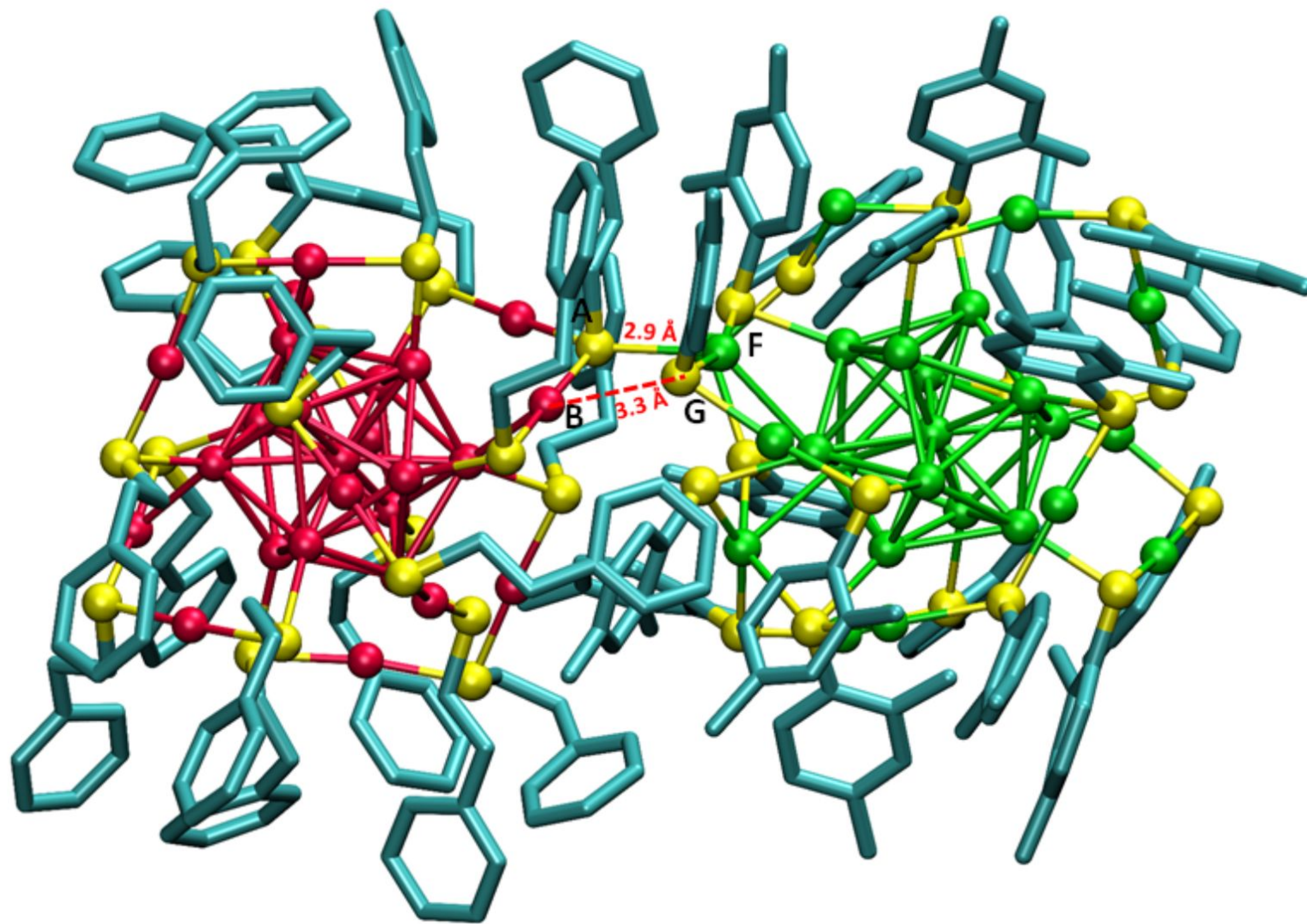
Evolution of alloy clusters from the dianionic adduct, $[\text{Ag}_{25}\text{Au}_{25}(\text{DMBT})_{18}(\text{PET})_{18}]^{2-}$

within 5 min

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

within 2 min

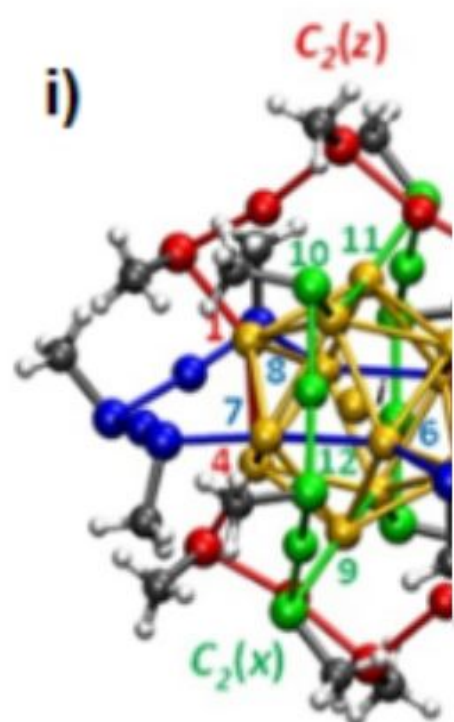
Optimized structure of $[\text{Ag}_{25}\text{Au}_{25}(\text{DMBT})_{18}(\text{PET})_{18}]^{2-}$



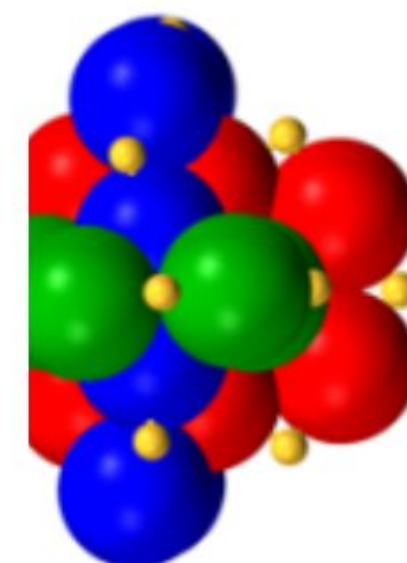
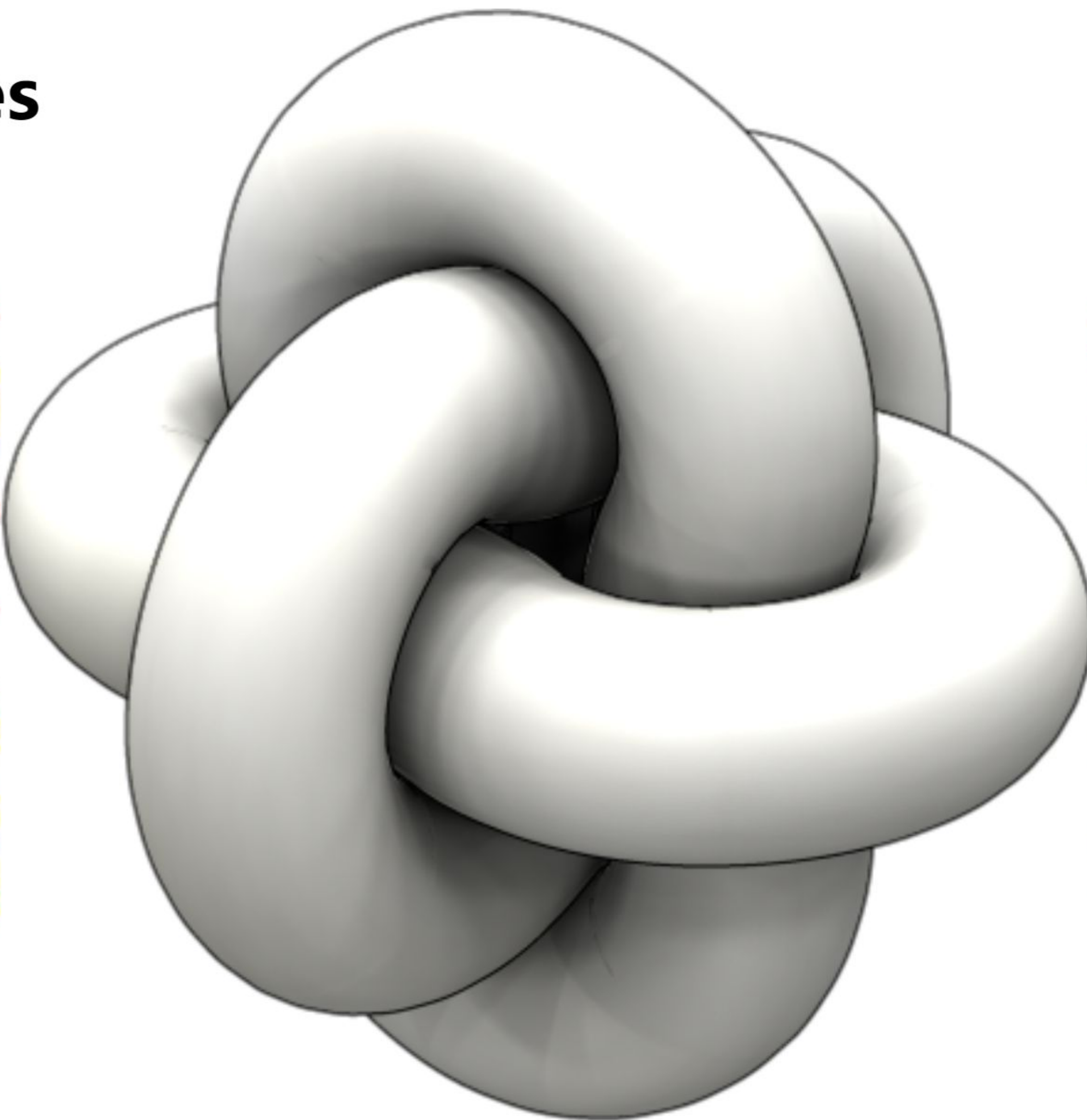
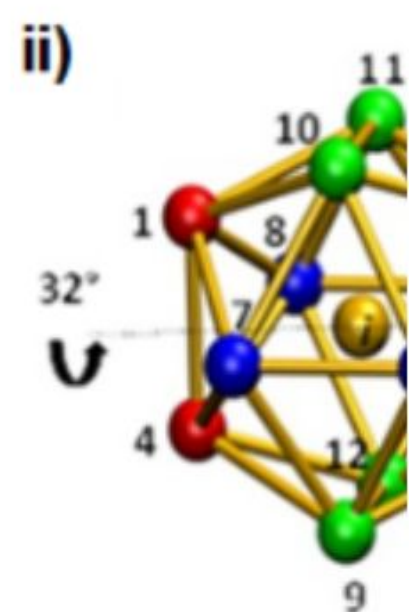
How do we comprehend th
is?

Nomenclatu
re

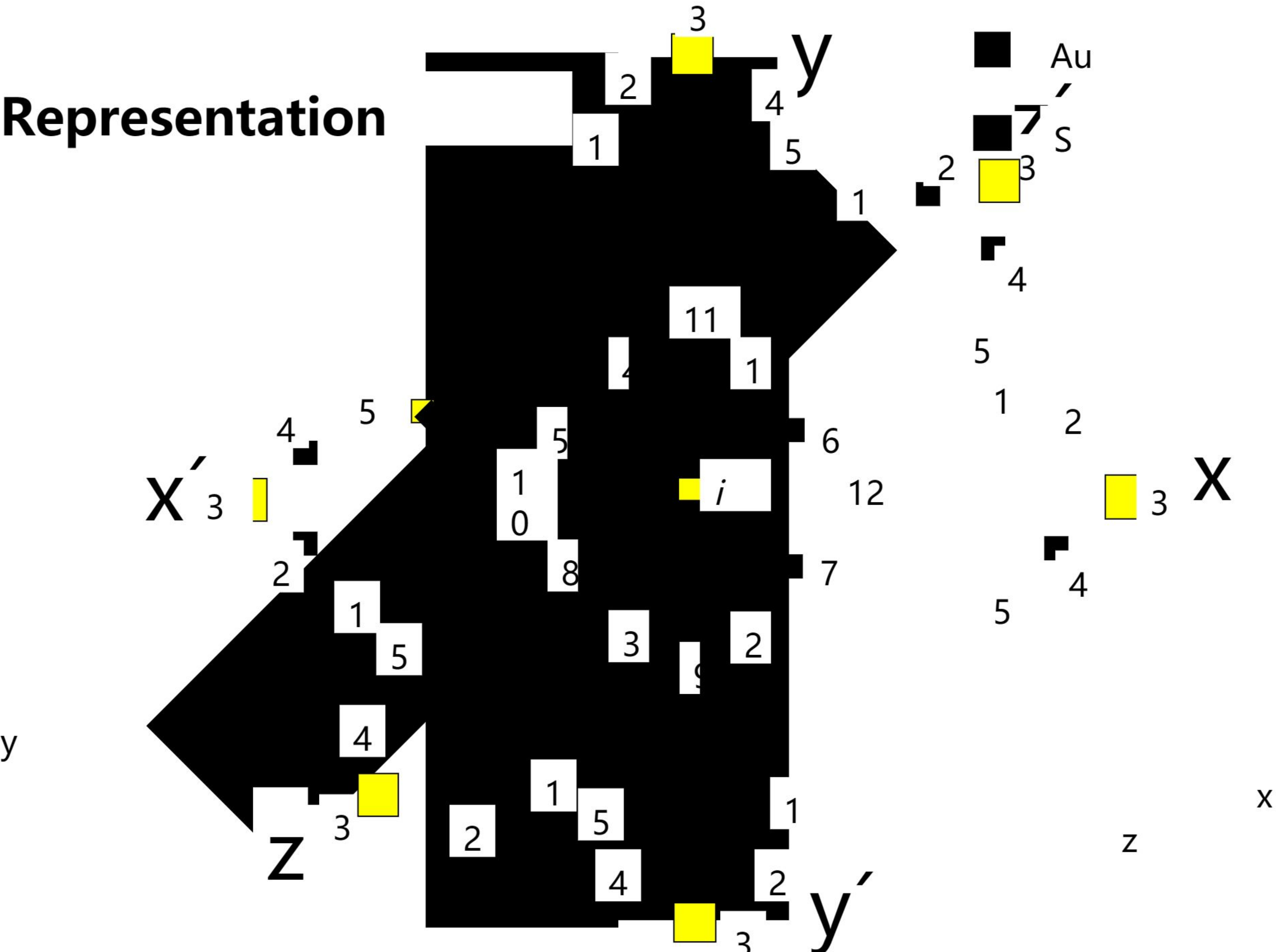
Aspicules



18(methylthiolato)-auro-



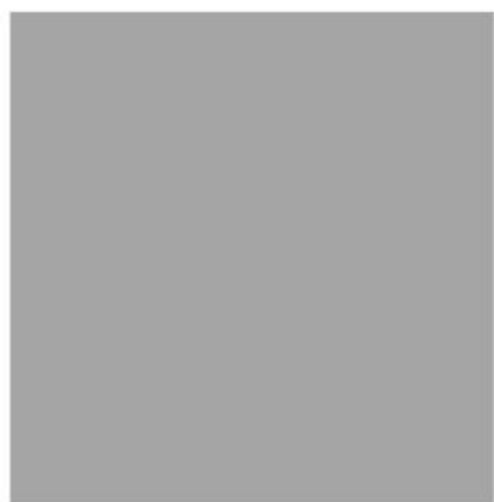
Representation



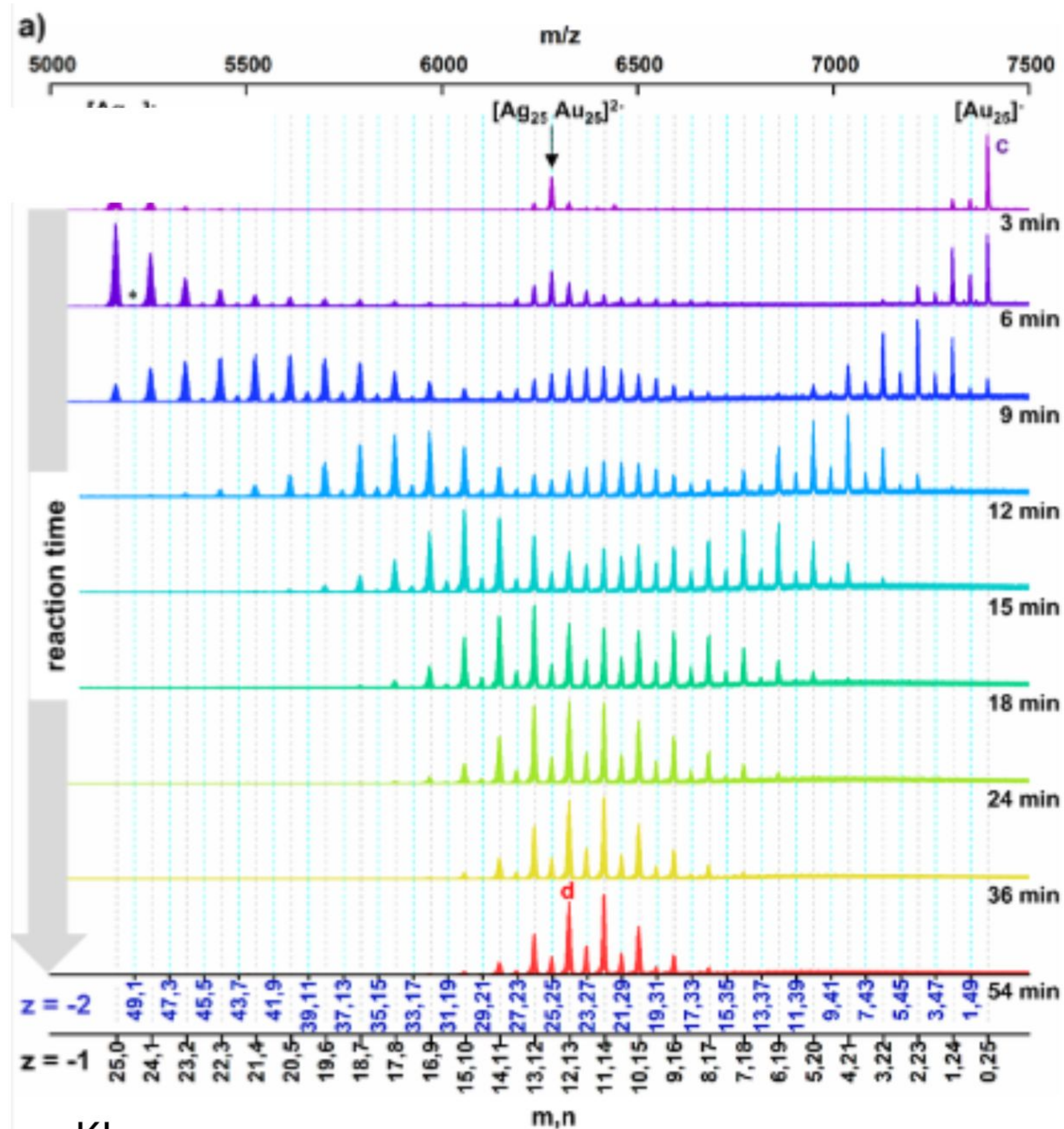
Naming

(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-)



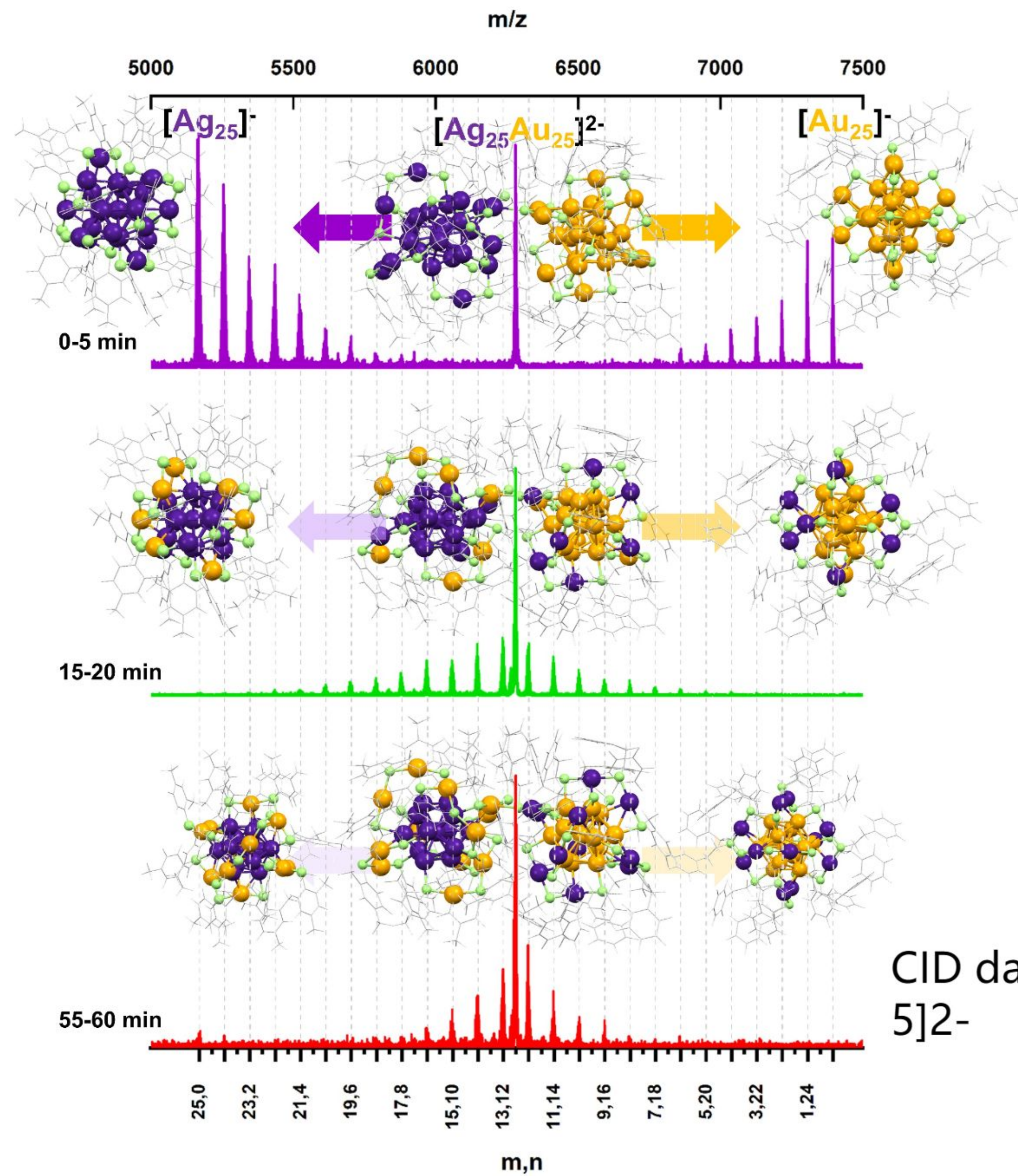
Complexities



Manfred Kappes, KI
T

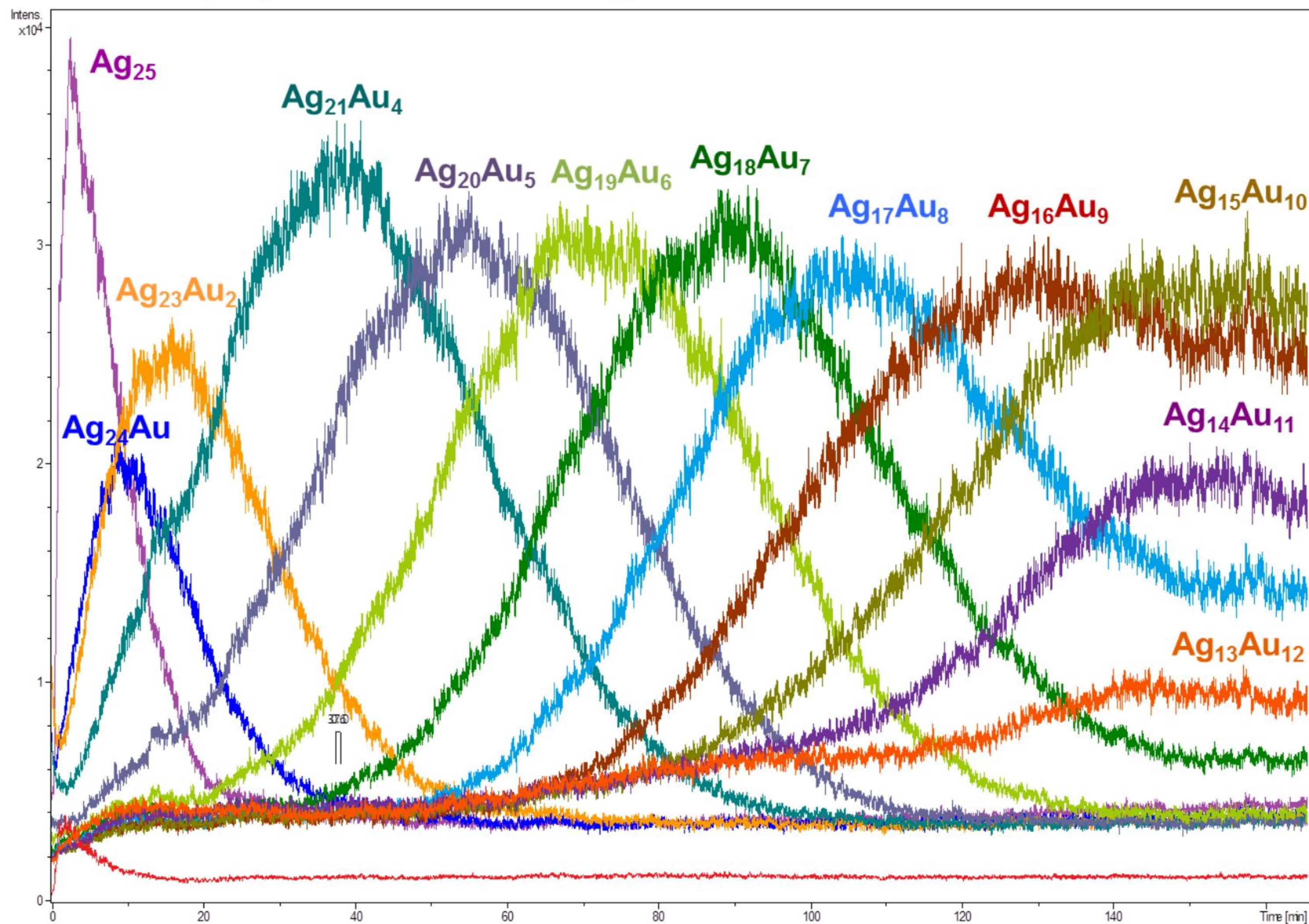
M. Neumaier, A. Baksi, et. al., *JACS* 20

21

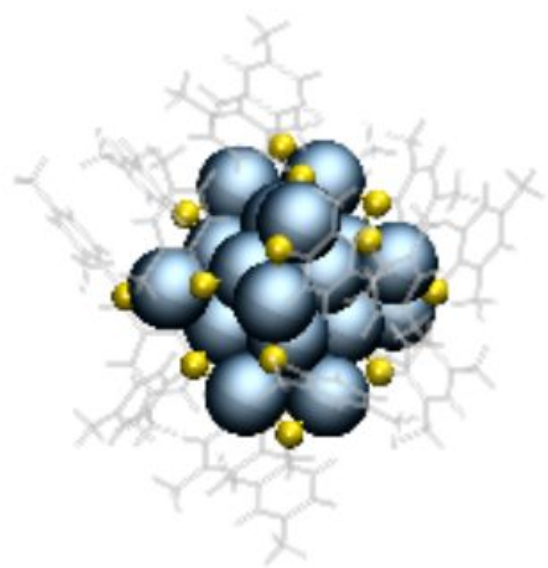


Kinetics of the exchange (monitored on the Ag25 sid

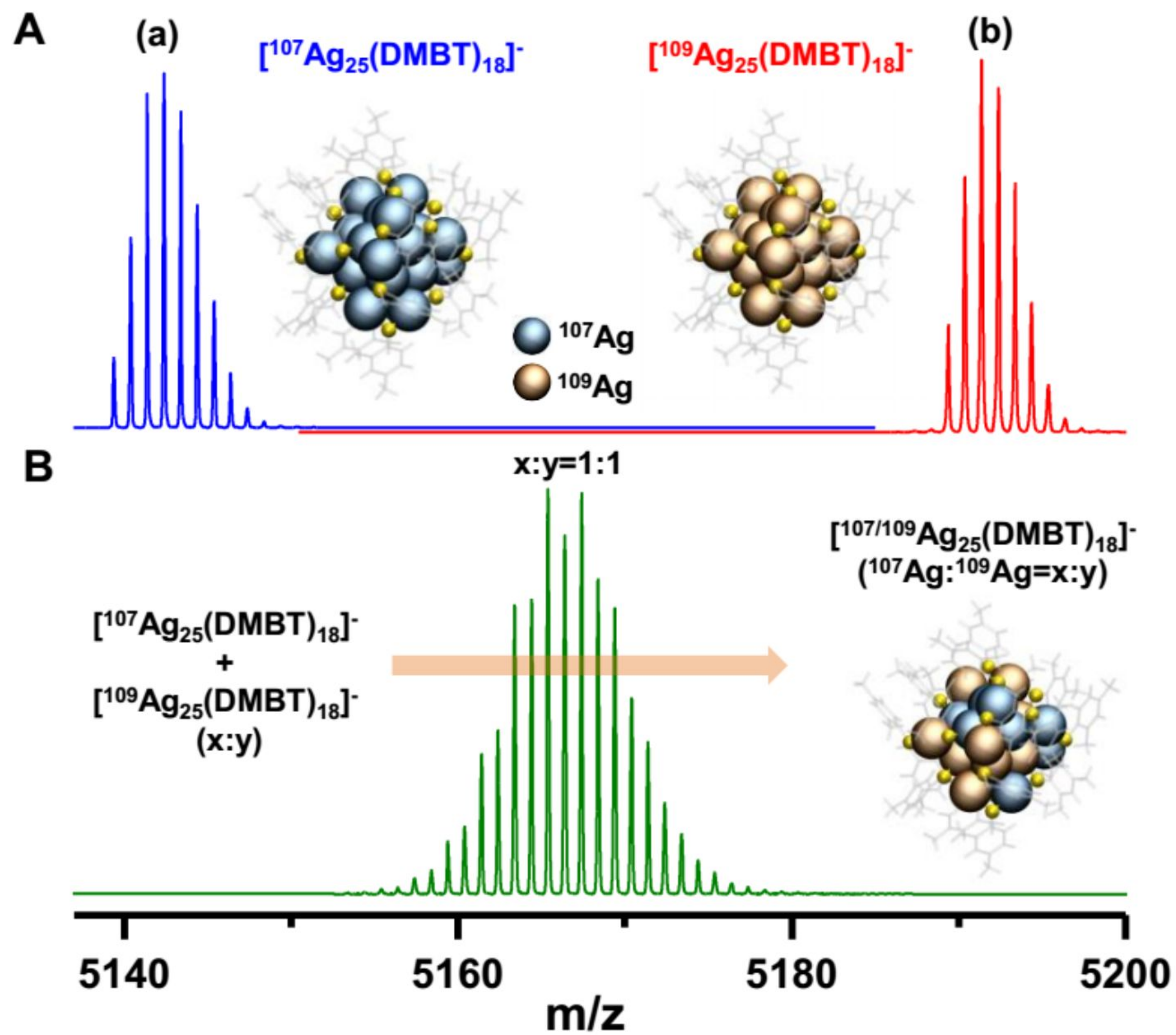
e)

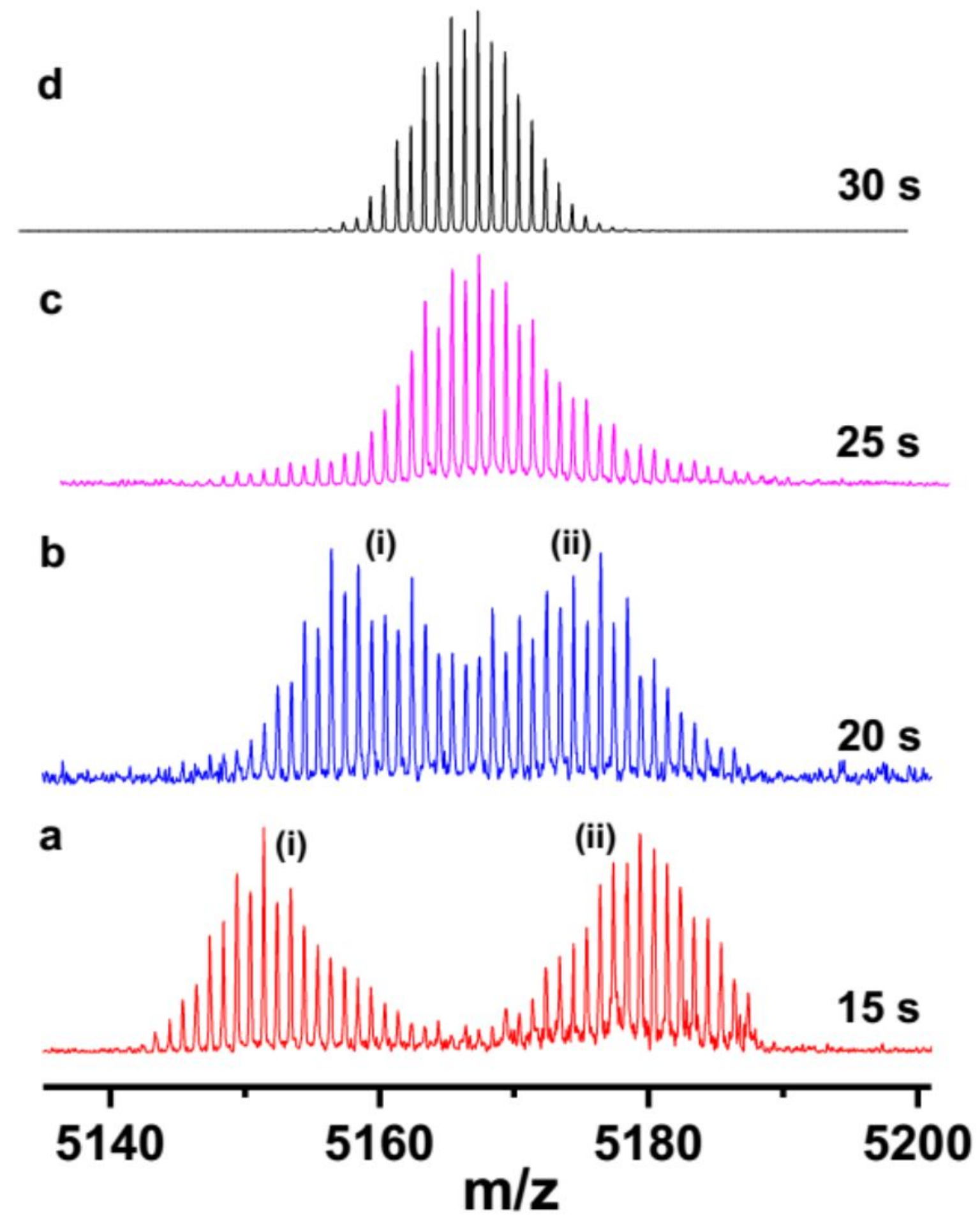


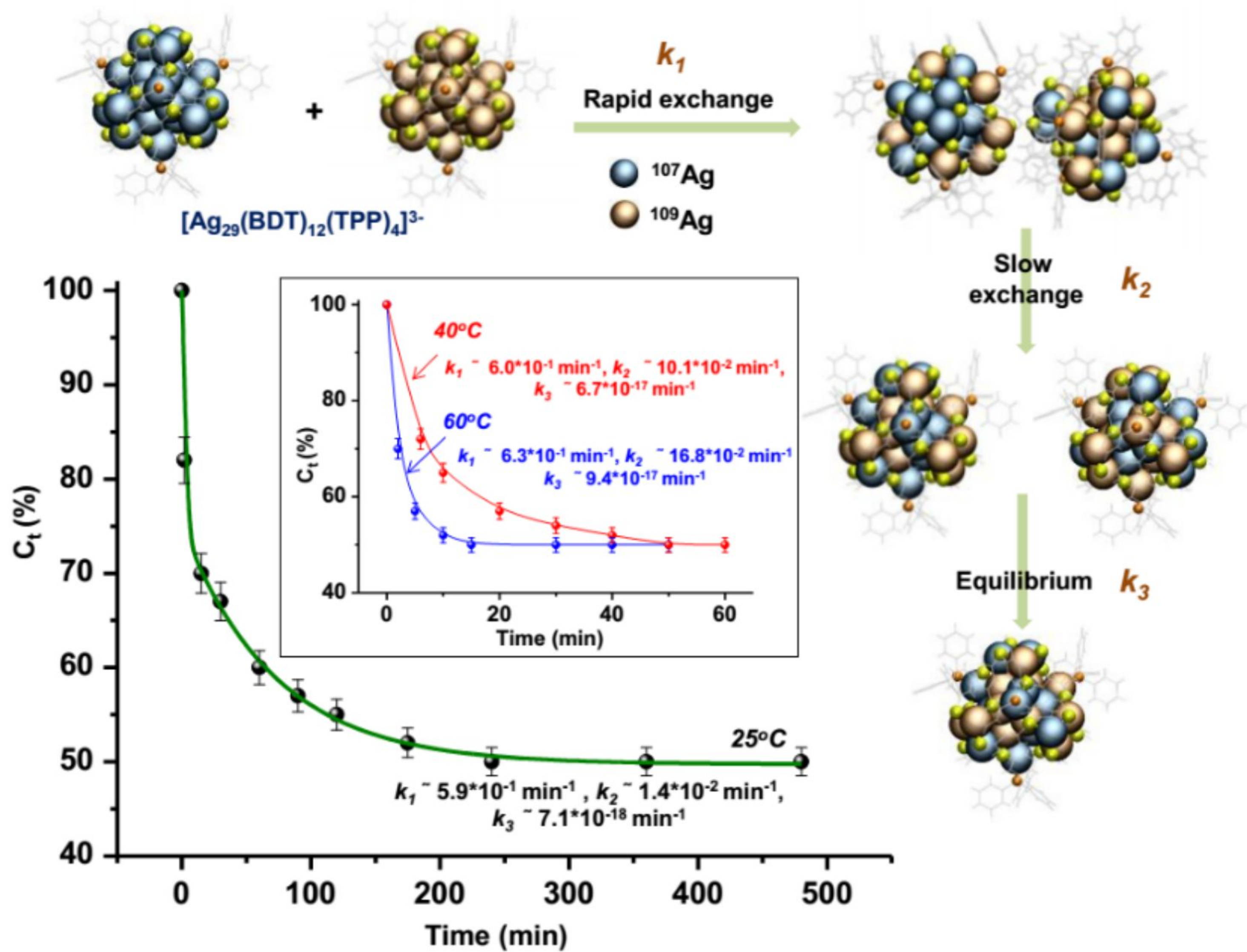
Coulomb adduc



ESI MS of **A)** $^{107}\text{Ag}_{25}(\text{DMBT})_{18}$ and **B)** $^{109}\text{Ag}_{25}(\text{DMBT})_{18}$. Insets shows the respective isotope patterns.







Clean water for everyone



ACS Sustainable Chemistry & Engineering Editorial, December 2016

Water positive materials

PNAS PNAS PNAS

Biopolymer-reinforced synthetic granular nanocomposites for affordable water purification

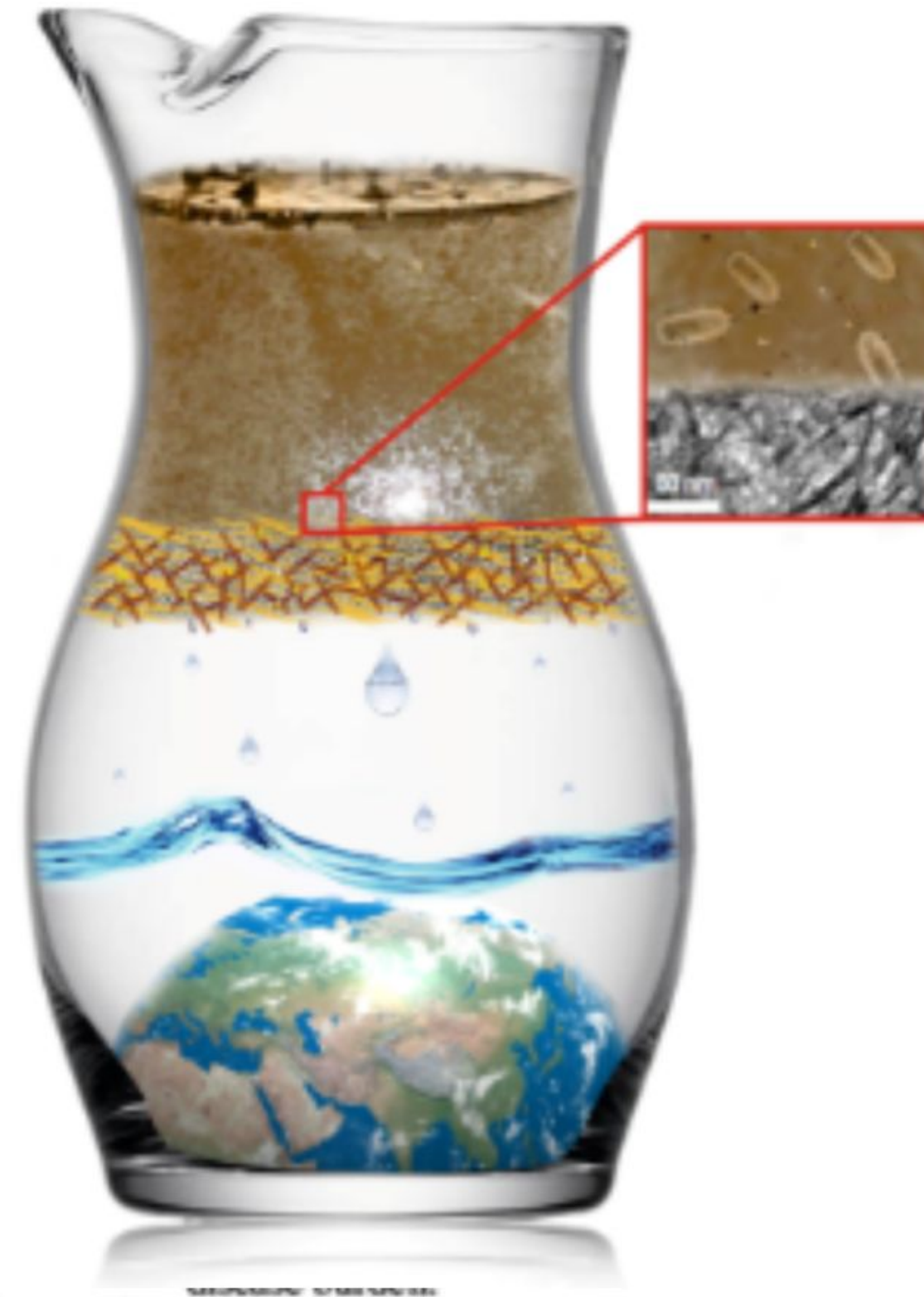
Mohan Udhaya Sankar¹, Sahaja Aigal, Kamalesh Chaudhari, and Thalappil Pradeep

¹Unit of Nanoscience and Thematic Unit of Excellence

Edited by Eric Hoek, University of California, Los Angeles

Creation of affordable materials for constant clean drinking water is one of the most promising ways to ensure water for all. Combining the capabilities of nanocomposites to scavenge toxic species such as heavy metals and other contaminants along with the above-mentioned materials to create an affordable, all-inclusive drinking water purifier without electricity. The critical problem is the synthesis of stable materials that can reliably function in the presence of complex species in drinking water that deposit and cause scaling on surfaces. Here we show that such constant clean water can be synthesized in a simple and effective fashion without the use of electrical power. The nanocomposites have sand-like properties, such as higher shear strength and stability. These materials have been used to create a water purifier to deliver clean drinking water. The ability to prepare nanostructured materials at ambient temperature has wide relevance for water purification.

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



Anil Kumar,

6, India

September 21, 2012

continued retention

of nanocrystalline materials prepared by the previous route. The high abundance of -OH groups help in the crystallization of strong covalent bonds. X-ray photoelectron spectroscopy (XPS) analysis confirmed the composition is rich in oxygen. The results were confirmed by X-ray photoelectron spectroscopy (XPS) analysis. The results were confirmed by X-ray photoelectron spectroscopy (XPS) analysis.

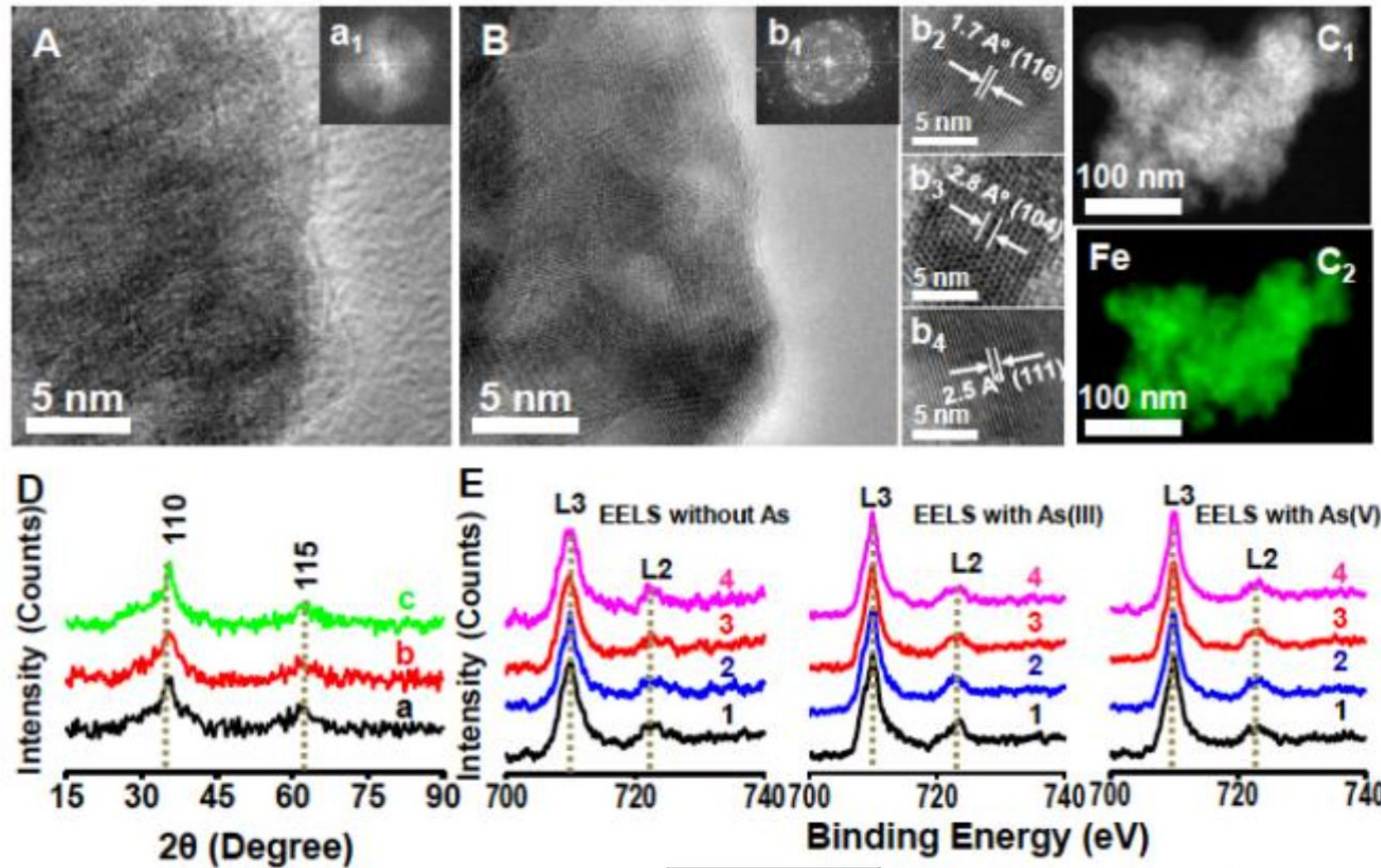
How to make?

What is special?

Live/dead staining experiments

No nanotoxicity

Variety of materials



www.advmat.de

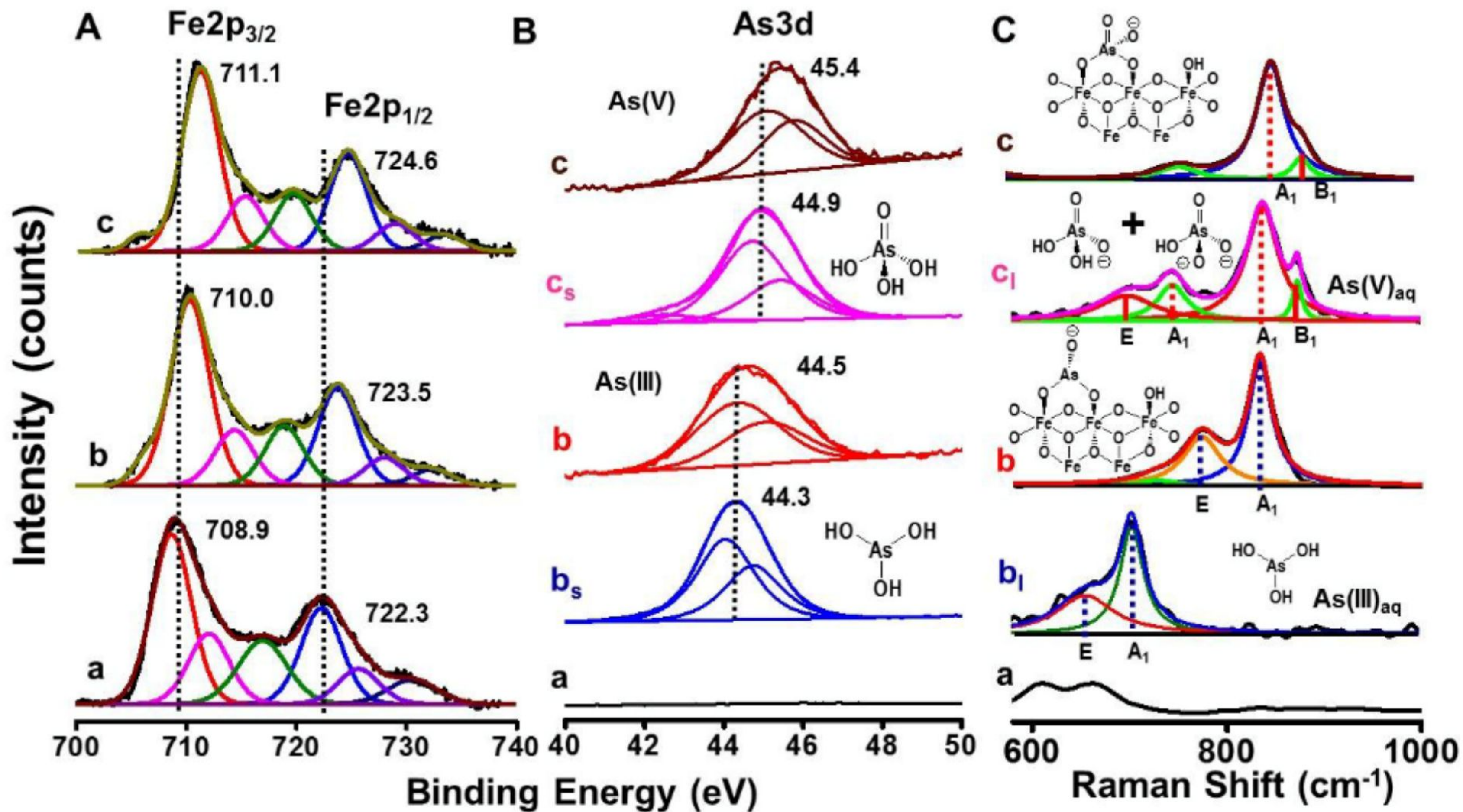
Author Pr ⁶ ADVANCED MATERIALS

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

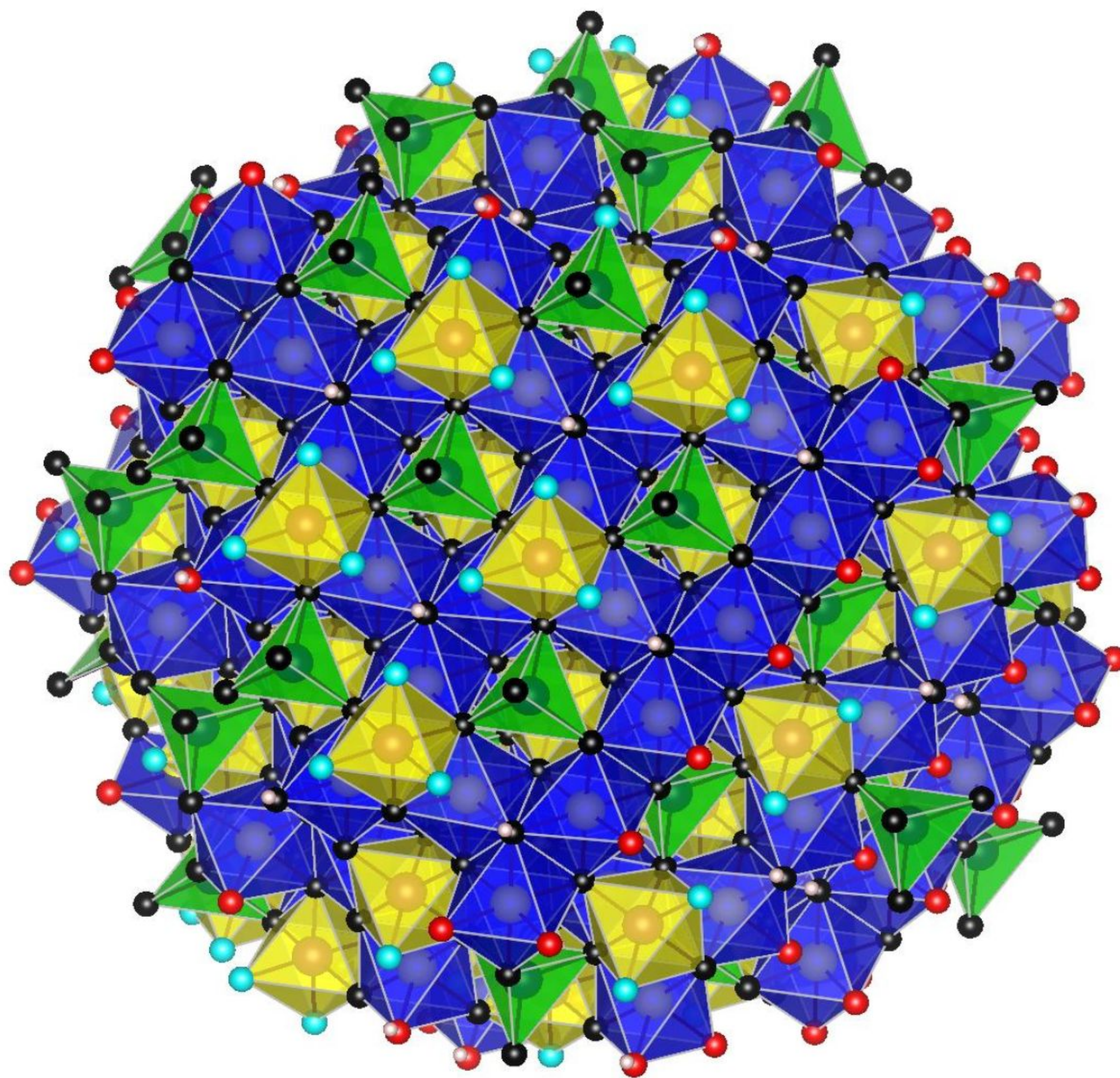
By Avula Anil Kumar, Anirban Som, Paolo Longo, Chennu Sudhakar, Radha Gobinda Bhuin, Soujit Sen Gupta, Anshup, Mohan Udhaya Sankar, Amrita Chaudhary, Ramesh Kumar, and T. Pradeep*

Communication

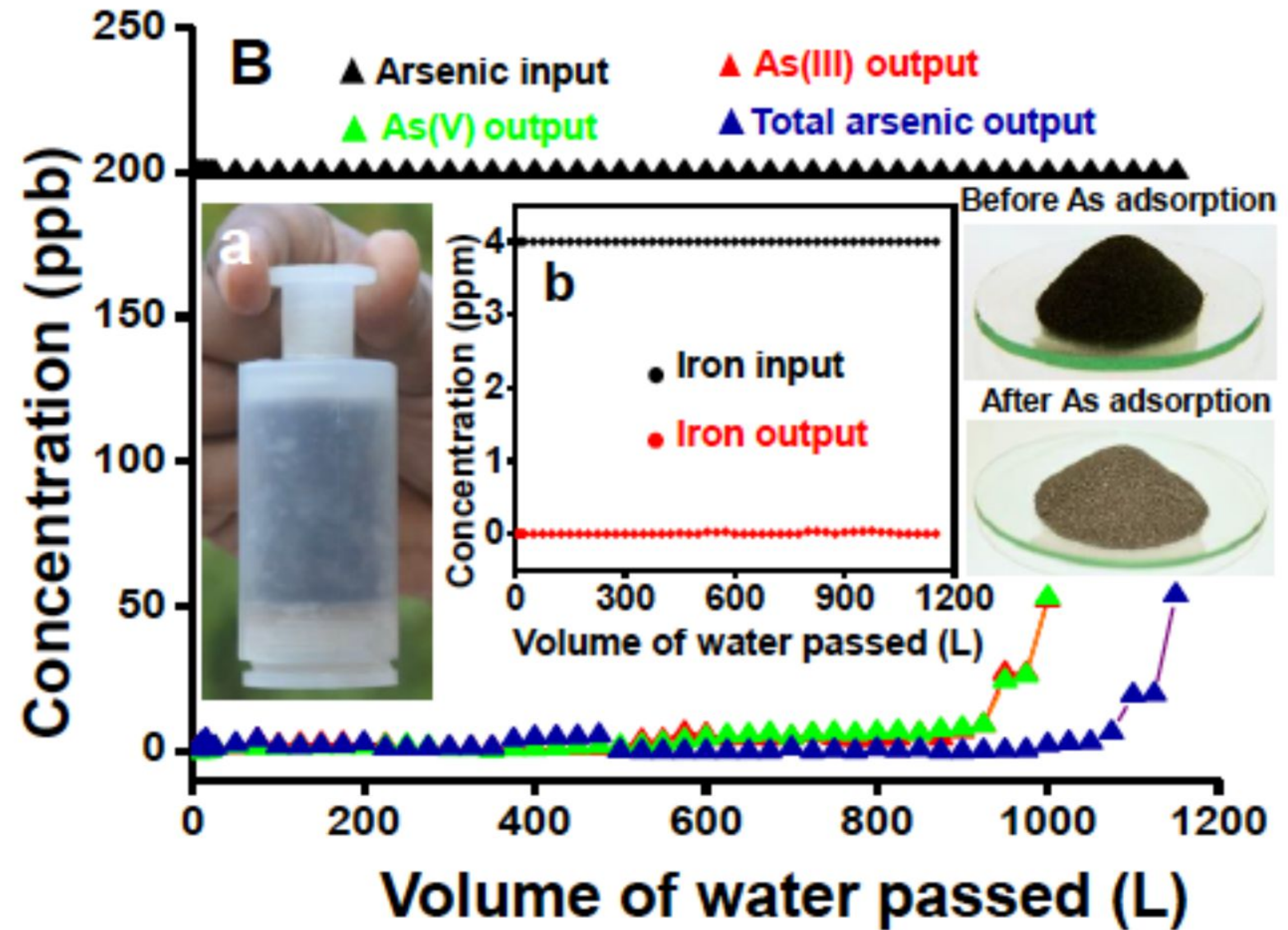
Mechanism – molecular tools



Modeling surfaces



Lab studies



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

Clean water at 2.1 paise per litre!



0.025 cent
s

Waste management

- Adsorbents conform to toxicity characteristic leaching procedure
- Elemental waste goes back to local environment
- Safe disposal of arsenic (or any other) laden waste
- Additional protection could be considered, if necessary
- Exploring viable uses

Policy, interface, governments

Now they are across the countr



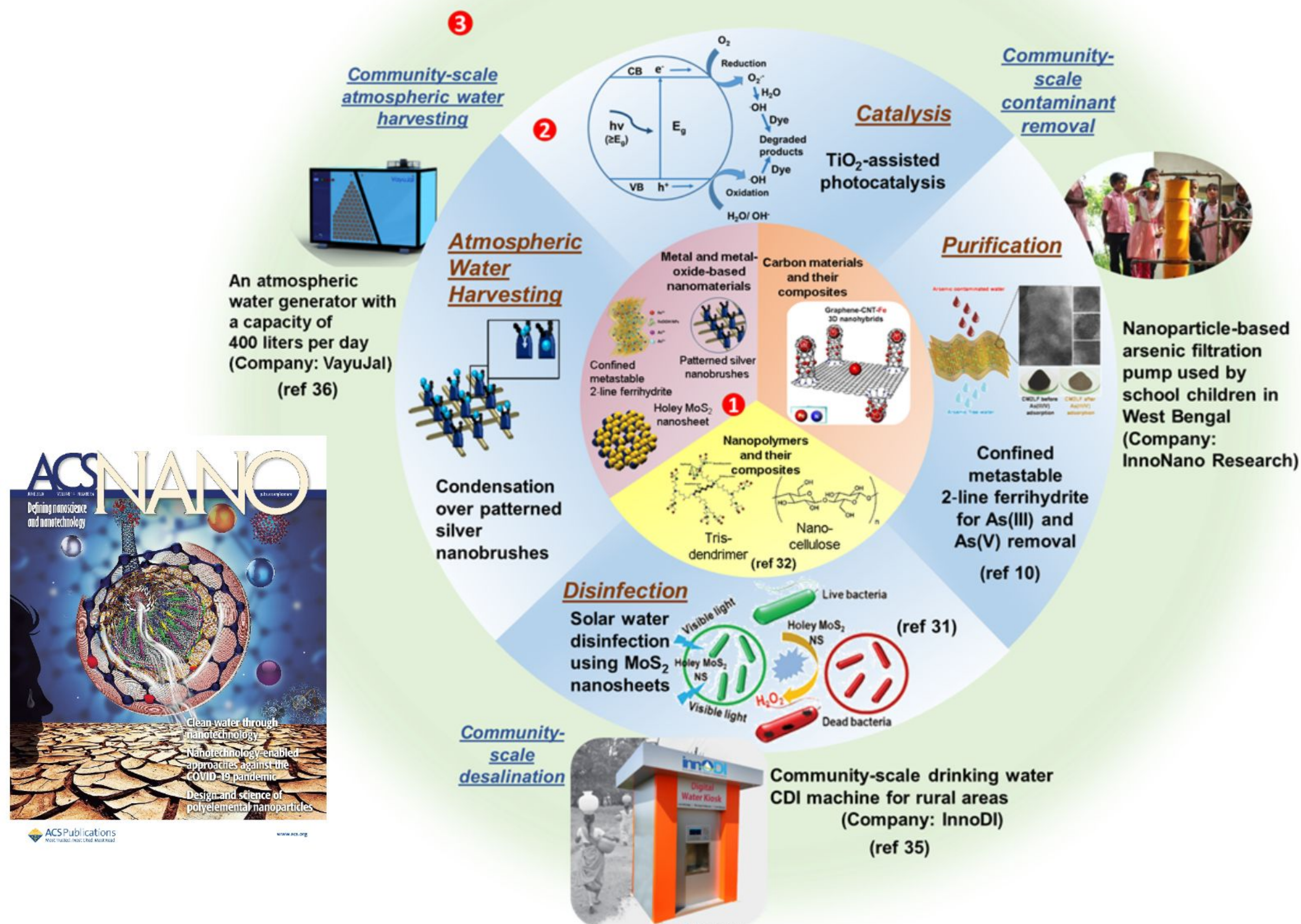
Components of IoT architecture implemented by DWSS, GoP



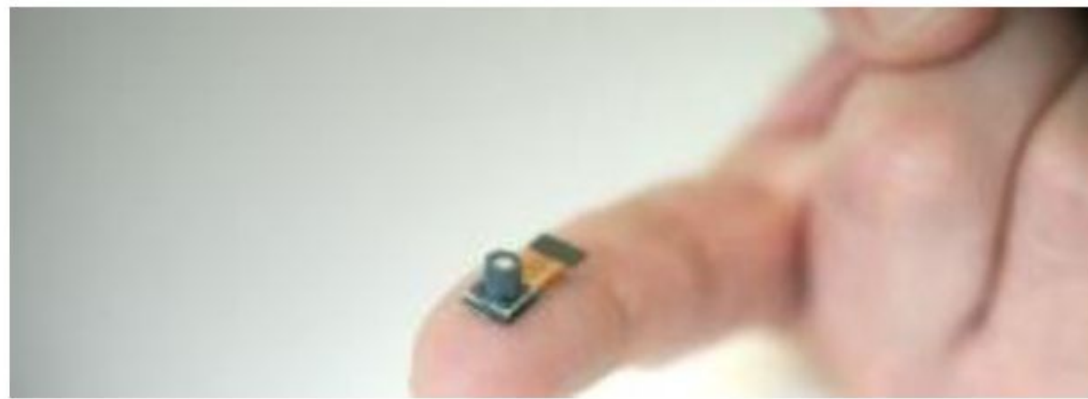
Typical IoT architecture comprises various sensors and meters, communication gateway, Cloud Server, SMS gateway, Webservices and mobile phone application for operator

Smart water purifiers and big data

Evolution of materials to products



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 solution. Inset: Free standing quantum cluster loaded film in visible light and UV light

Approaching detection limits of tens of Hg₂

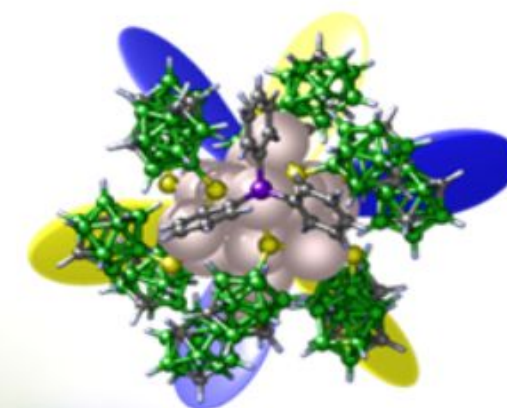
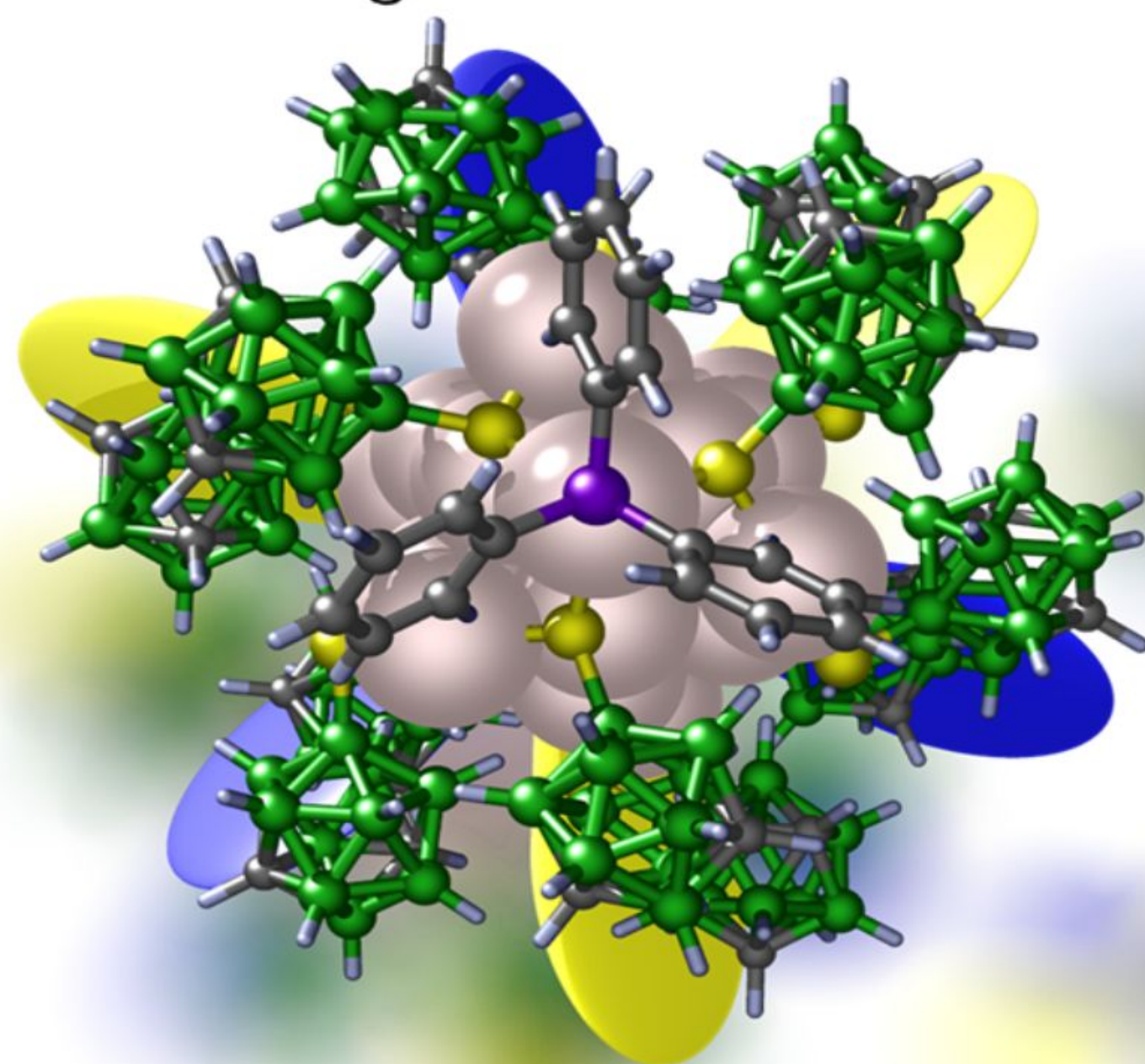
+

Mercury quenching experiment using nanofiber

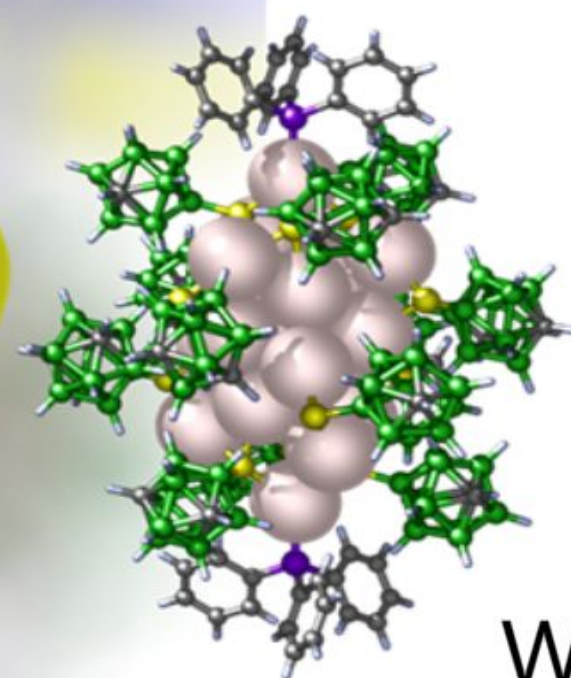


Carborane-thiol protected silver nanomolecule

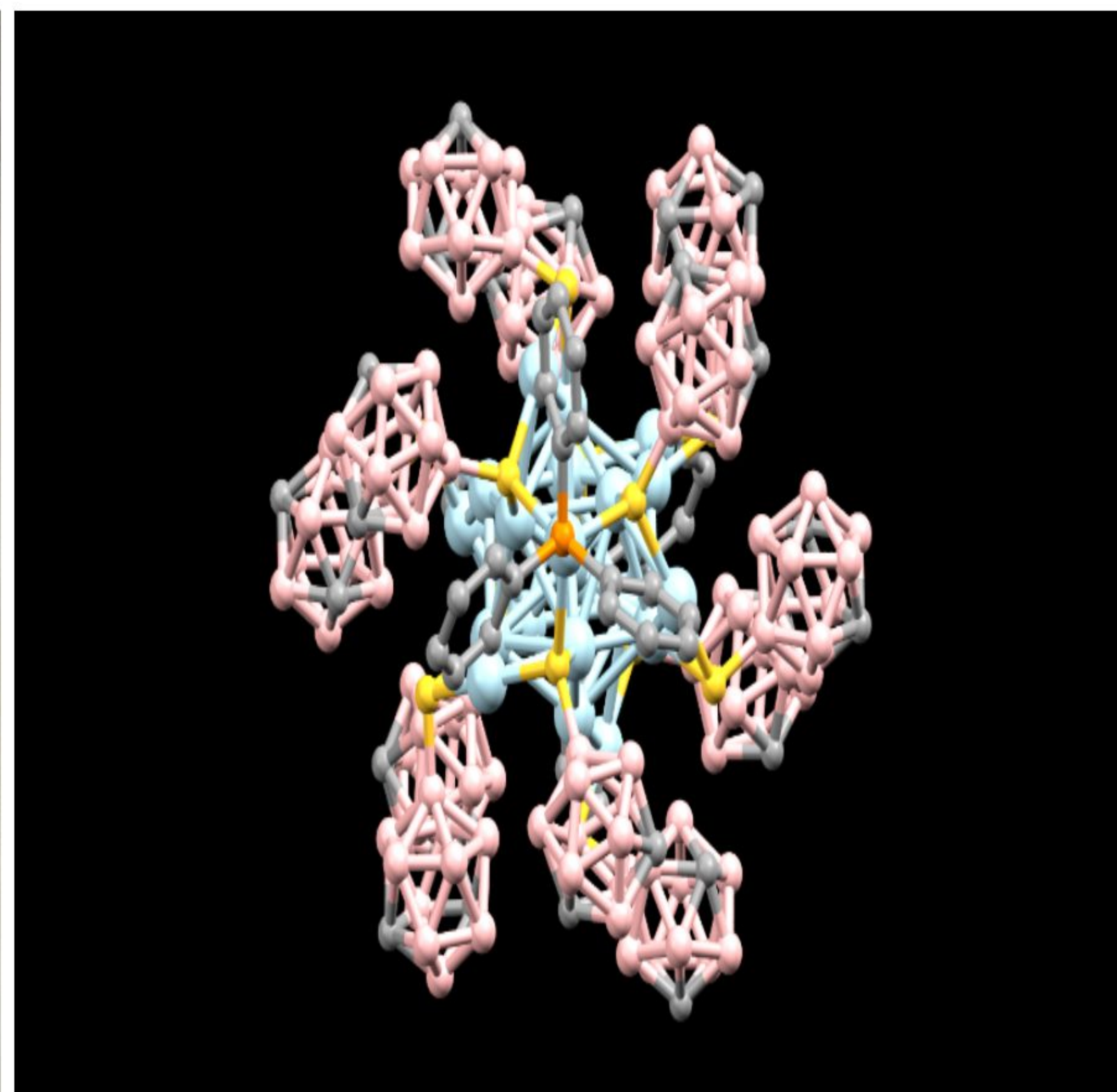
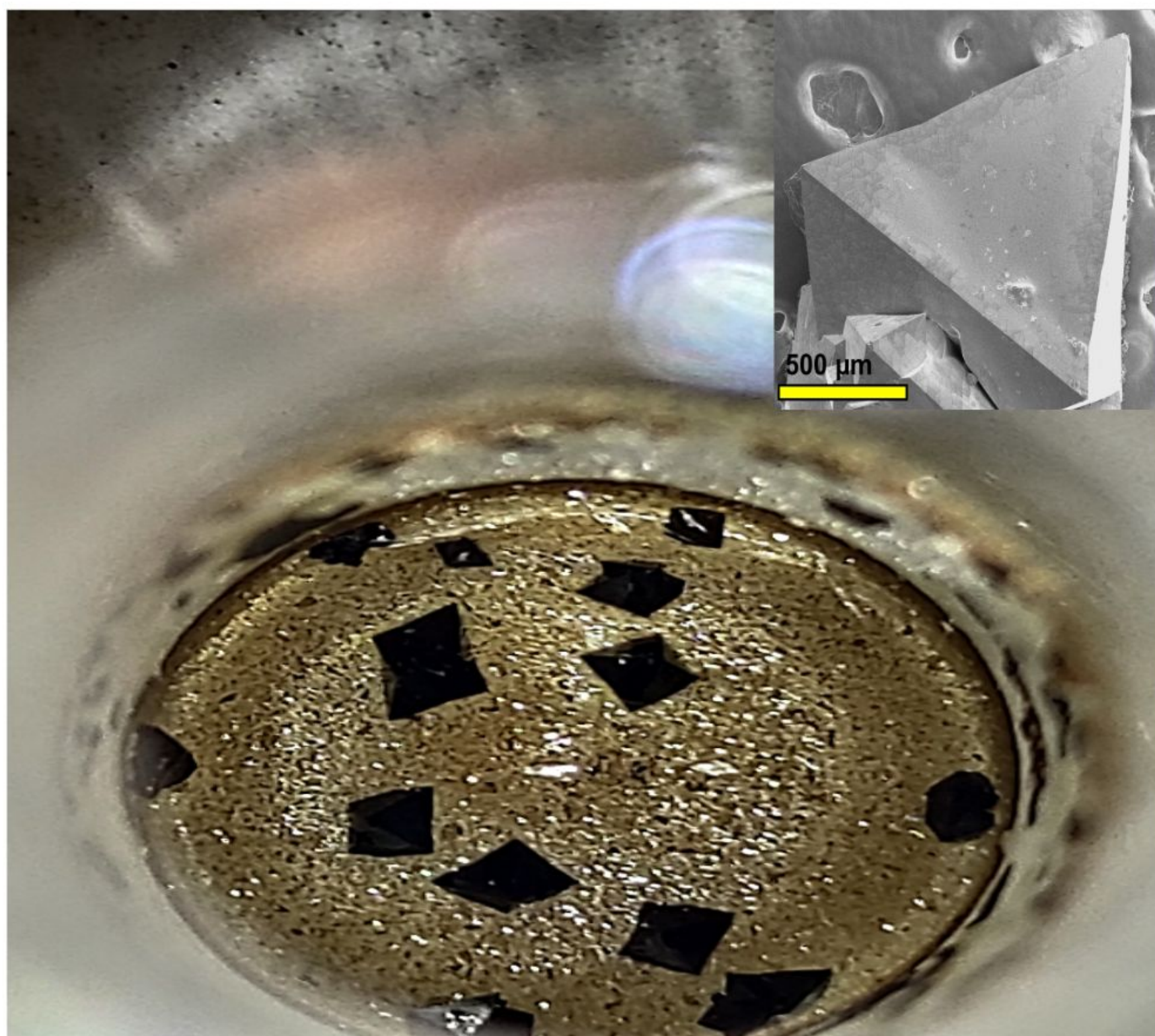
Rotary nanomolecule



Double rotors

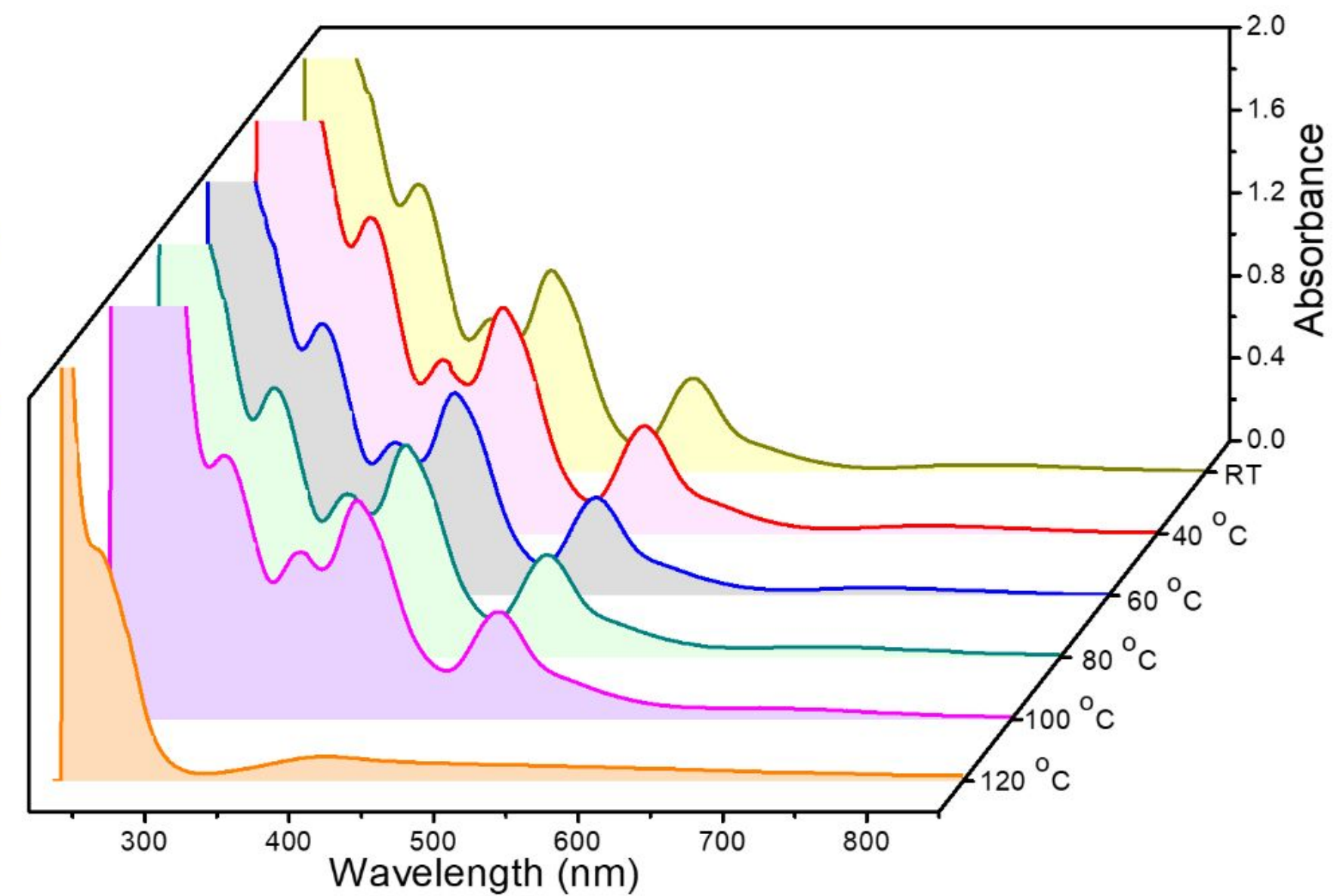
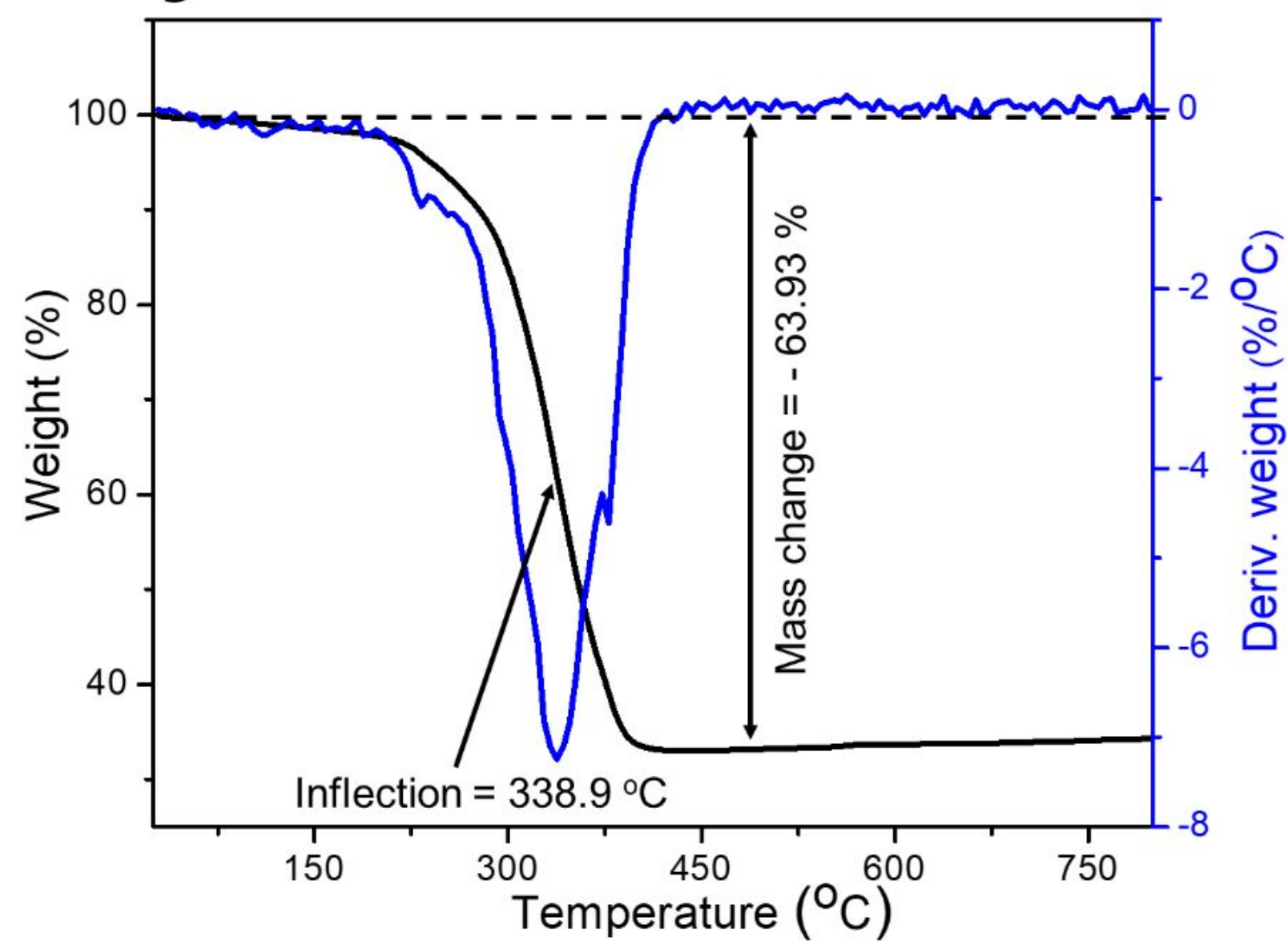


With Tomas Bas
e



Thermal stability

y

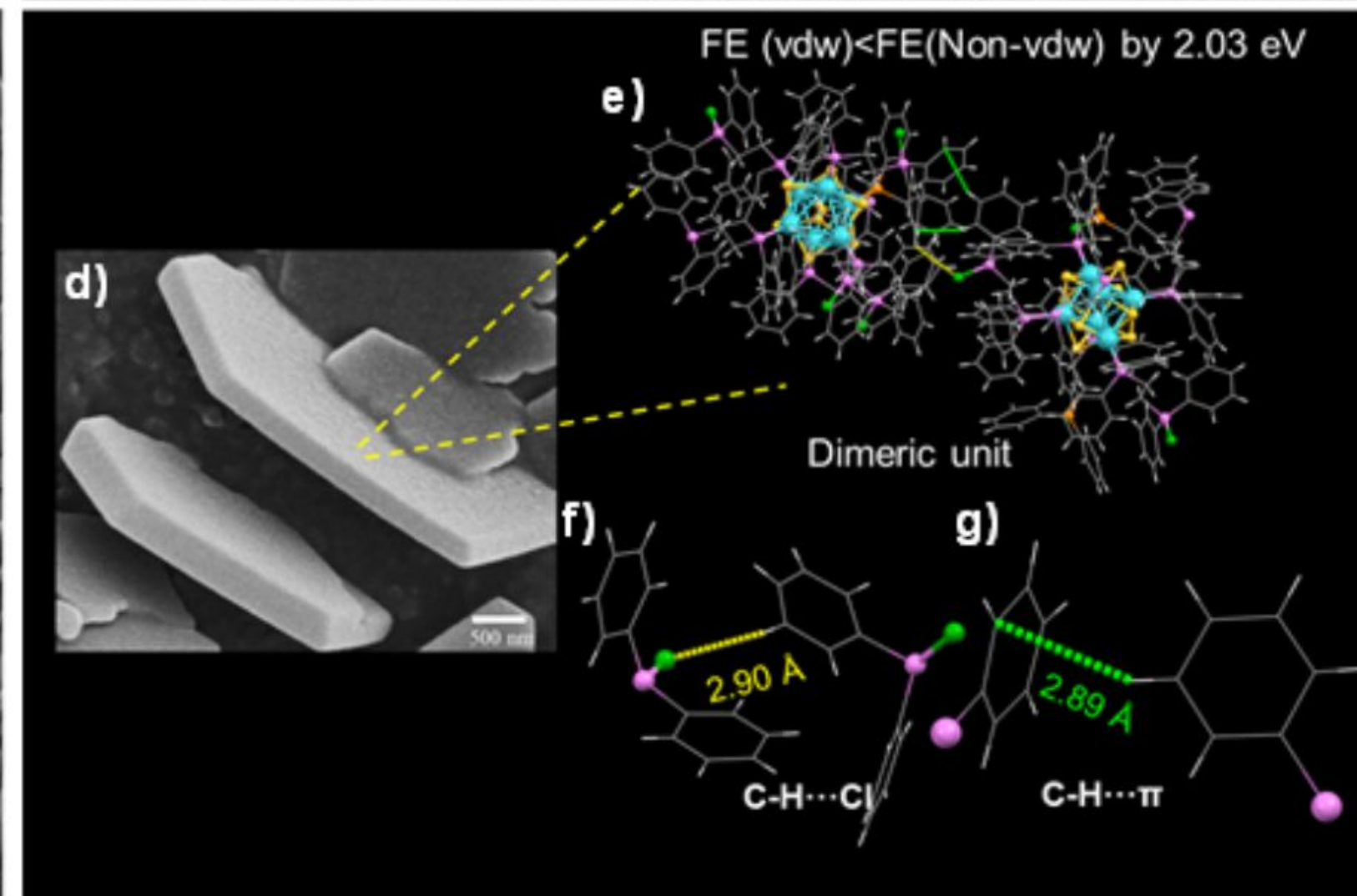
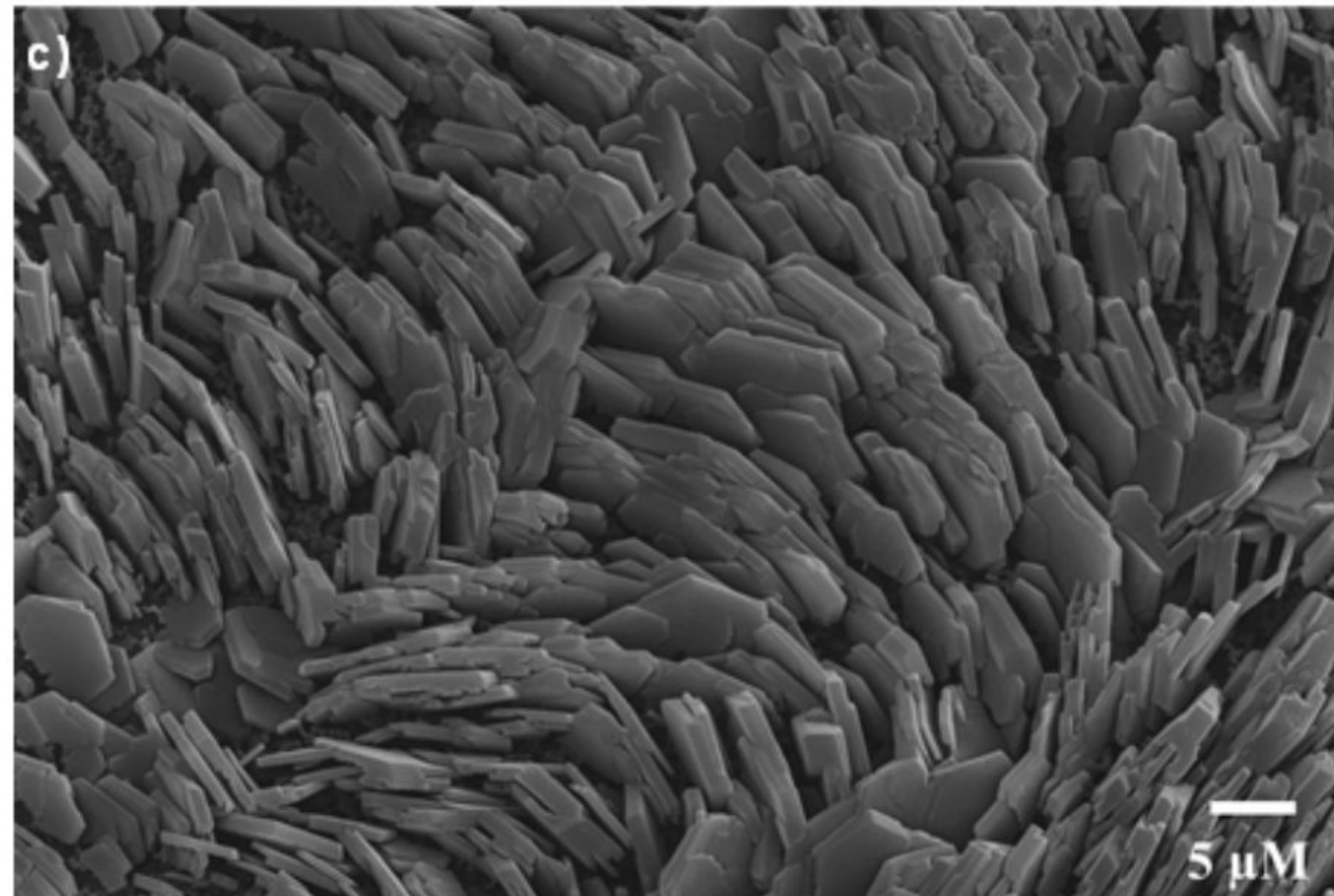
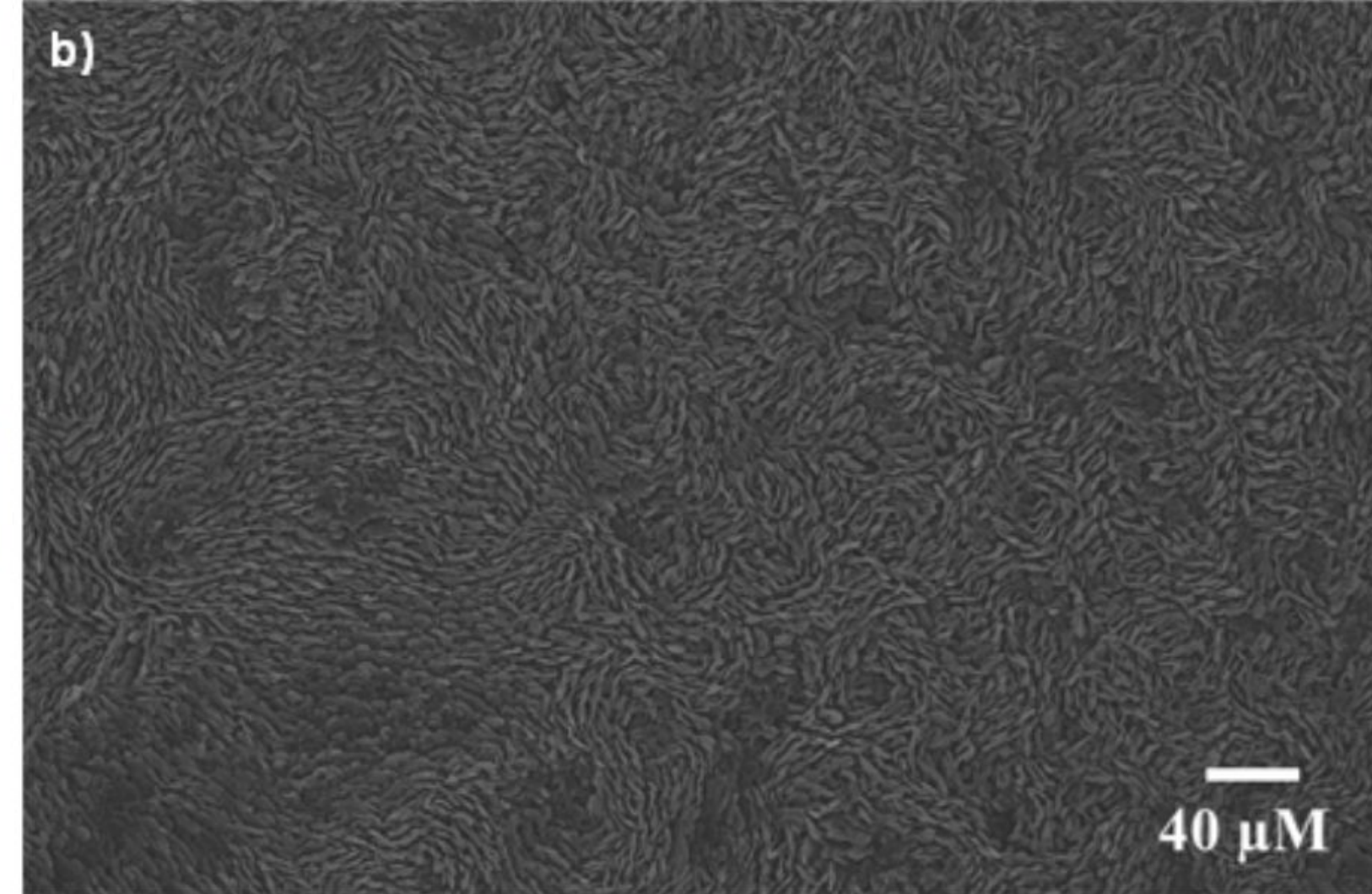
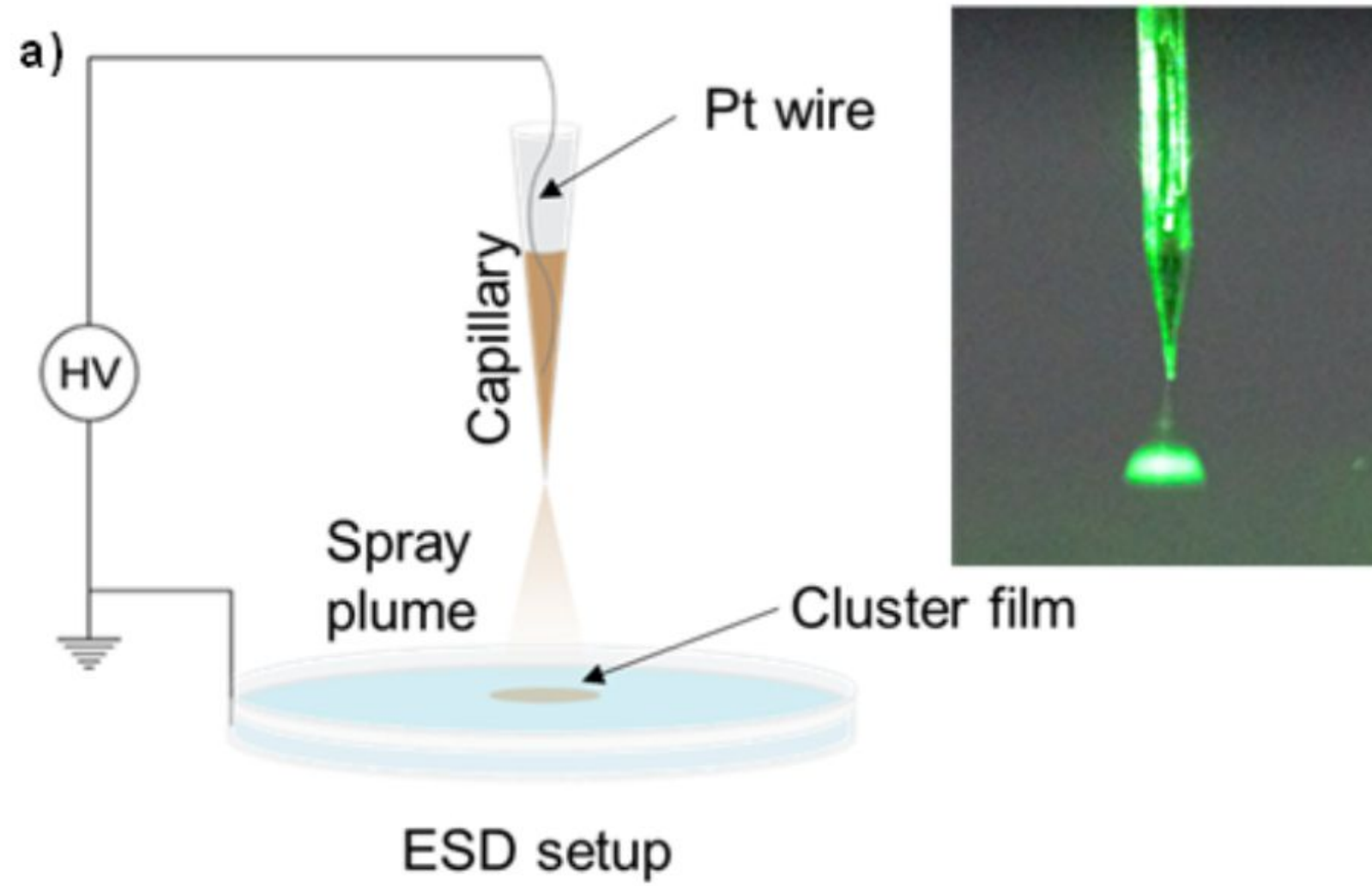


New electrodes - Aligned nanoplates of Co₆S

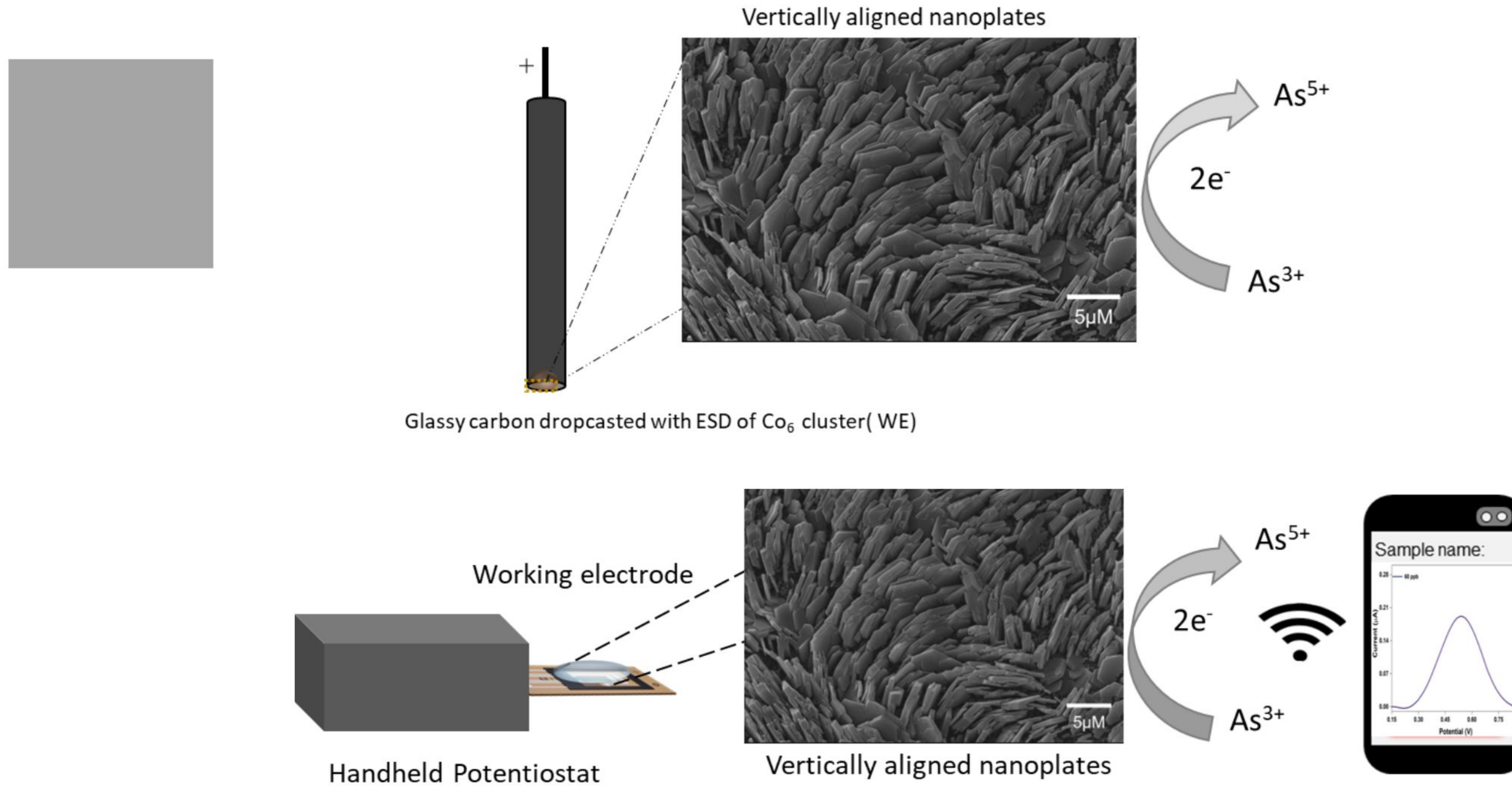
8

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

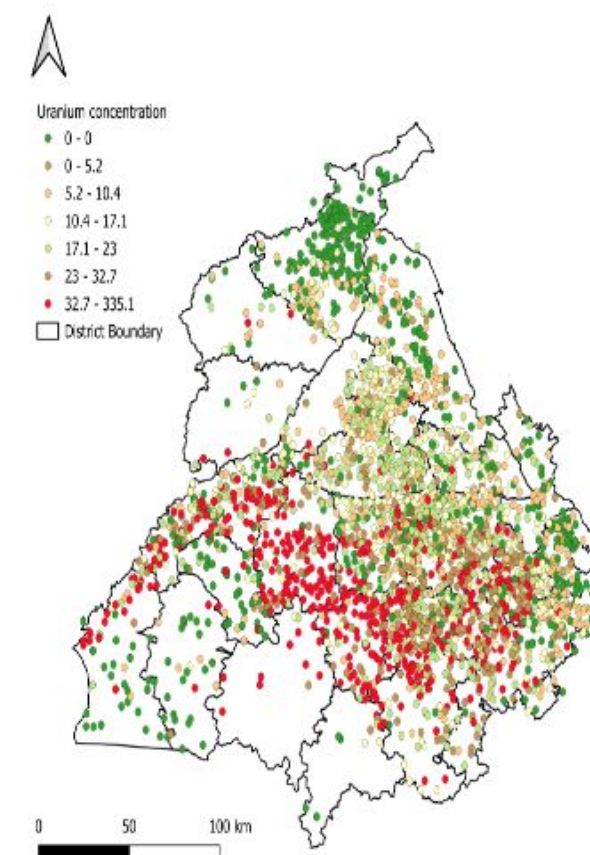
Electrospray deposition



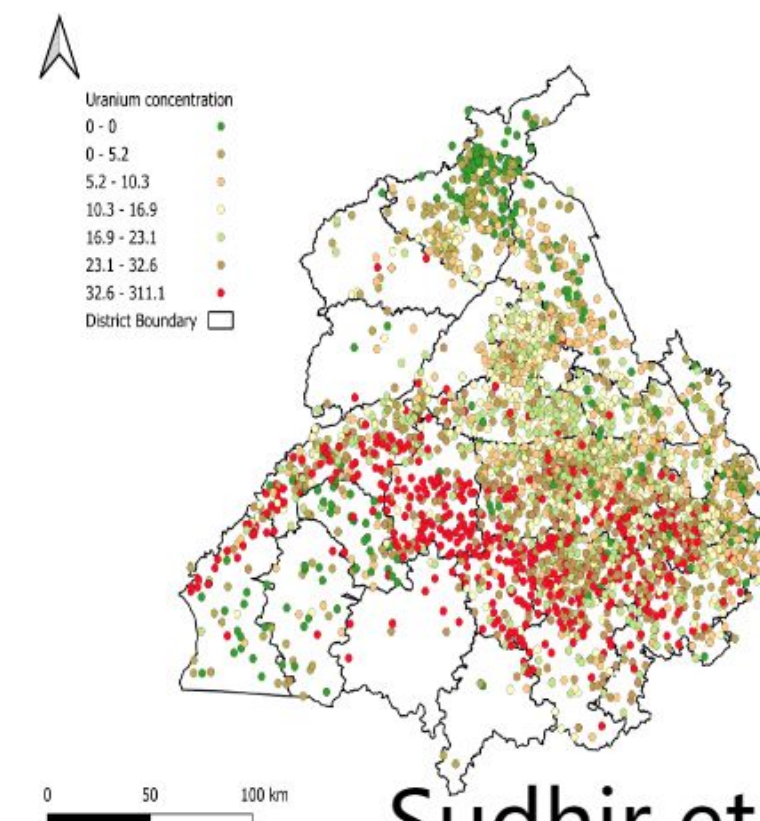
Sensing



Arsenic poisoning across the world



[1]



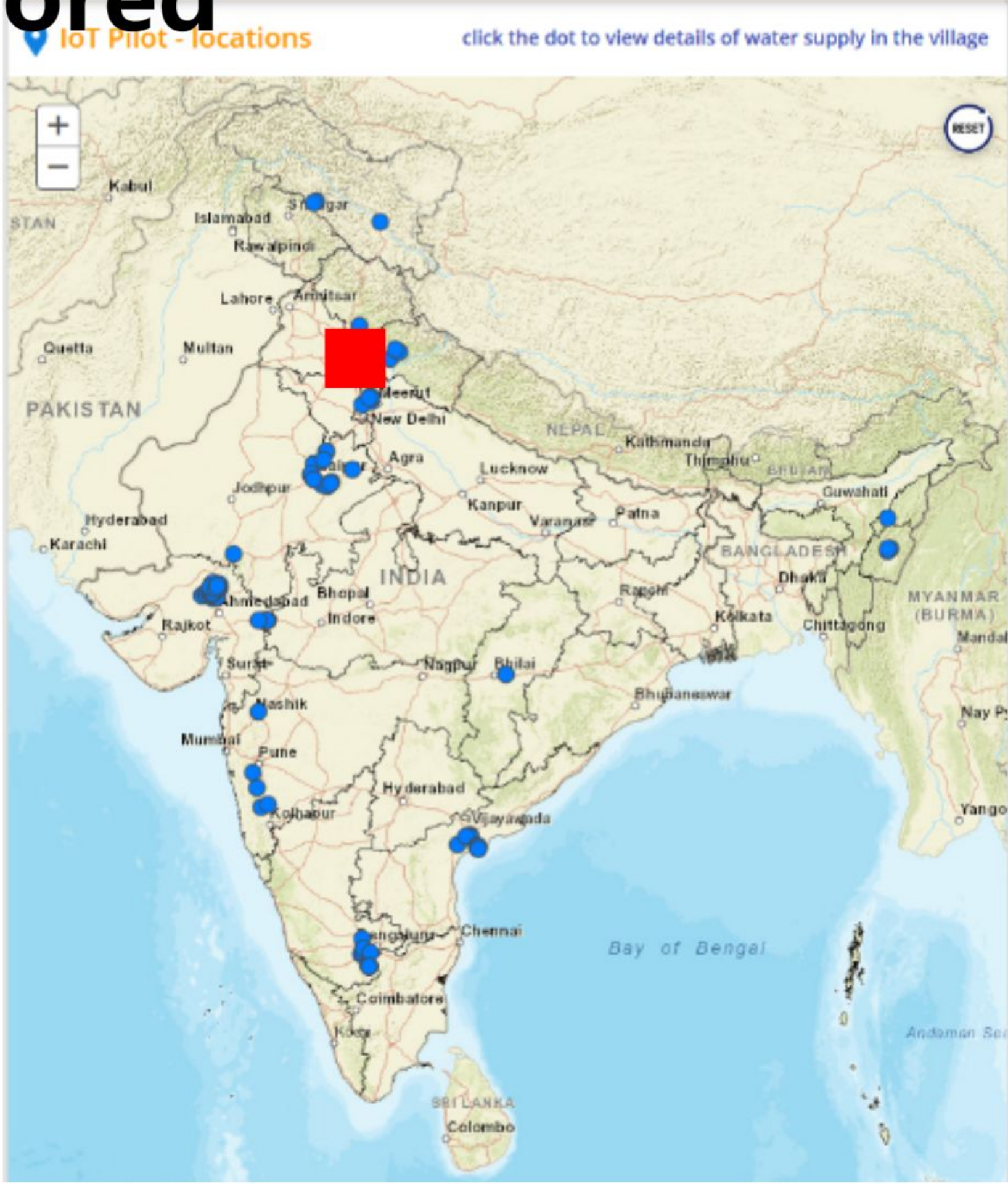
Sudhir et. al. Unpublish

ed

scale has been added like figure 1

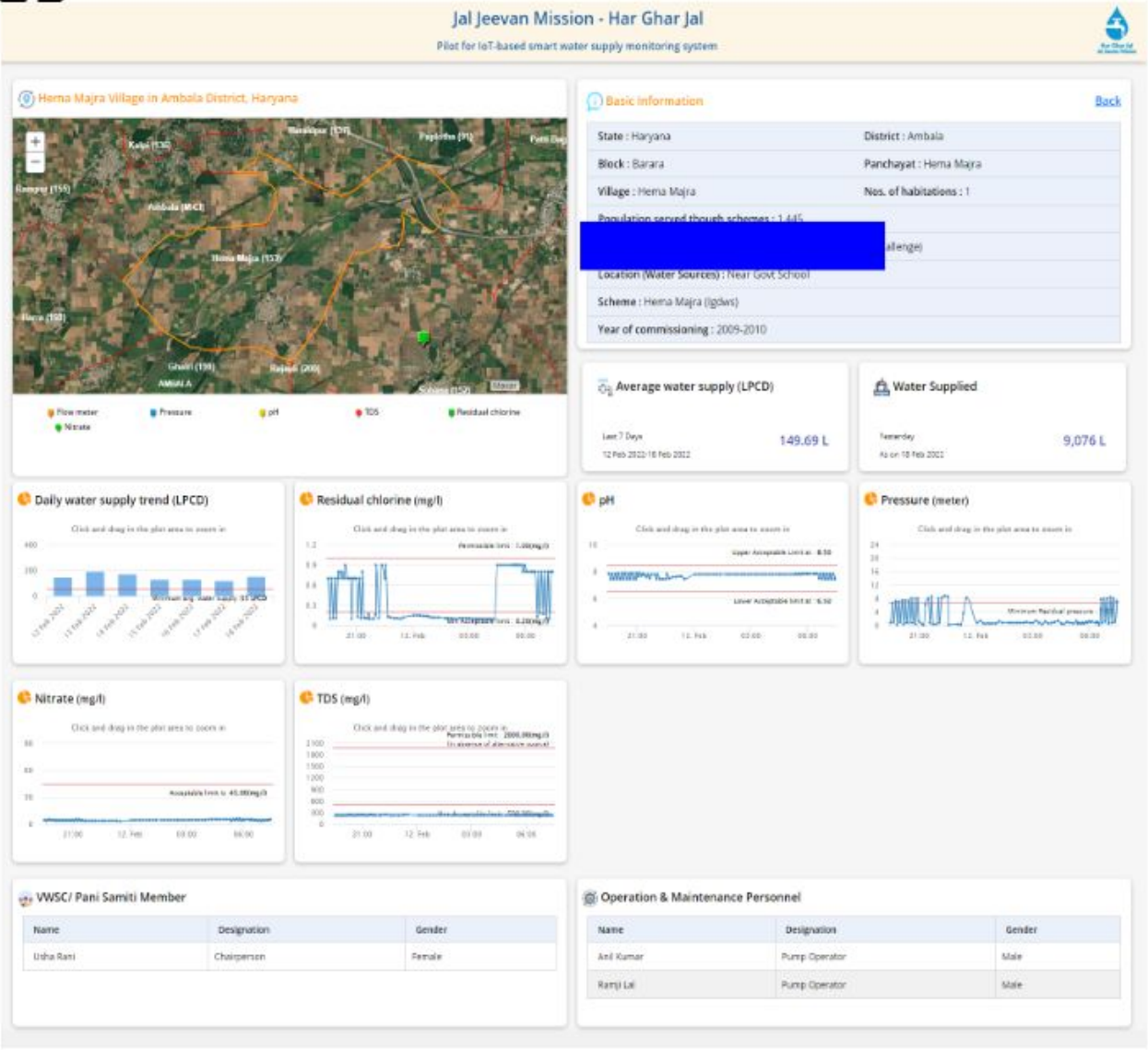


India's water is being monitored



IITM/IIS

Installations made by four companies





Water that Heals

A TRAVELOGUE



a SURESH MENON film

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



Clean water for a II

<https://preview.peopleswaterdata.org>

Can Water Microdroplets Make Soil?

A path to sustainable nanotechnology



Science

**A scale of 100
0**

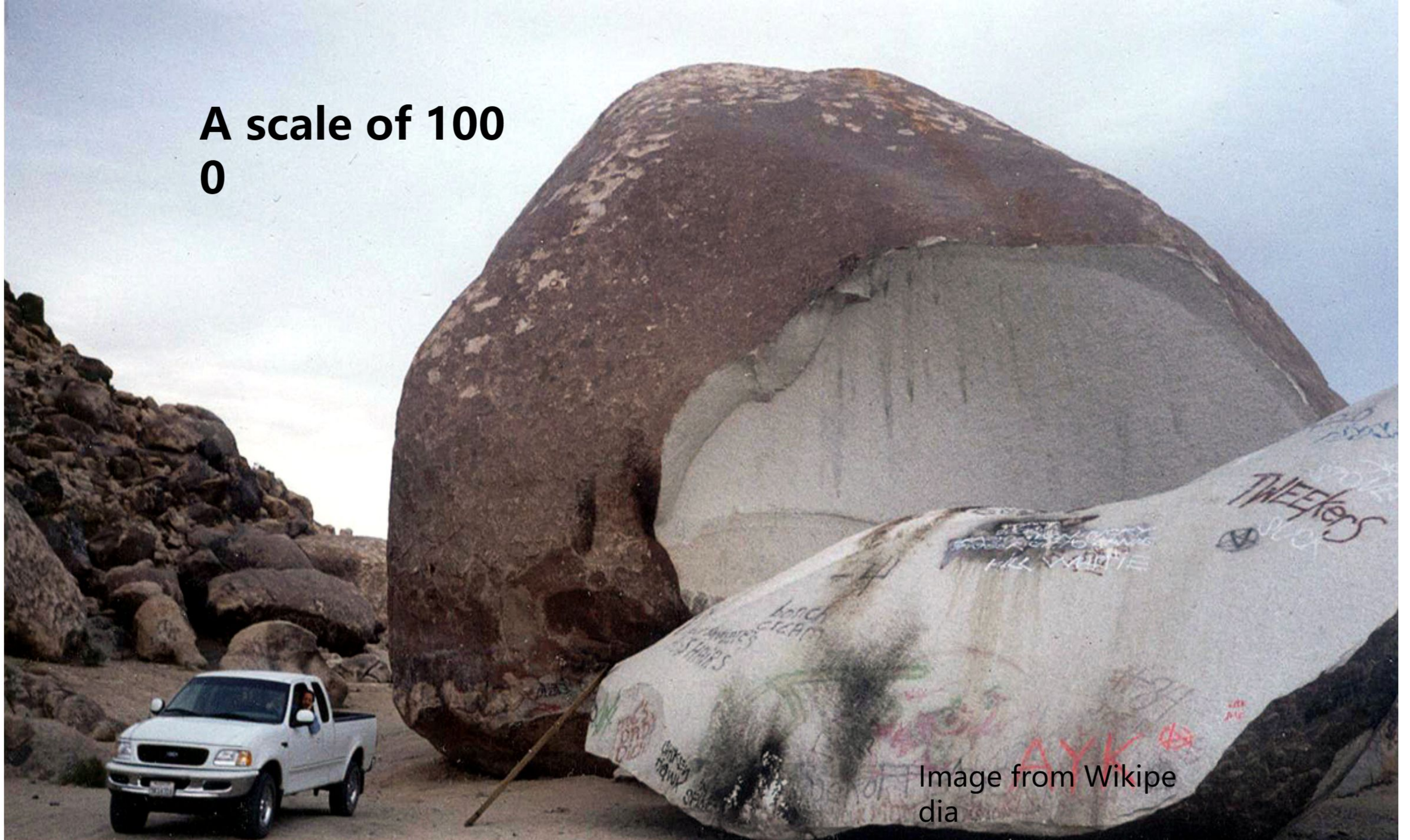


Image from Wikiped
ia

Functional Nanomaterials



Thanks to ChatGP

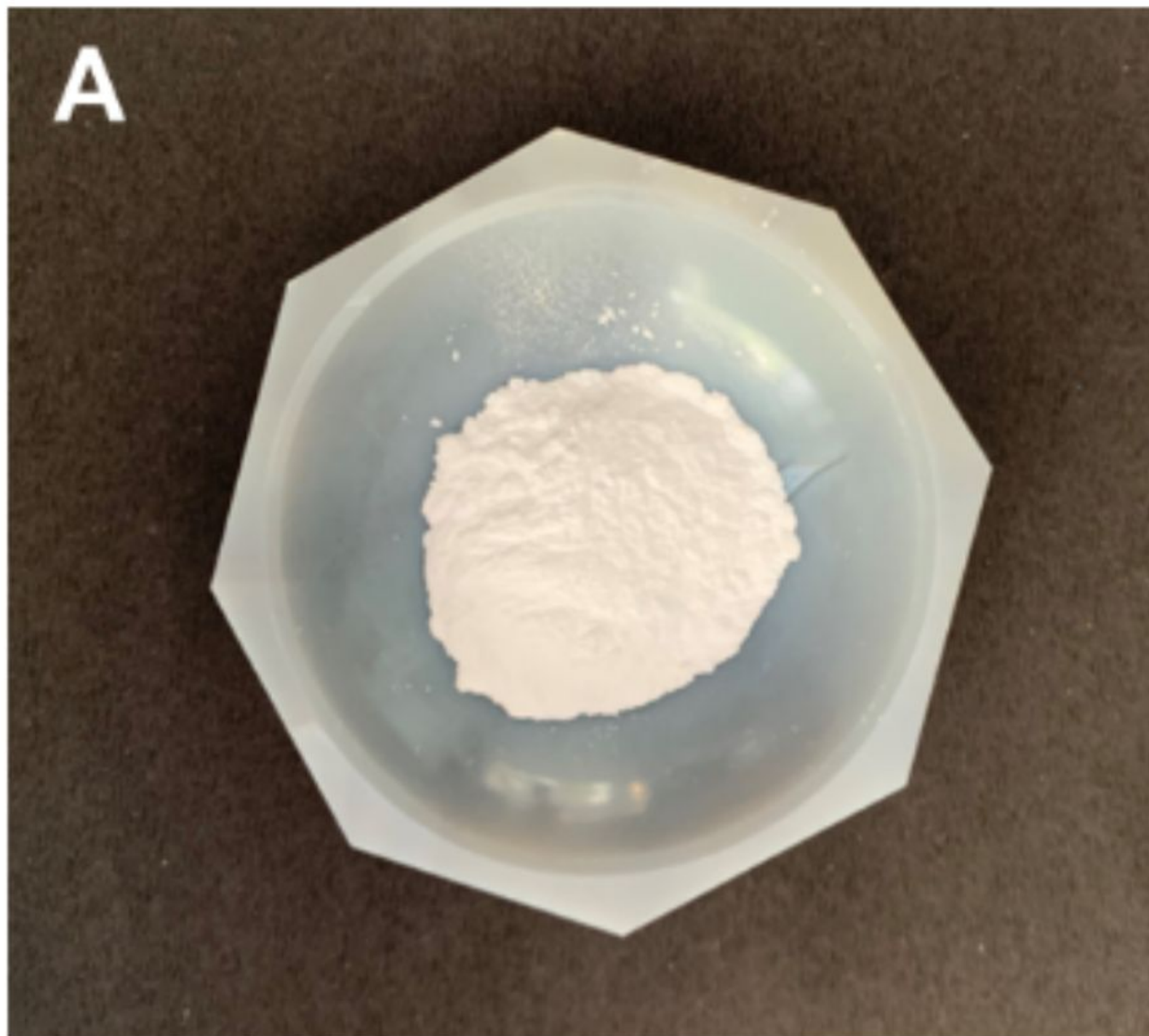
T

Sand, the Ubiquitous Material

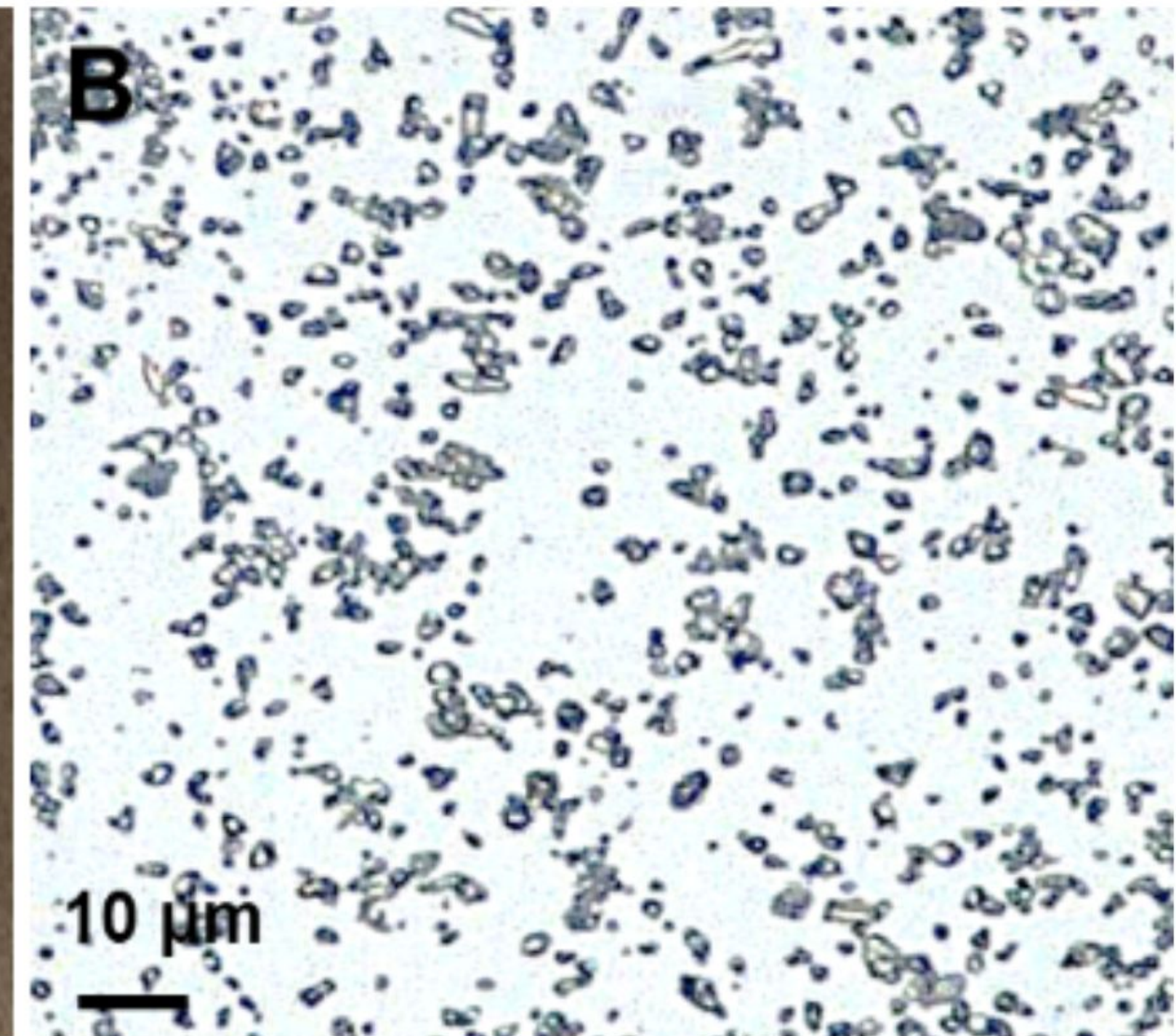


Images from Wikipedia
dia



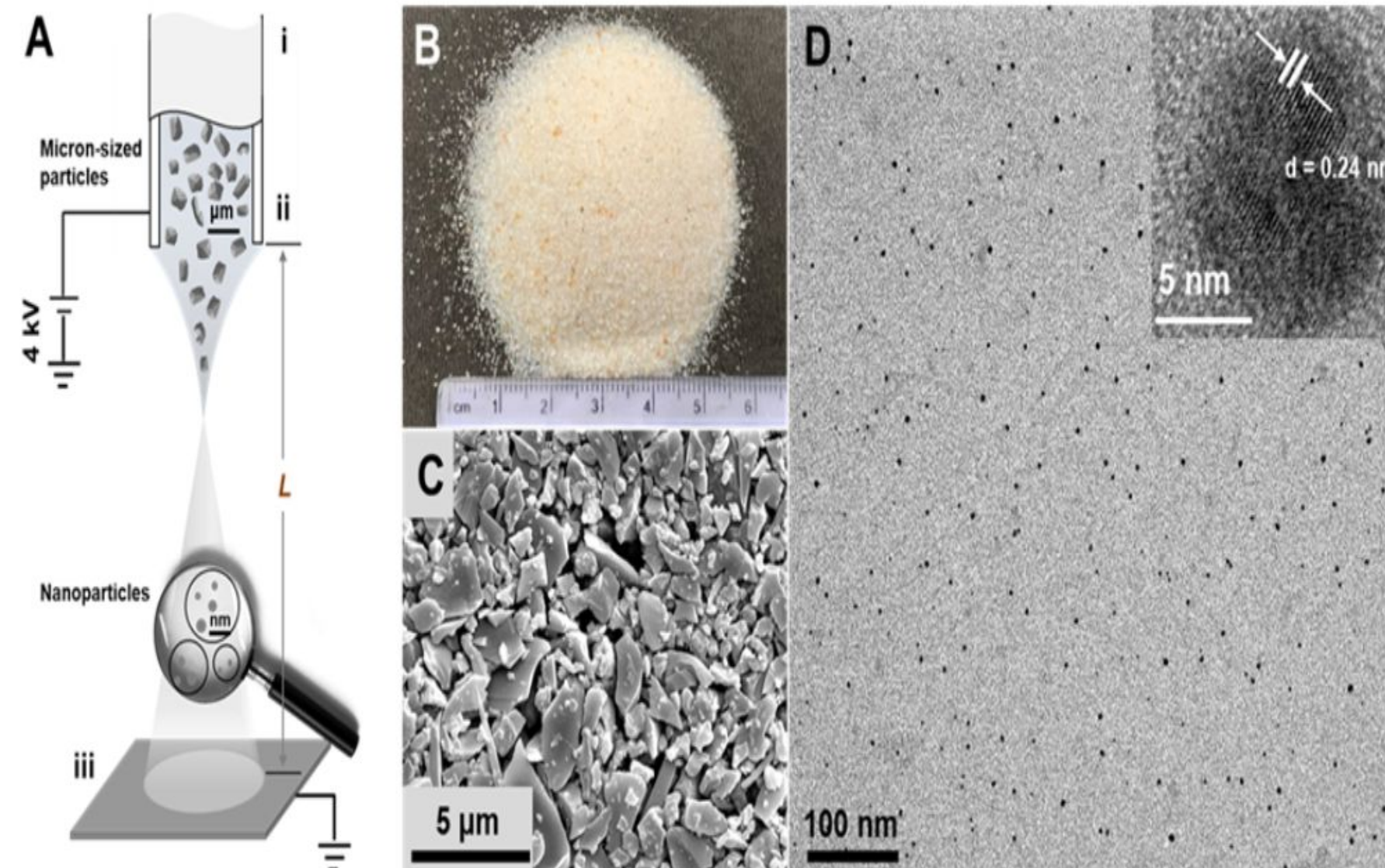
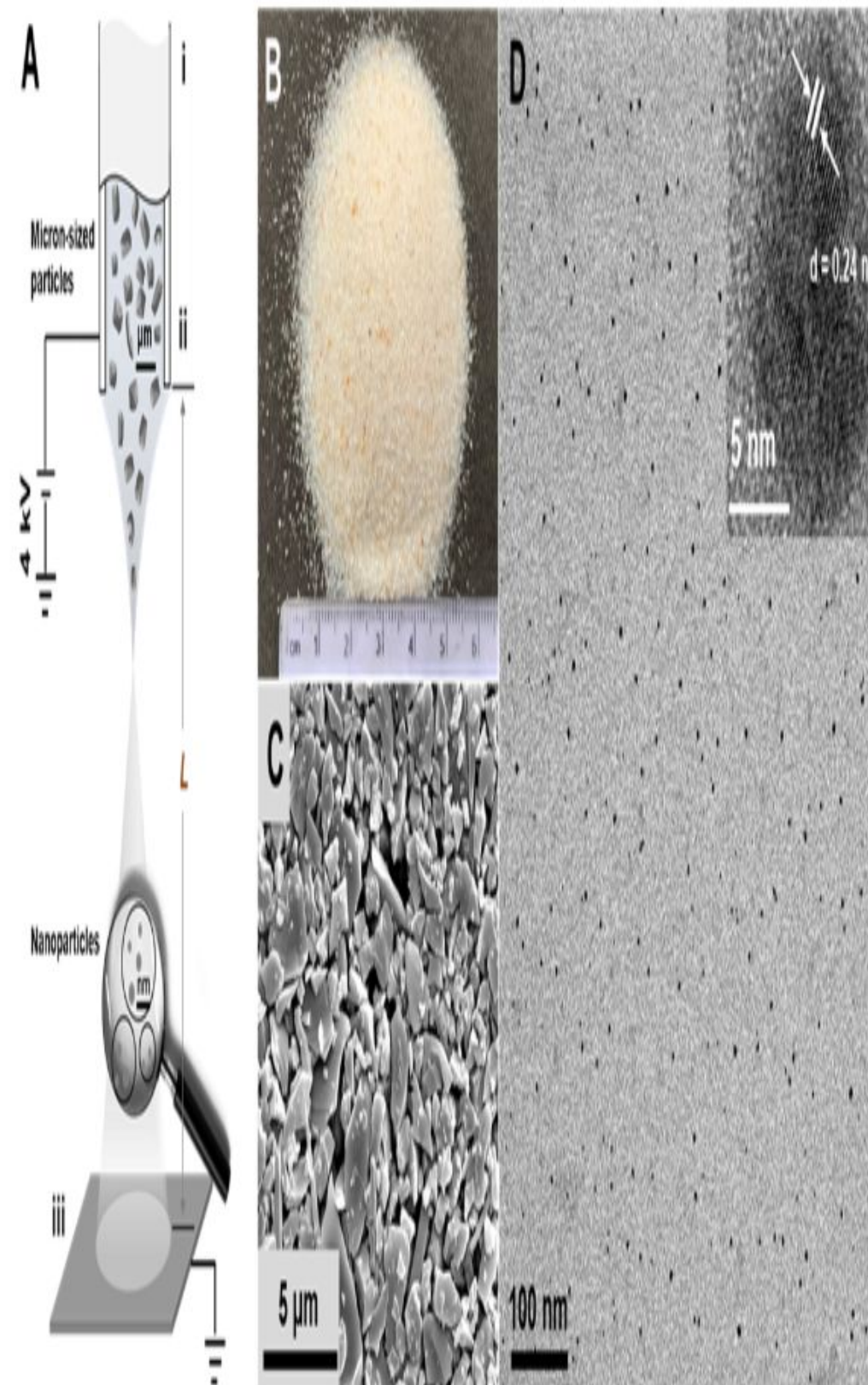


Ground silica



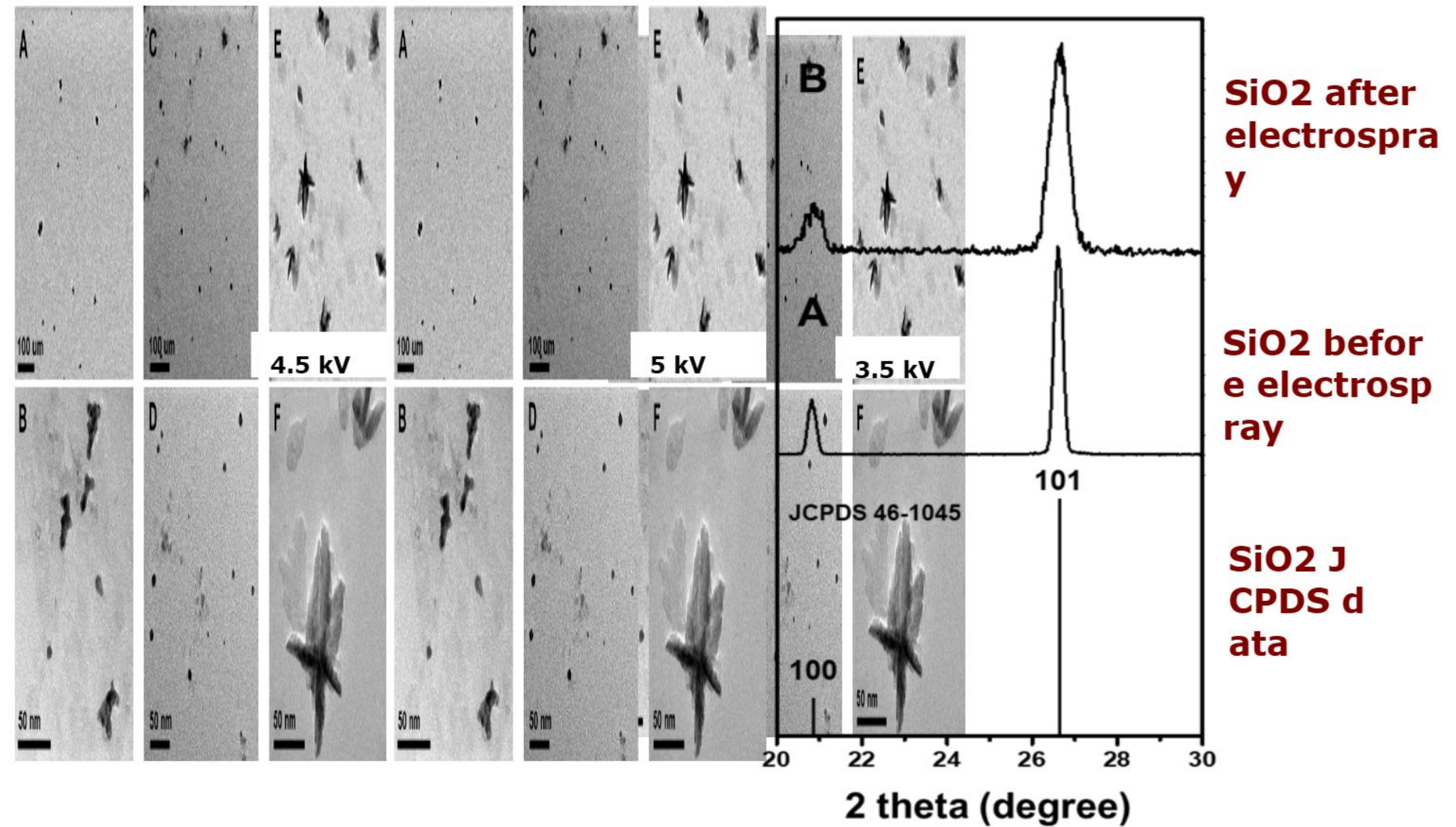
Optical image of silica

Weathering of Minerals in Microdroplets



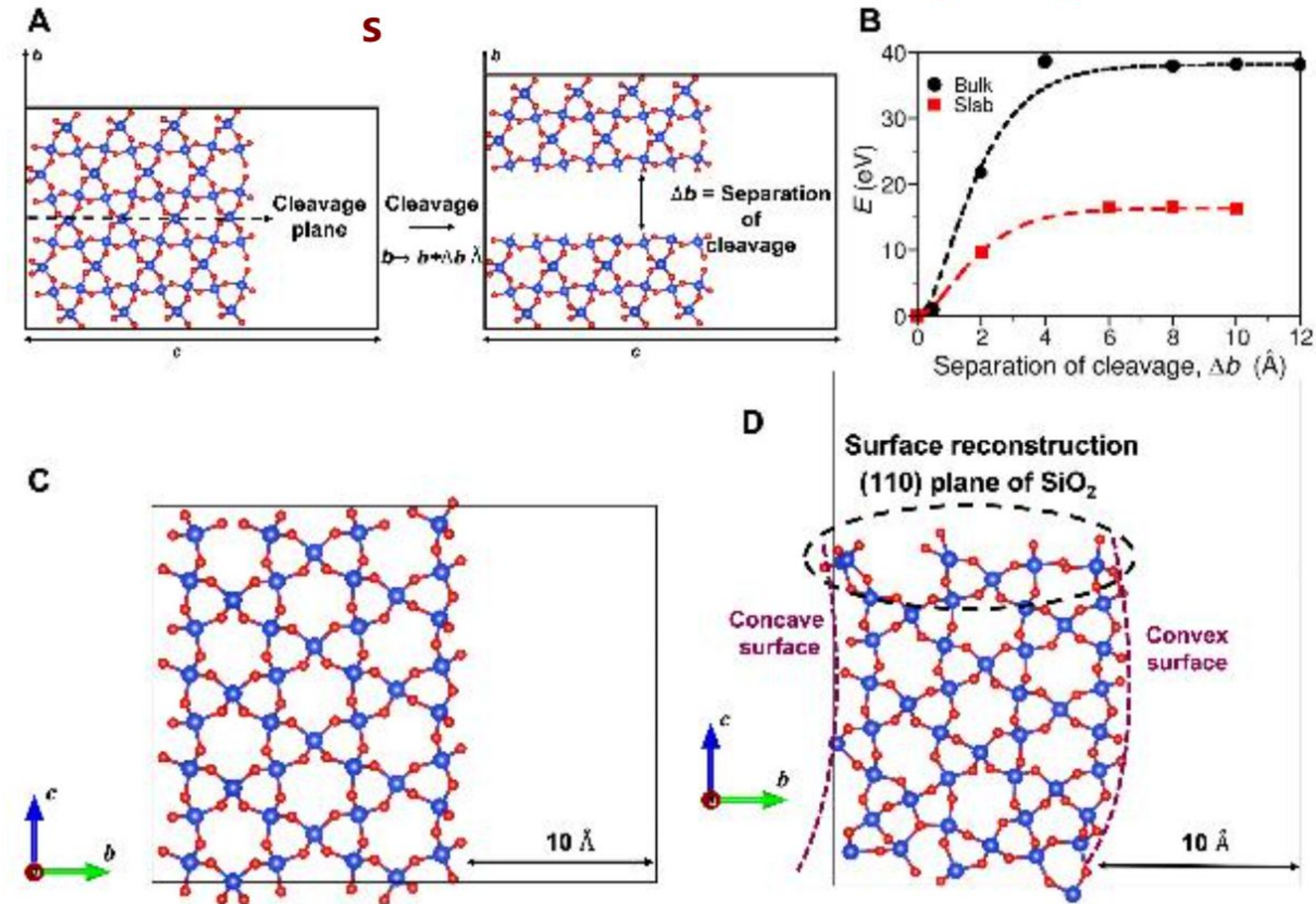
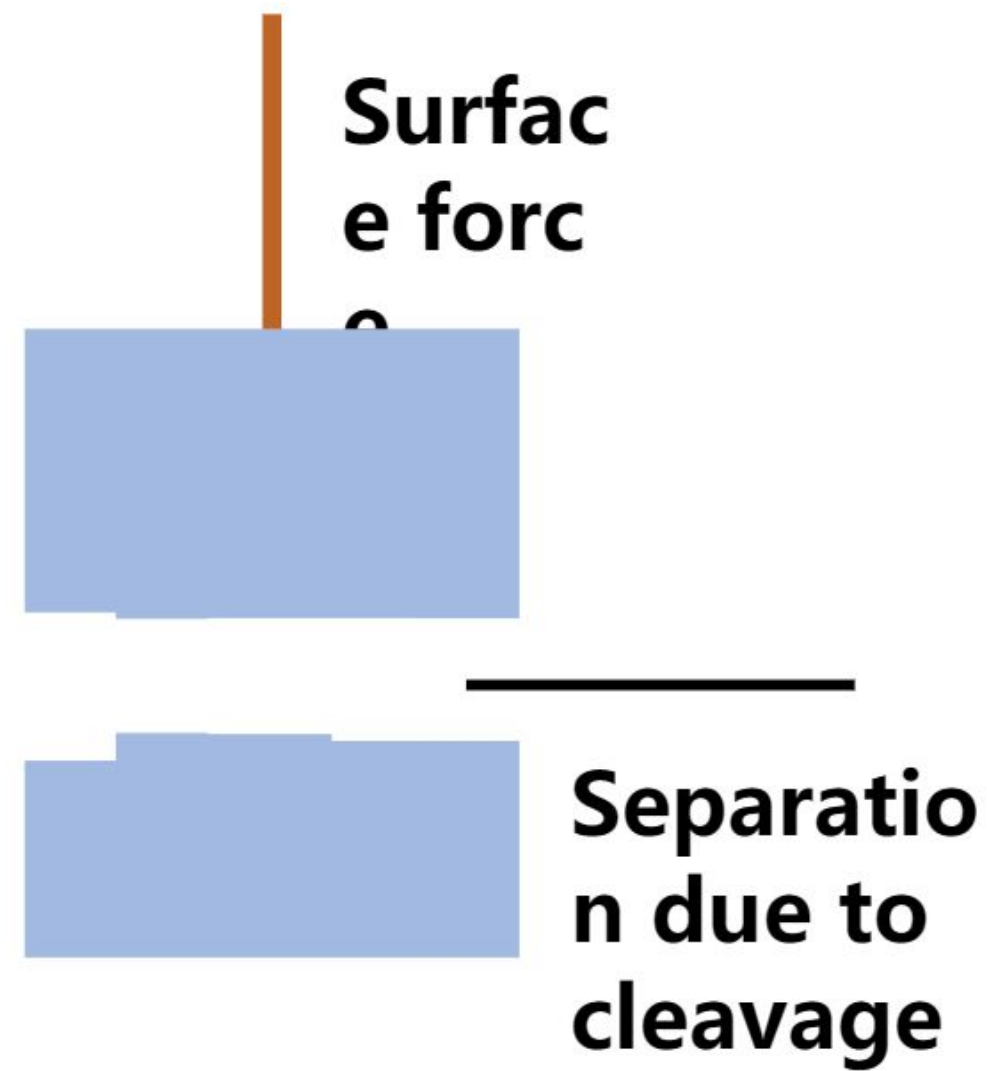
Ruby, Fused Alumin a

Fragmentation of Silica – Varying Conditions

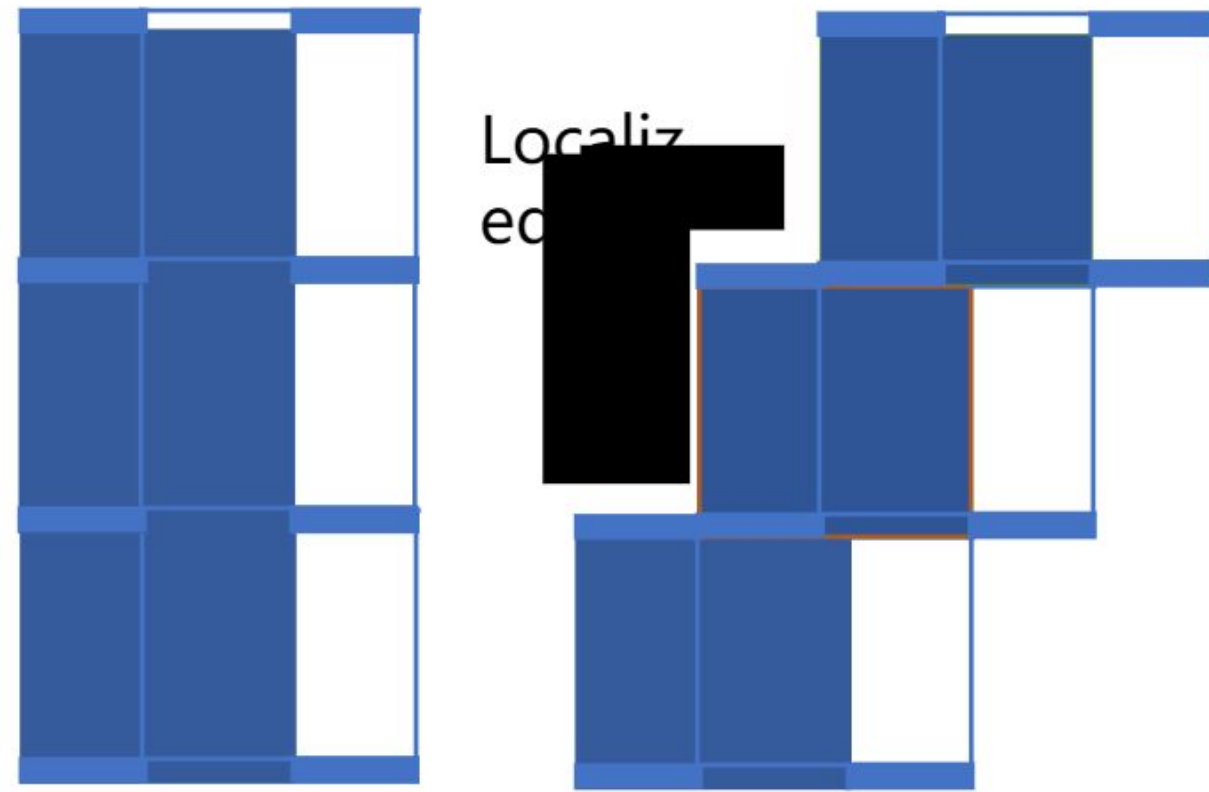


Mechanism: Cleavage

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



Mechanism: Slip

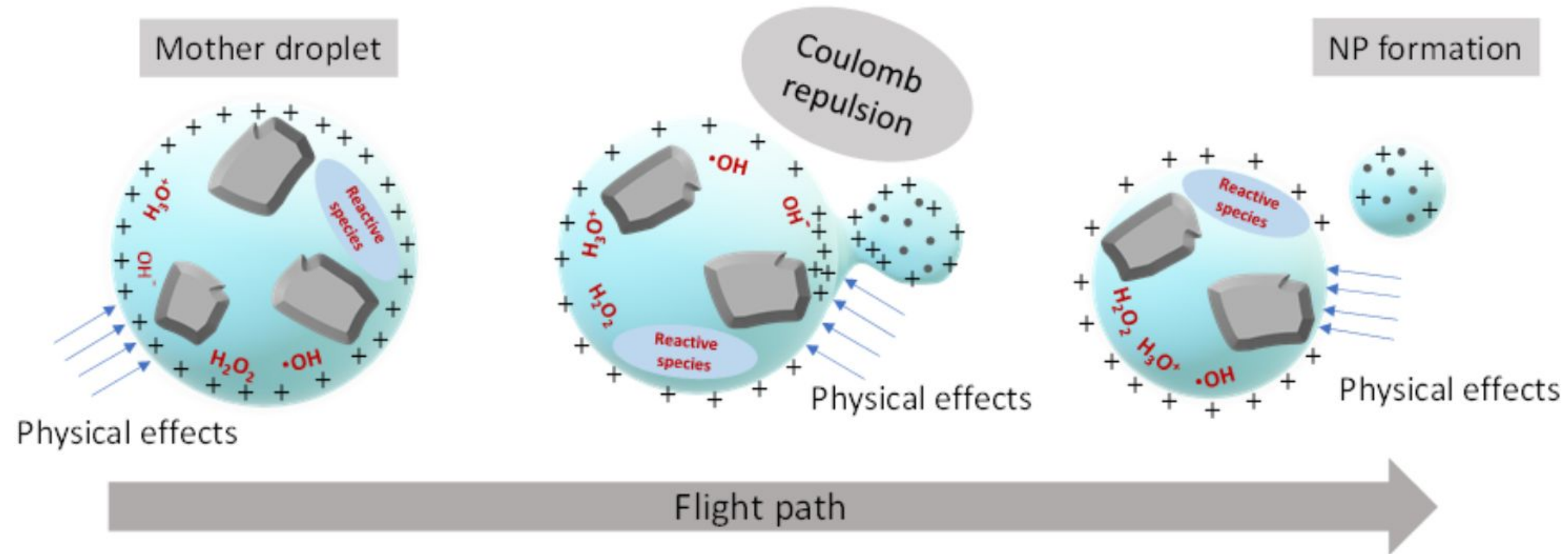


This instability leads to the formation of a stacking fault on the (010) plane, achieved with slip localized at (010) plane

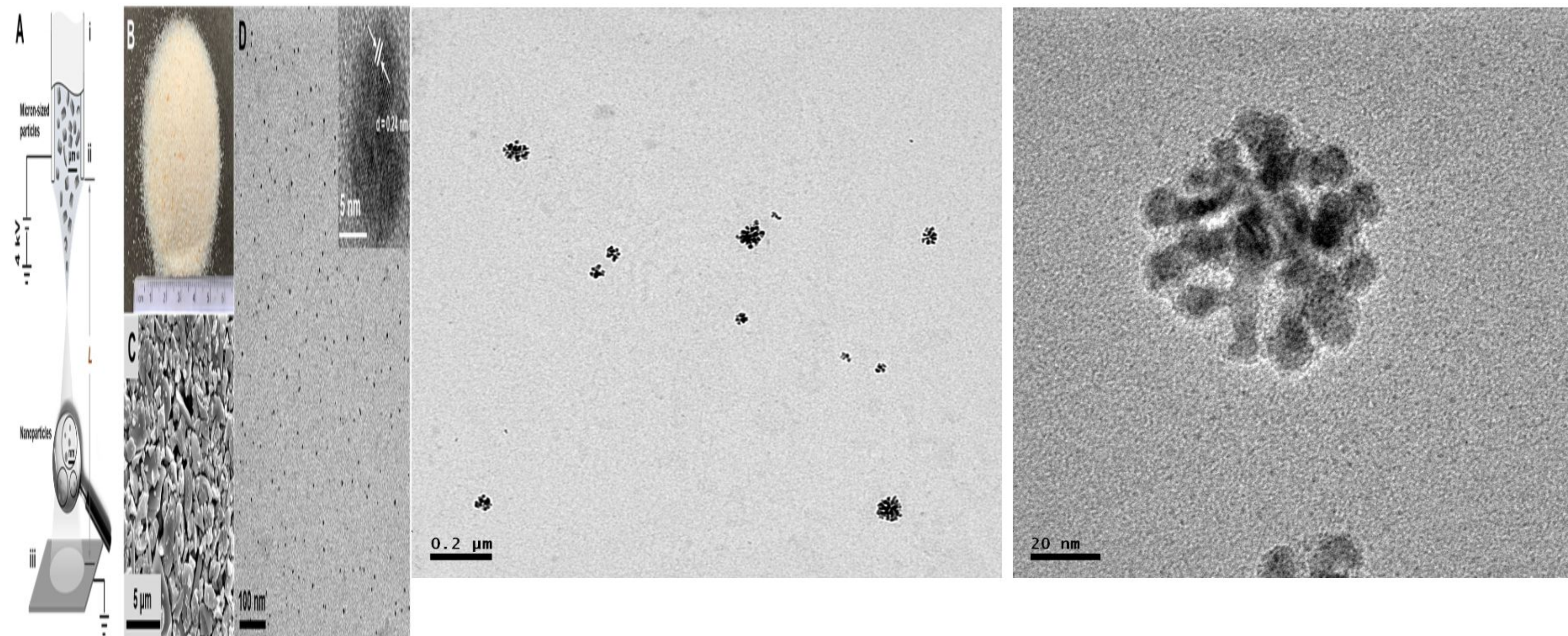
Stacking fault
 $\vec{b} \rightarrow \vec{b}_0 + (x, 0, z)$

$(\diamond\diamond, \diamond\diamond \in [0,1])$ - fractional coordinates

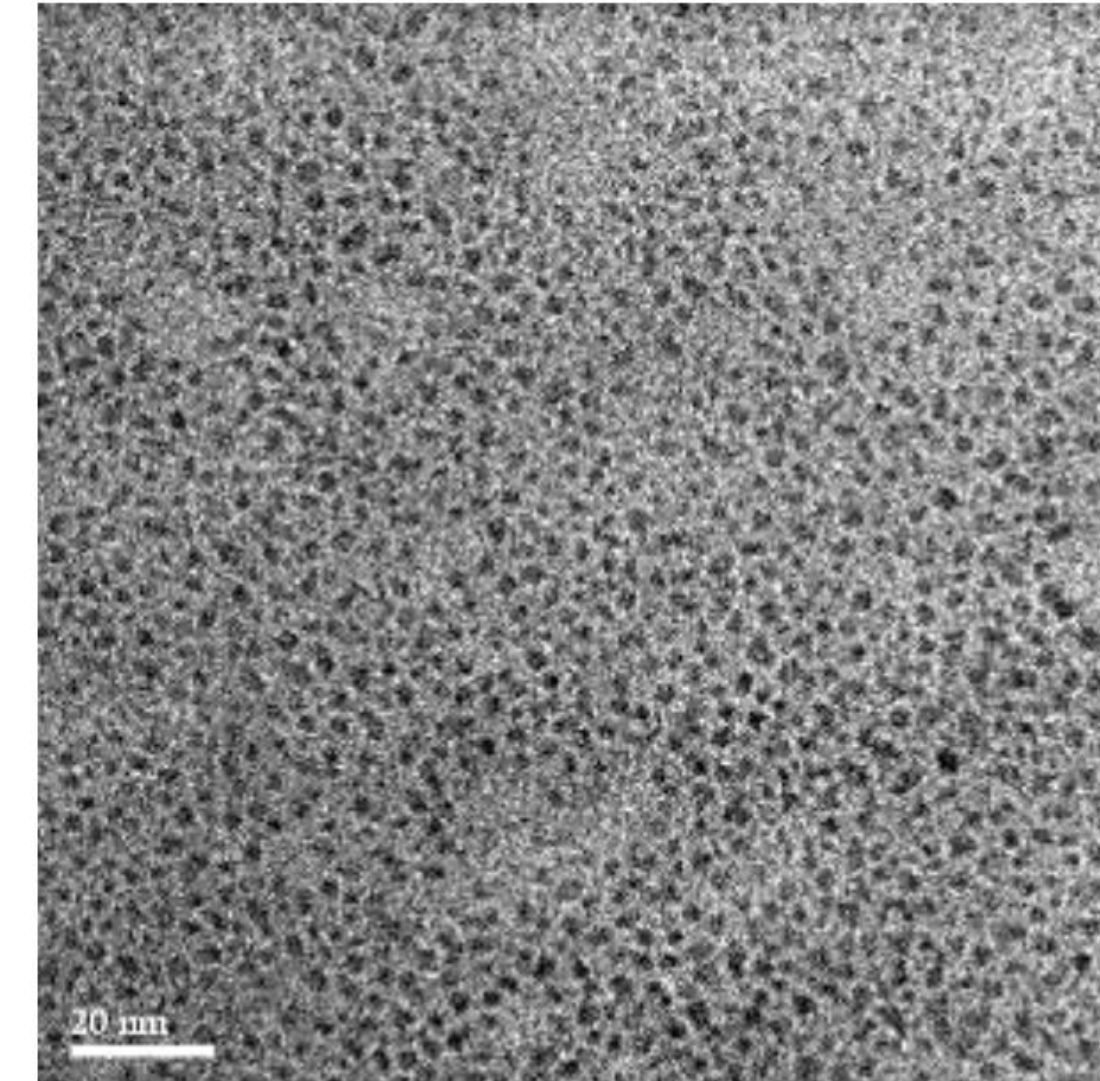
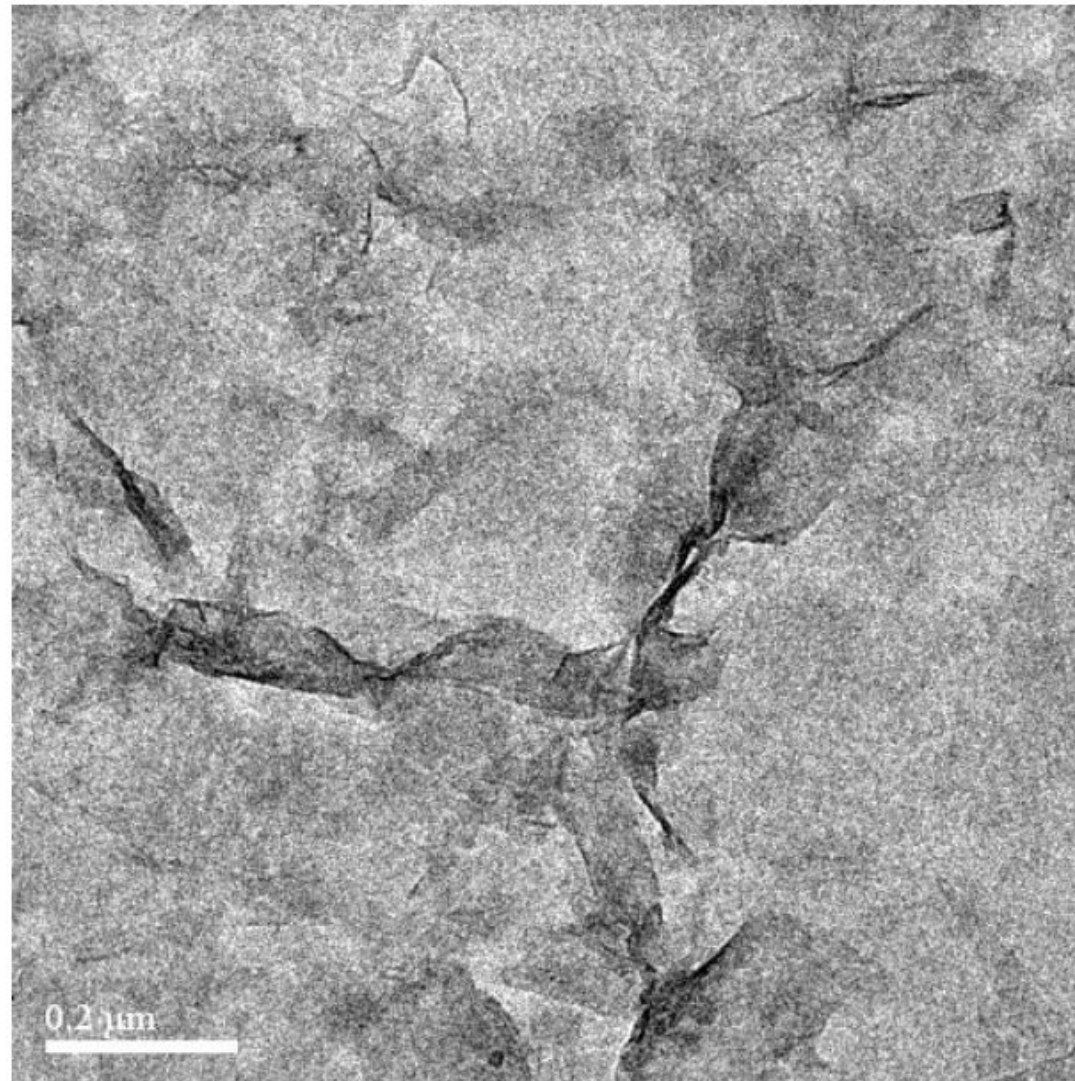
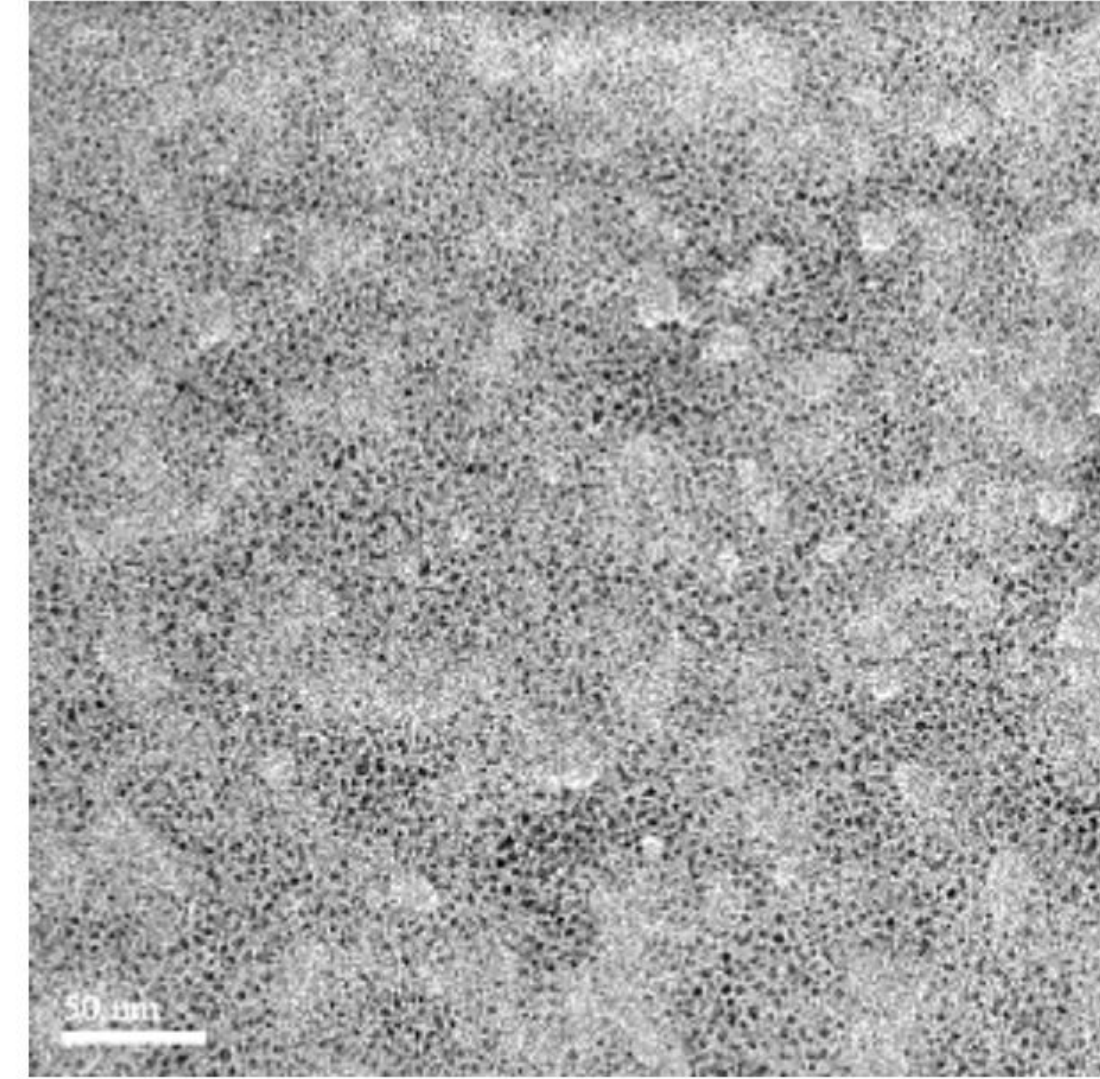
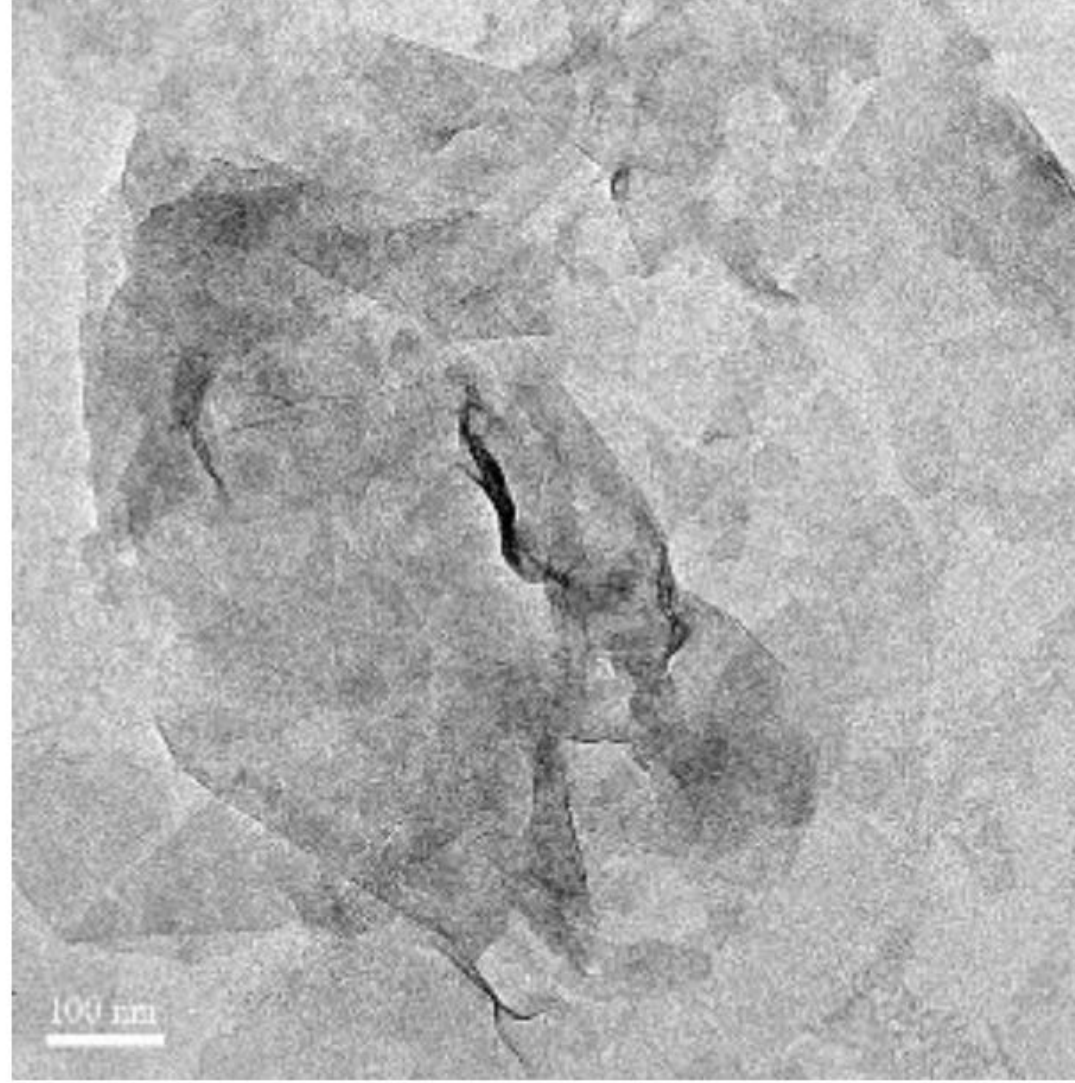
Mechanism of nanoparticle formation



How do they form?



MoS₂ Nanosheets



MoS₂ Nanosheet

MoS₂ Nanoparticles



Thanks to ChatGP
T

Vision

Make soil using processed wastewater and make deserts bloom.

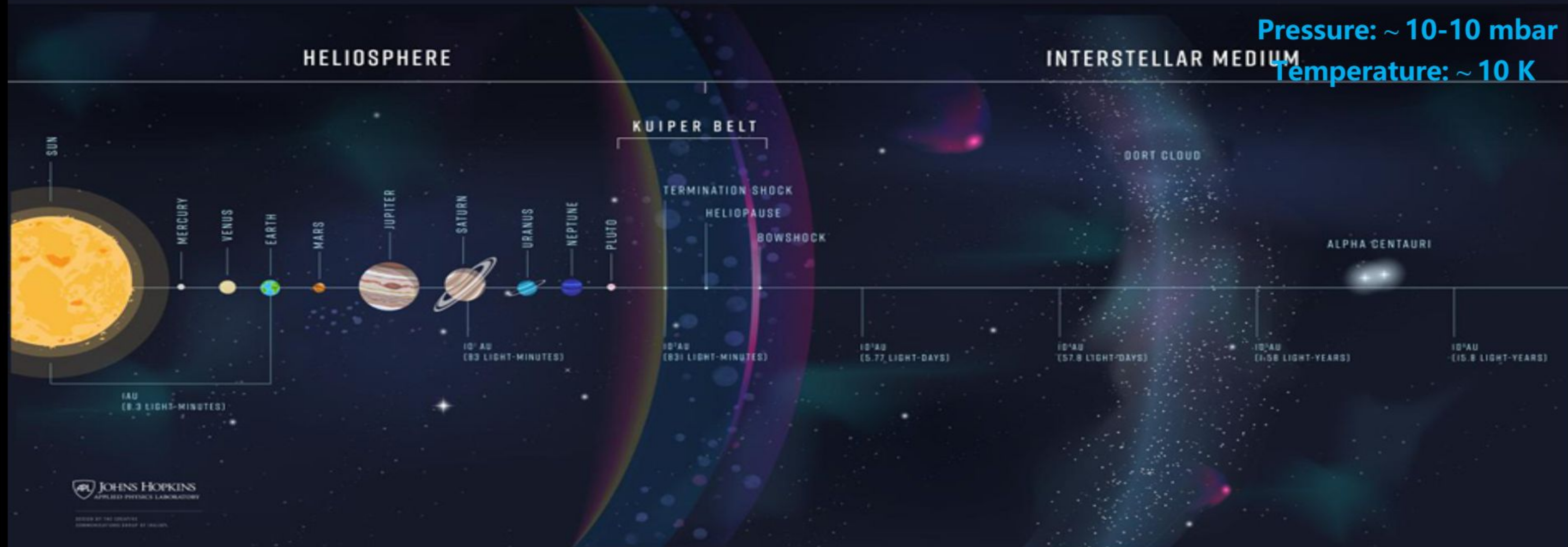


Thanks to ChatGP
T

Can Clathrate Hydrates Exist in Space?

Exploring astrobiology

Interstellar medium

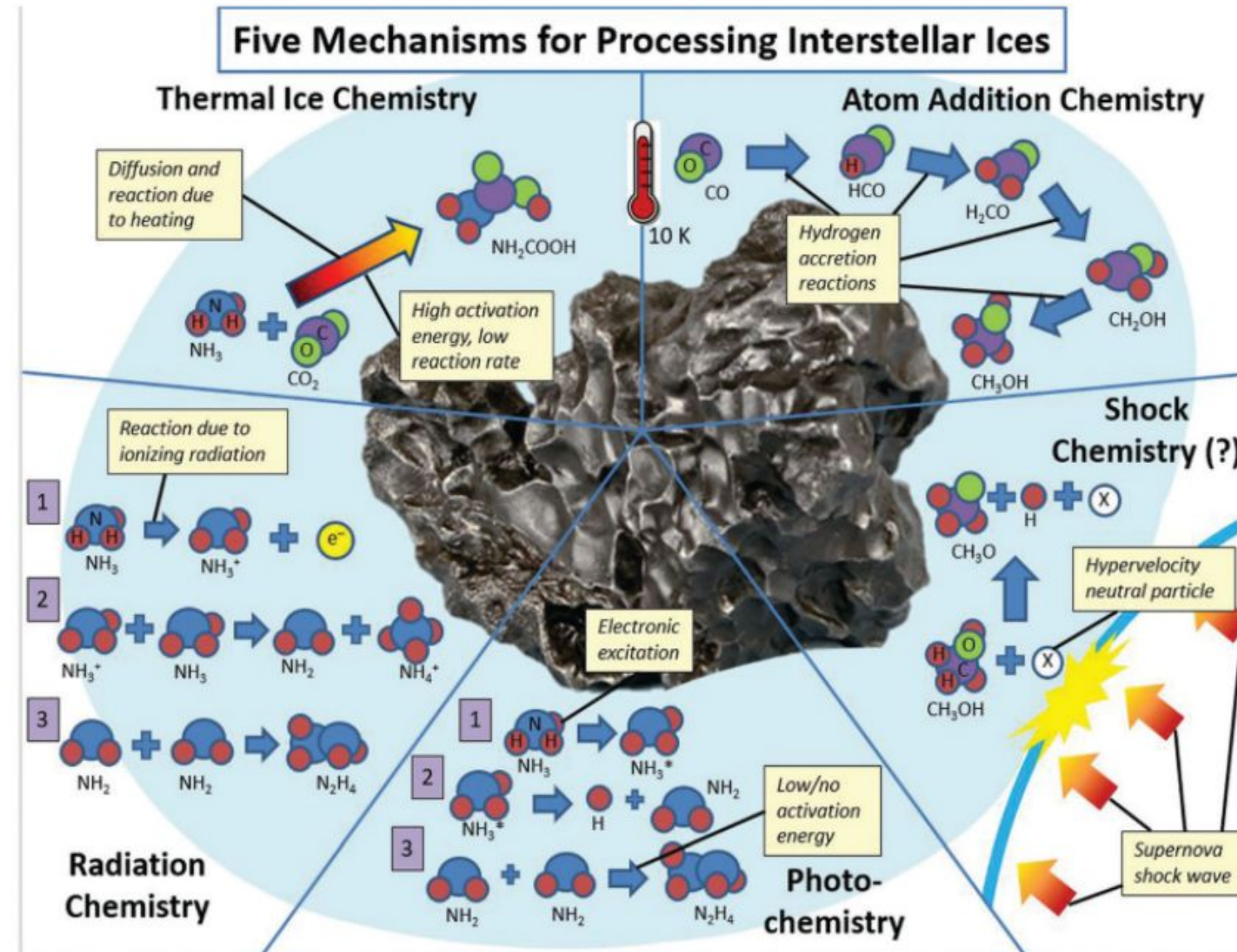
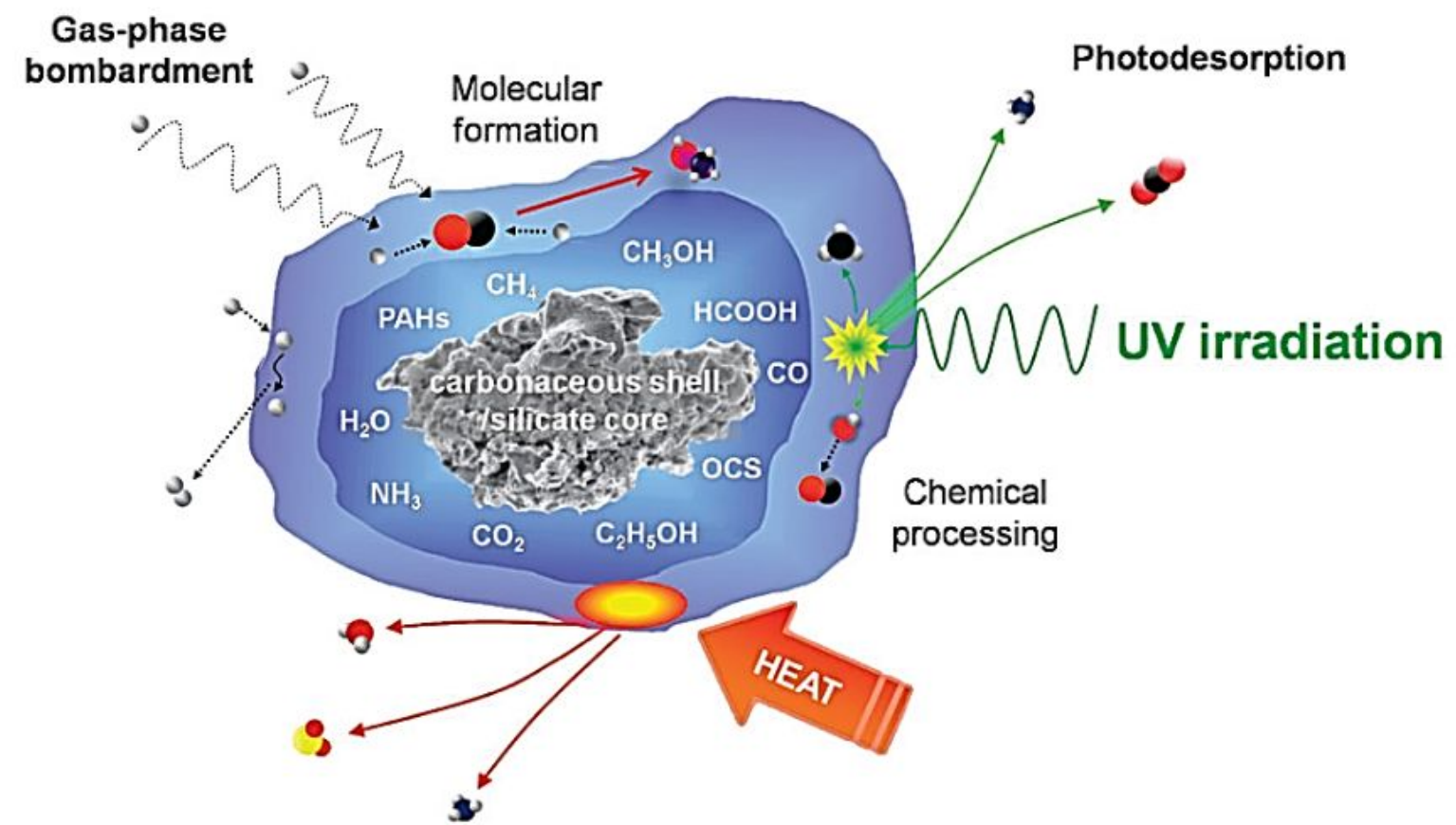


Diffuse clouds: $T \sim 100$ K, $n \sim 100$ molecules per cm^3

Dense clouds: $T \sim 10$ - 100 K, $n \sim 10^4$ - 10^8 molecules per cm^3

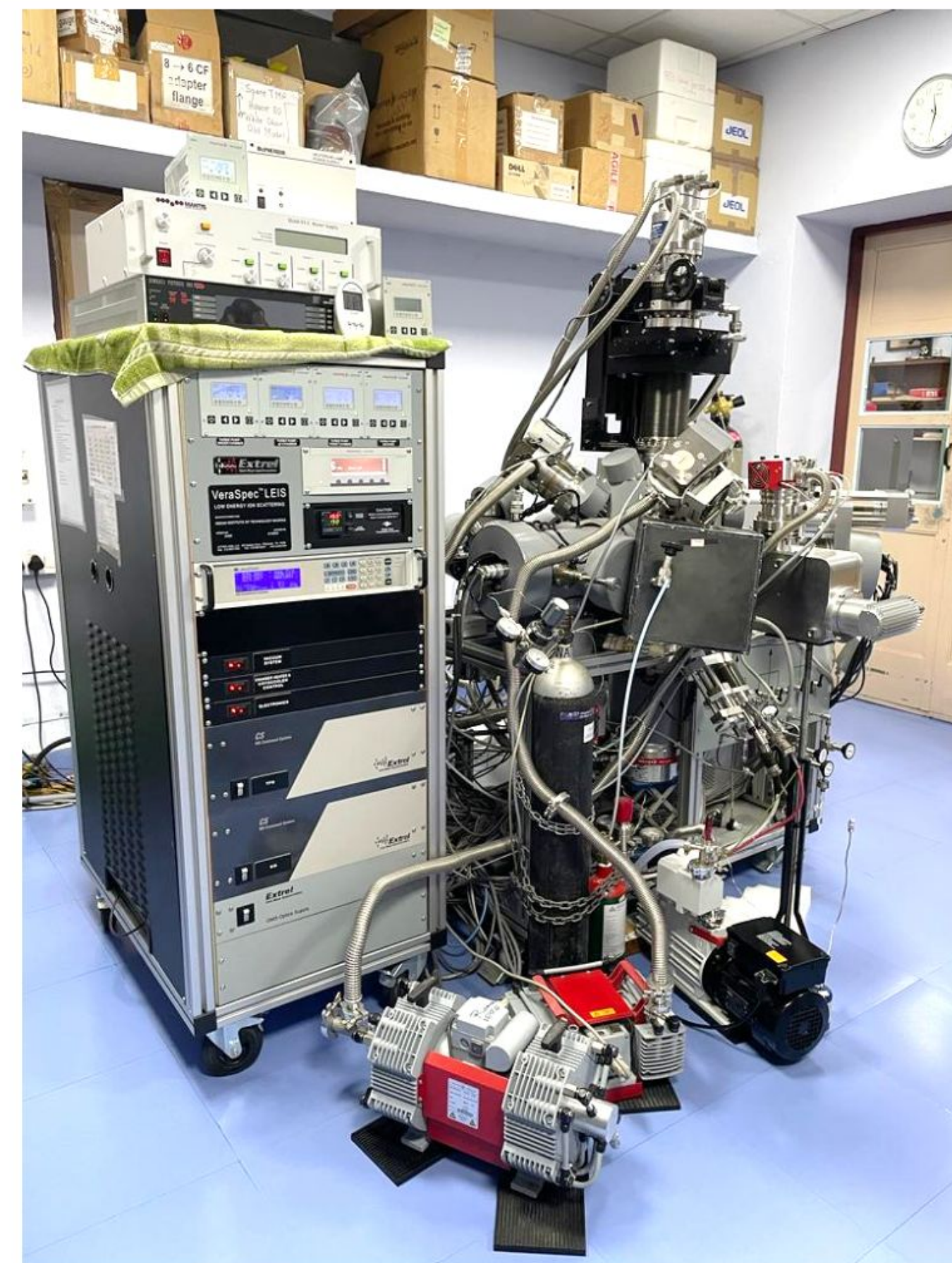
On Earth sea level: $T \sim 300$ K, $n \sim 3 \times 10^{19}$ molecules per cm^3

Interstellar ices



Silicates and carbonaceous material – 0.01-0.5 μm

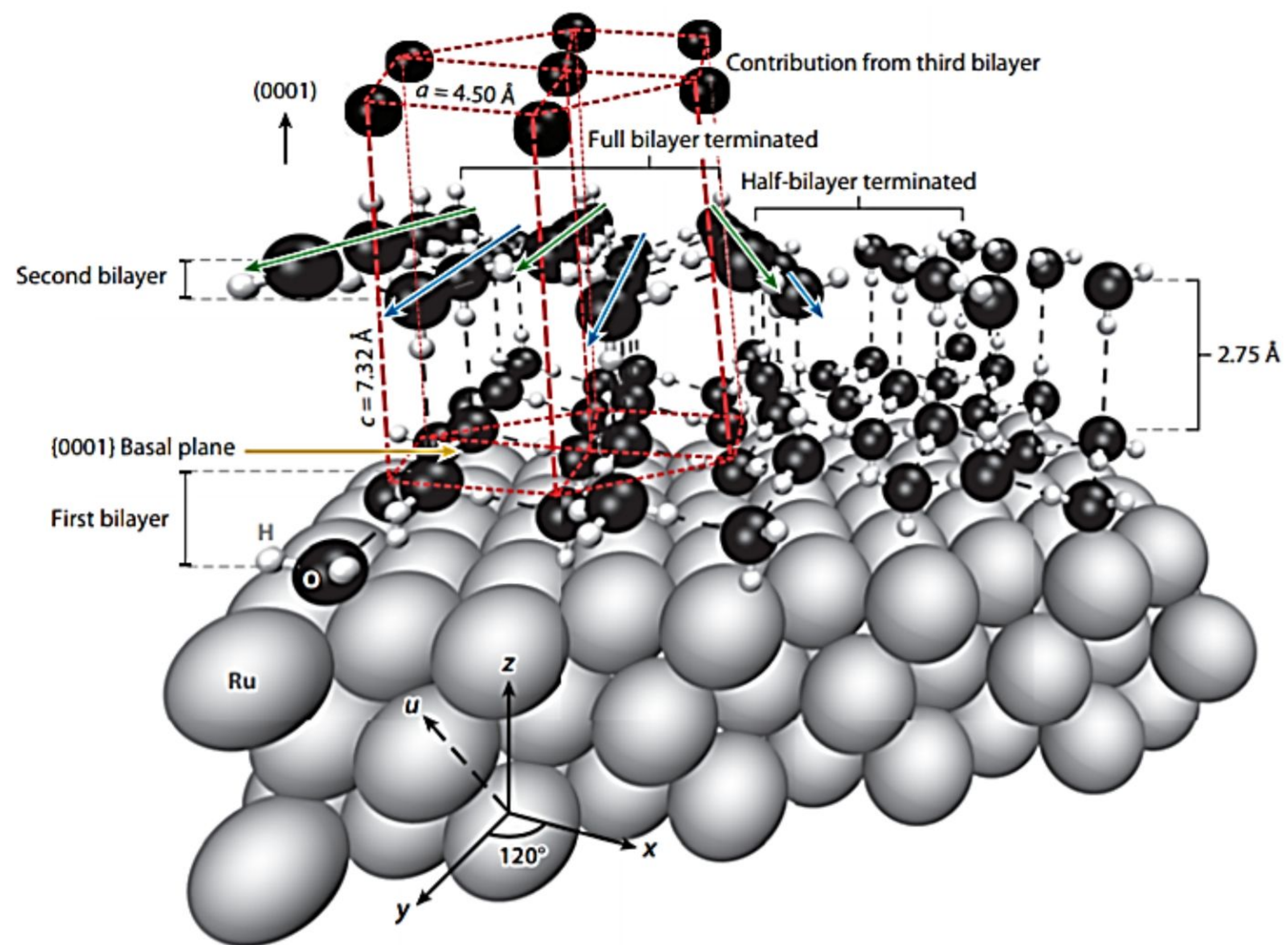
Instrumentation



115-400 nm

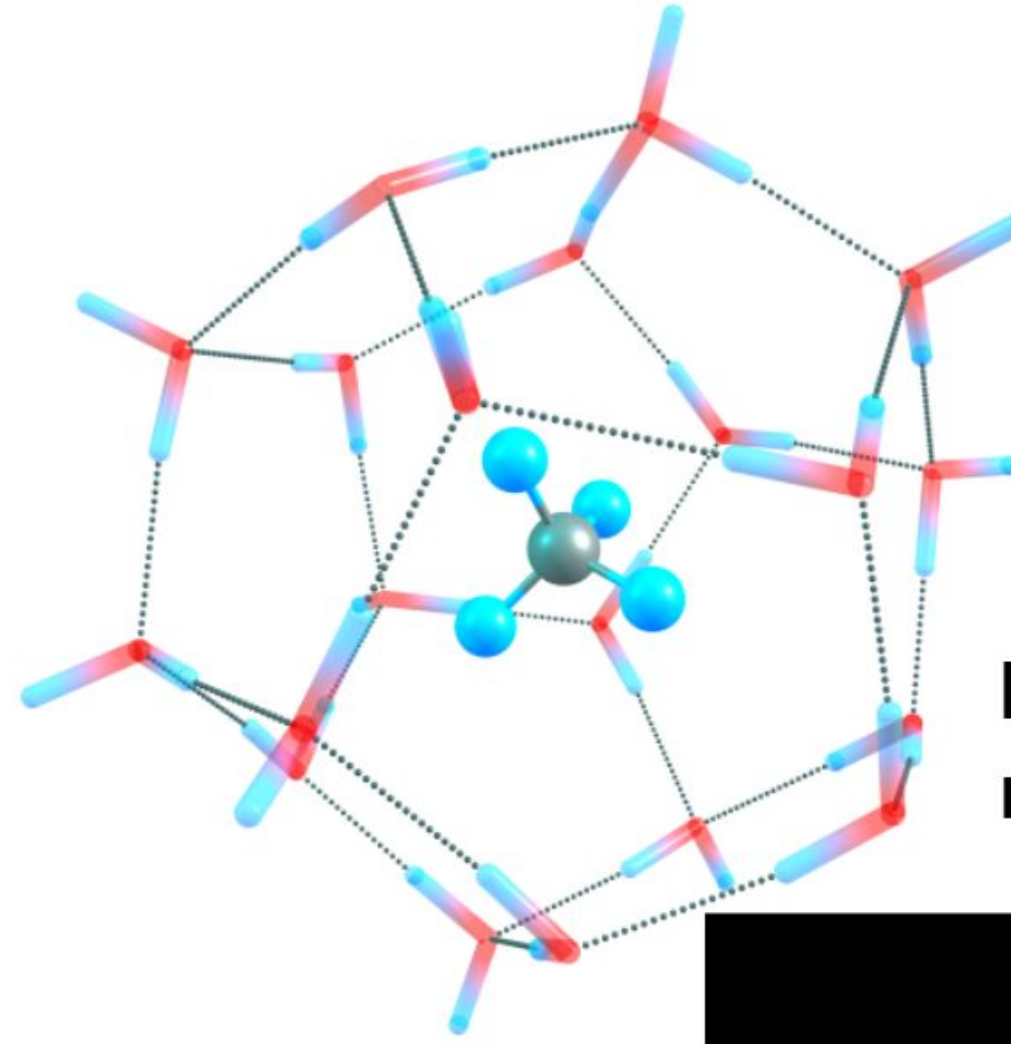
Bag, S. *et al.*, *Rev. Sci. Instrum.* **2014**, 85, 014103/1-014103/7

Viswakarma, G. *et al.*, *J. Phys. Chem. Lett.*, **2023**, 14, 2823–28



Clathrate hydrates in interstellar environment

Sample inlet tubes



Methane hydrate structure; 512 cage

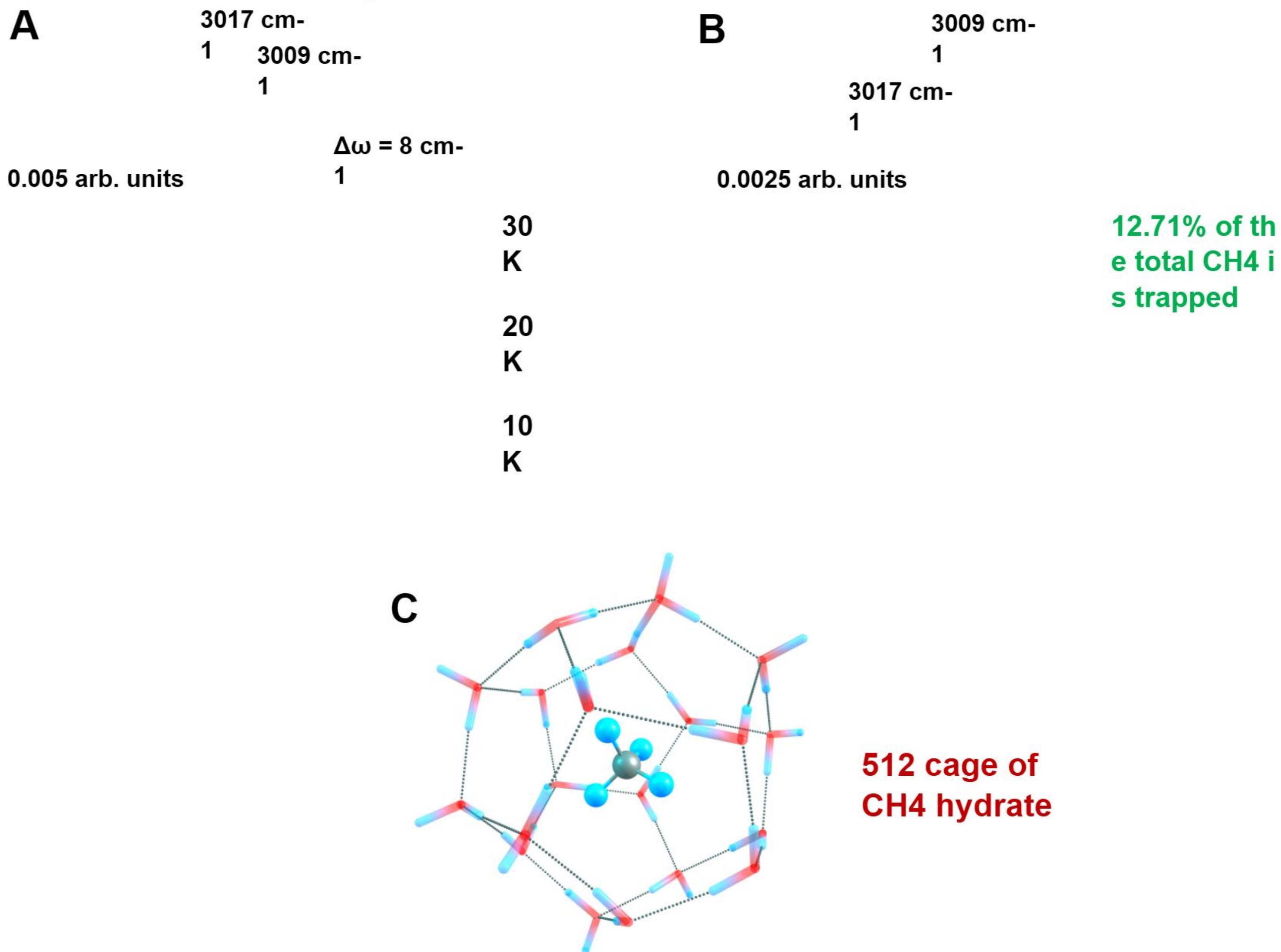
Annealing

Varying T, depending on the gas

Co-deposition at 10 K

Clathrate hydrate (CH)

Clathrate hydrates in interstellar environment



Formation and Transformation of Clathrate Hydrates under Interstellar Conditions

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



Cite This: <https://doi.org/10.1021/acs.accounts.3c00317>



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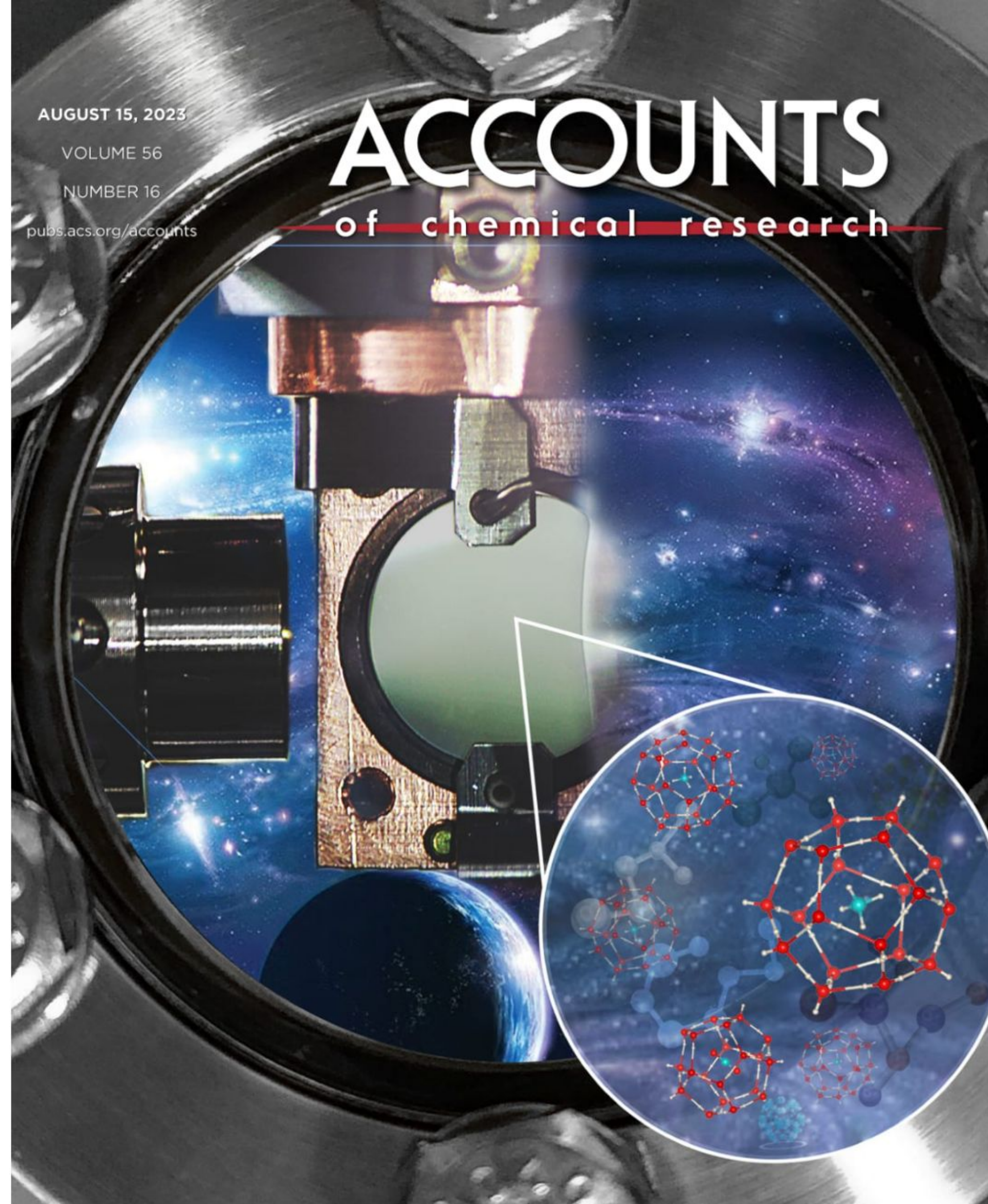
AUGUST 15, 2023

VOLUME 56

NUMBER 16

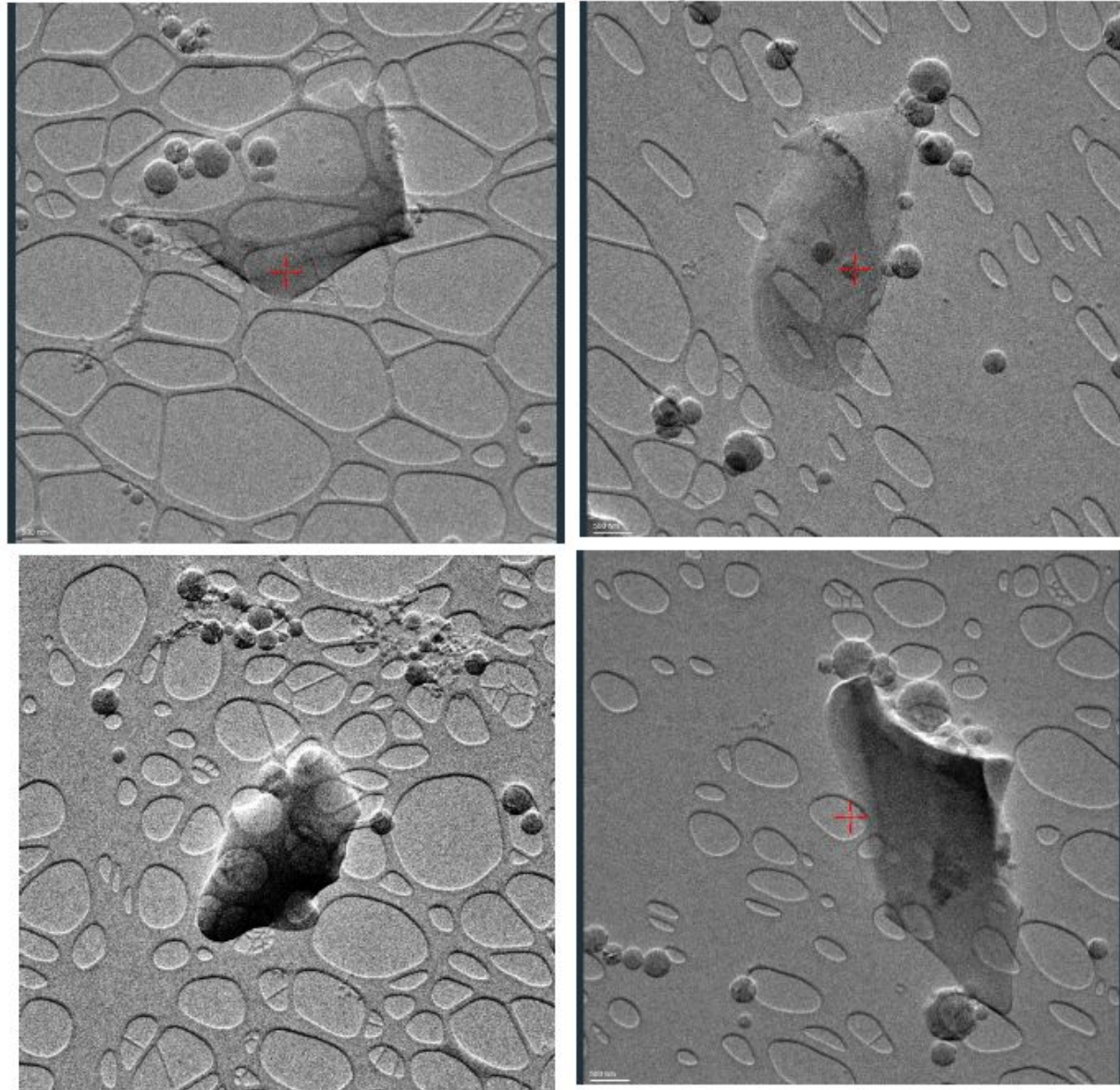
pubs.acs.org/accounts

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of chemical research

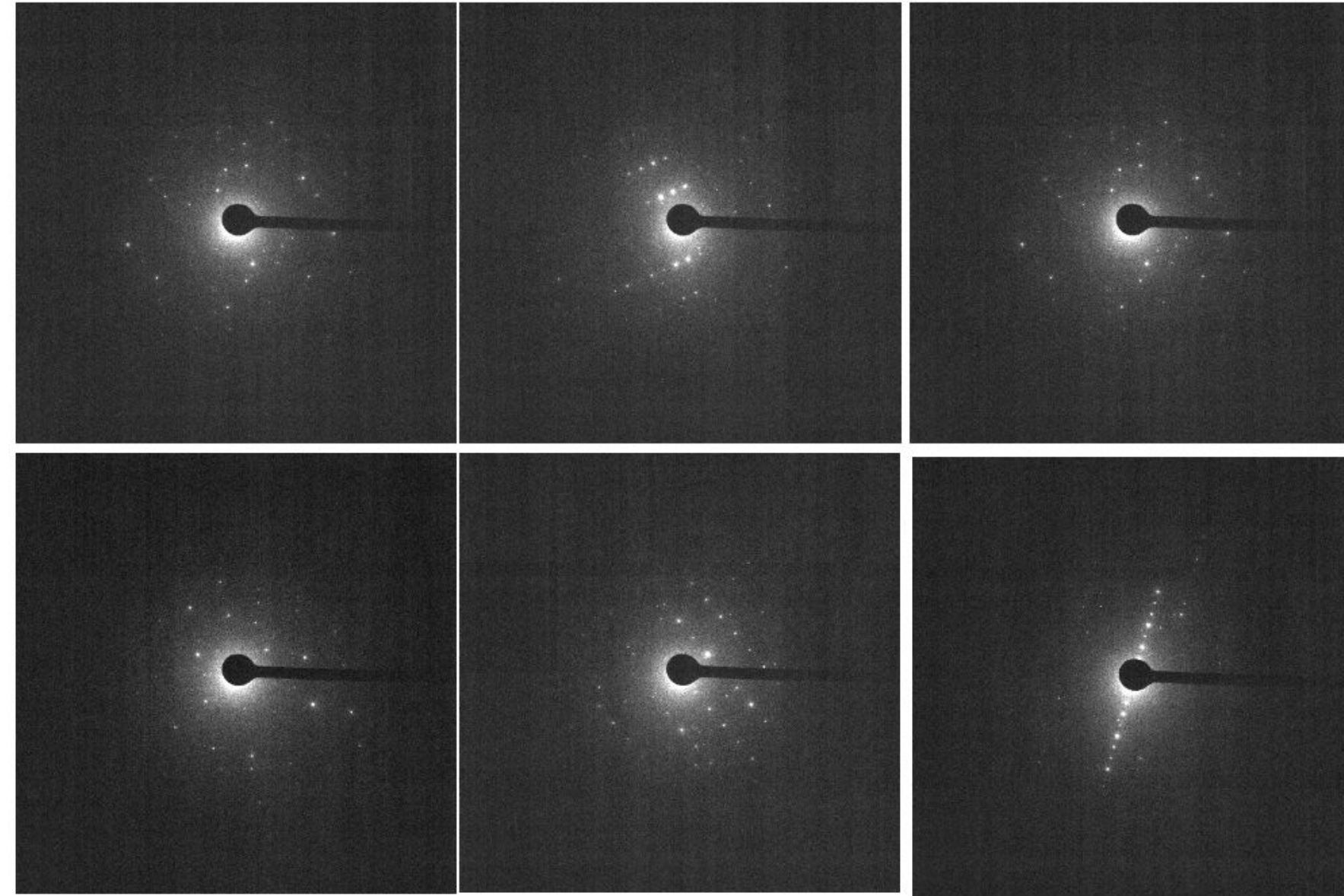


Electron diffraction of nanometer-scale crystals of clathrate hydrate

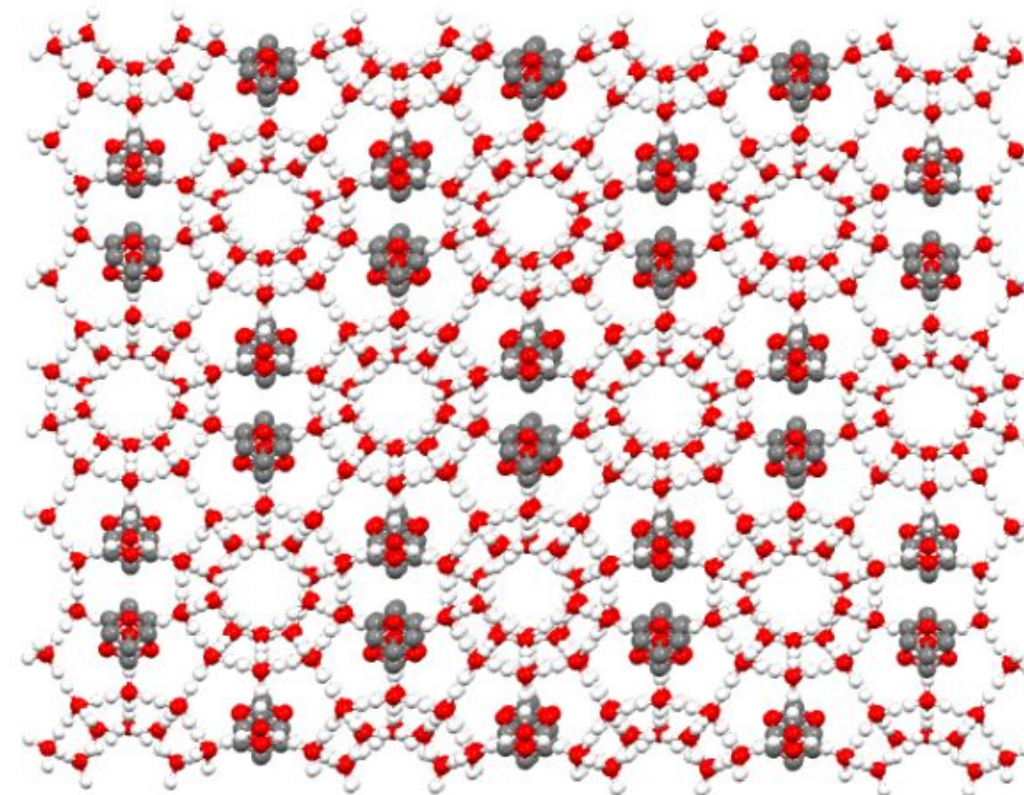
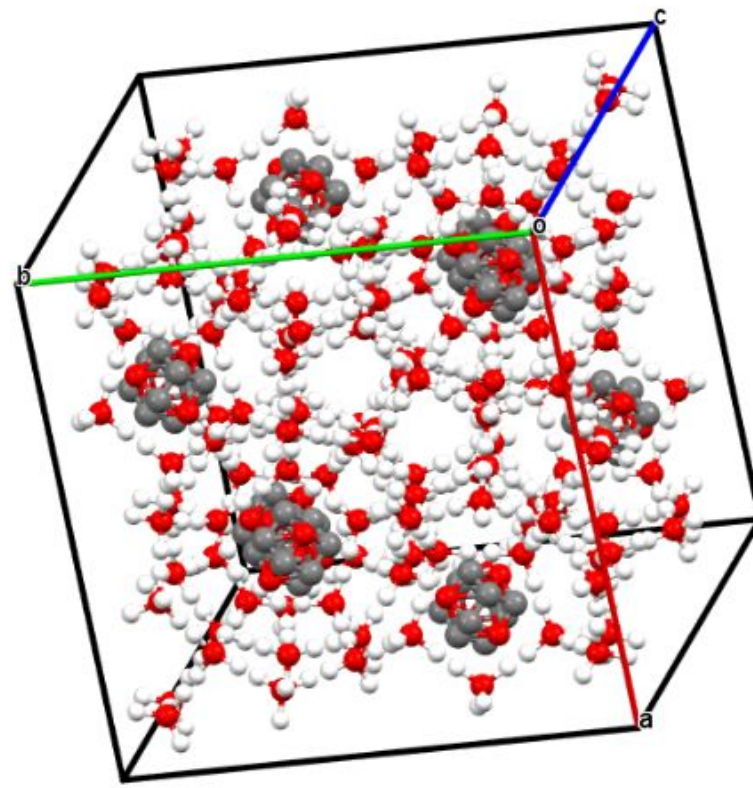
(a) THF-CH₄ Clathrate hydrate crystal
)



(b) 3 D electron diffraction
)

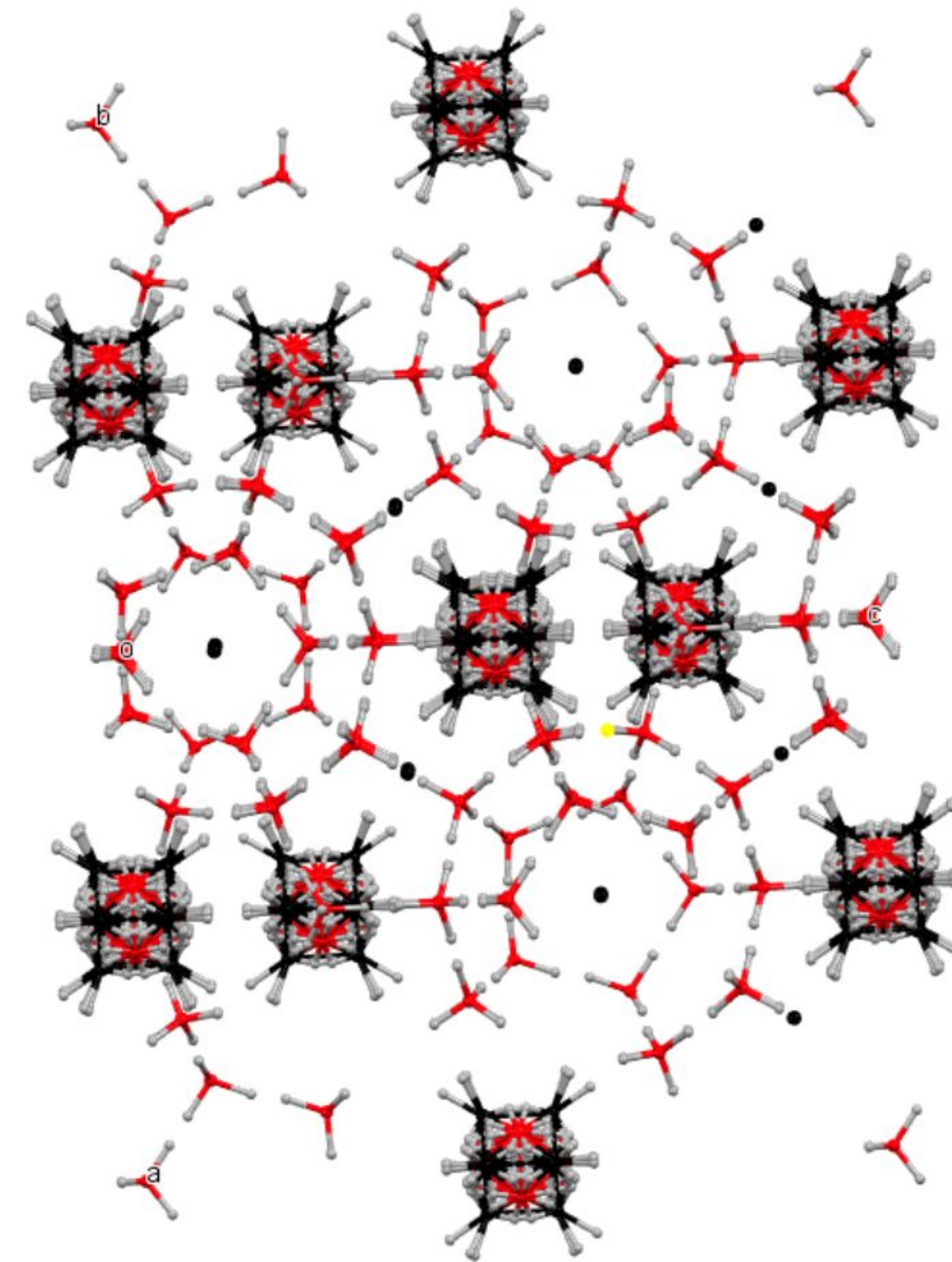
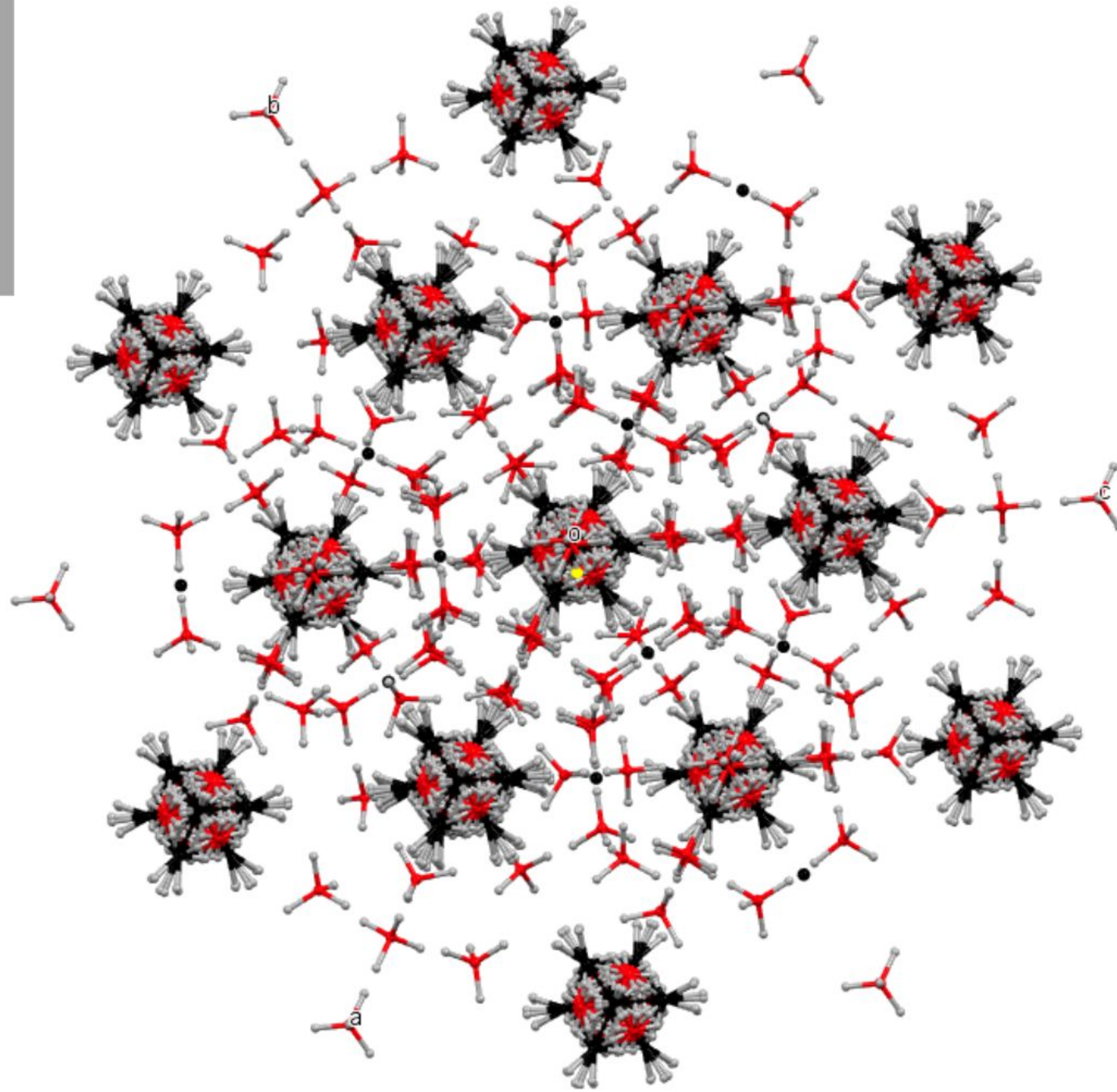
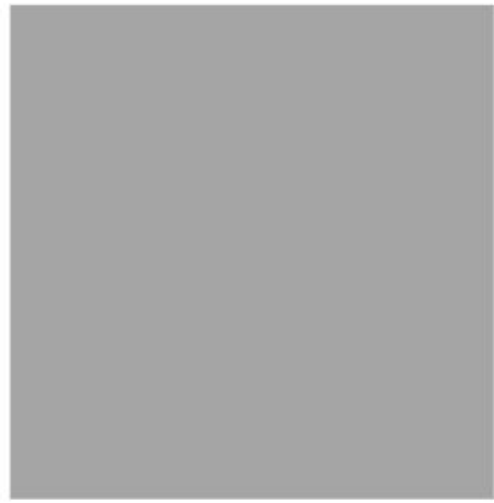


(c)
)



Crystal structure

MicroED – THF CH₄ clathrate hydrate



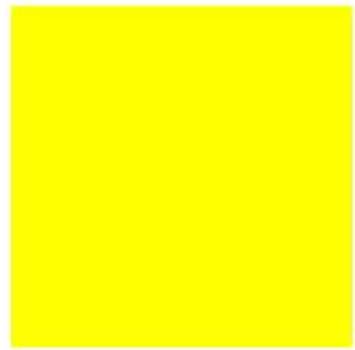




International Centre for Clean Water

<https://iccw.world>

Our dreams become reality with materials

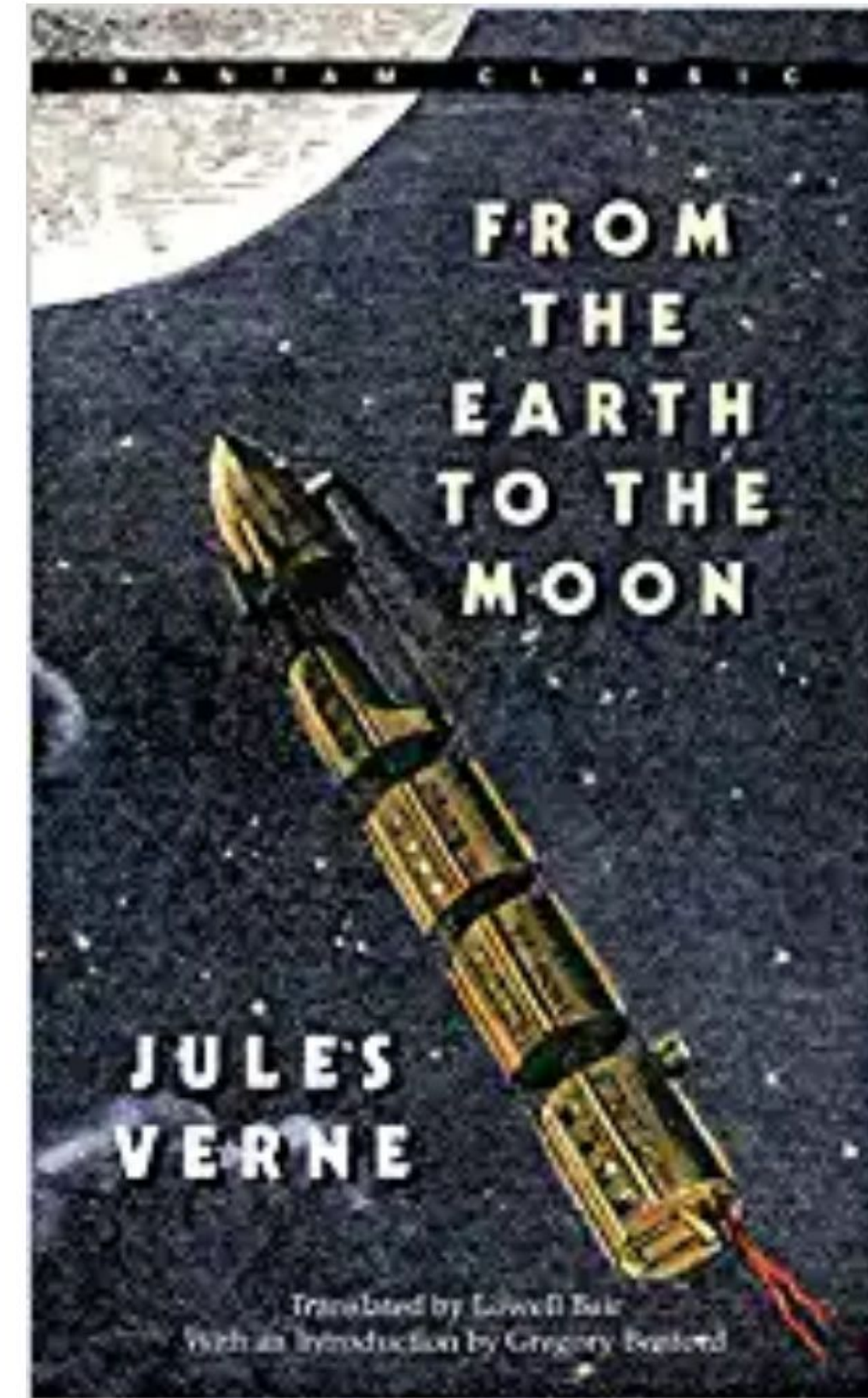


H₂O

Energy



Clean water



An ocean of opportunities

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

Conclusions

Affordable clean water with advanced materials is demonstrated at scale.

Natural minerals break spontaneously in charged water microdroplets.

Clathrate hydrates exist in ultrahigh vacuum.

Implications of all these are profound.

New research is needed in these areas.

Affordable, inclusive, sustainable and contextual excellence





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. Sajanla I, 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

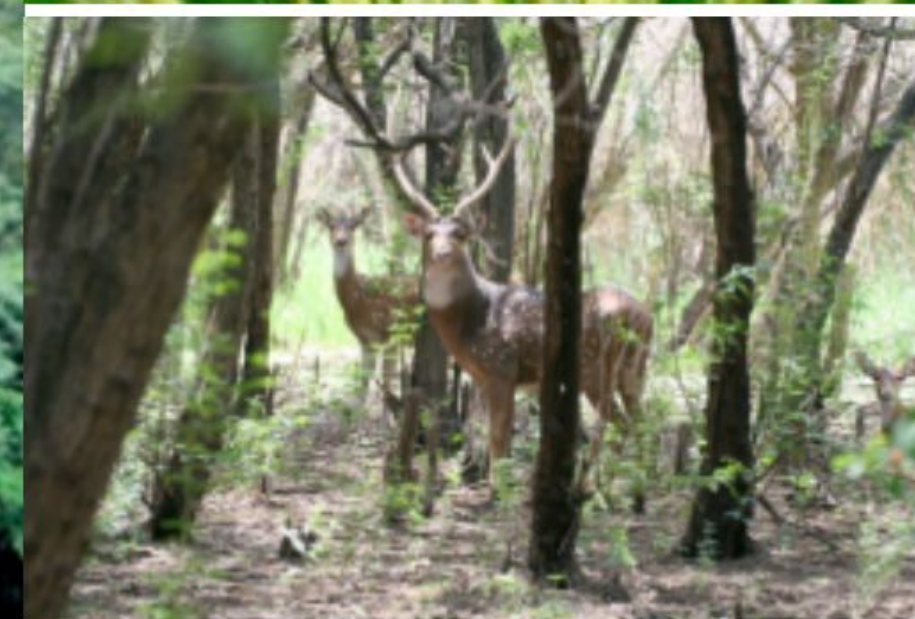
MS Theses: Ananthu Mahendranath, Ramesh Kumar Soni

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





Indian Institute of Technology Madras



Associate Editor
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