



Using ChatGP
T

Water: A Molecular Foundry

From Atomically Precise Clusters to Droplets and Ice for Sustainability

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<https://pradeepresearch.org>

Co-founder

InnoNano Research Pvt. Ltd.

InnoDI Water Technologies Pvt. Ltd.

VayuJAL Technologies Pvt. Ltd.

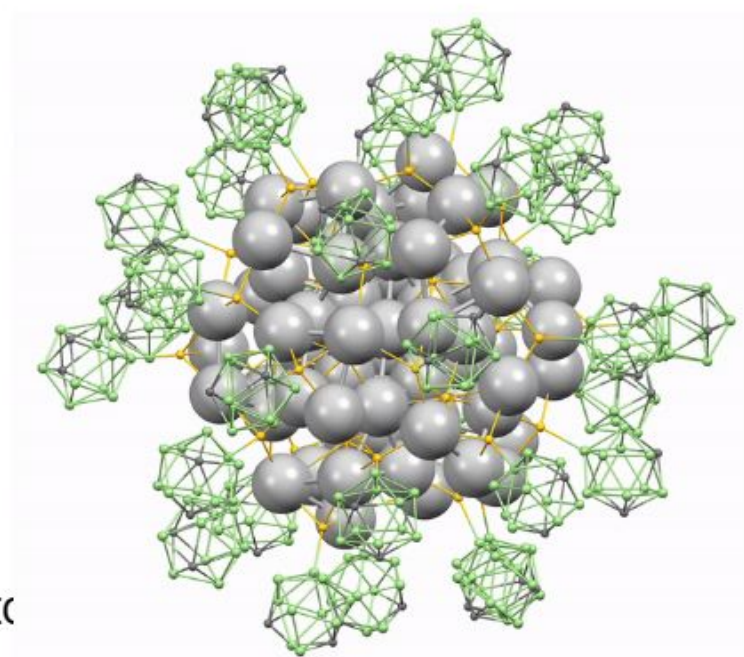
Aqueasy Innovations Pvt. Ltd.

Hydromaterials Pvt. Ltd.

EyeNetAqua Solu

DeepS

Associate Editor
Innovations Pvt. Ltd.



Professor-in-charge



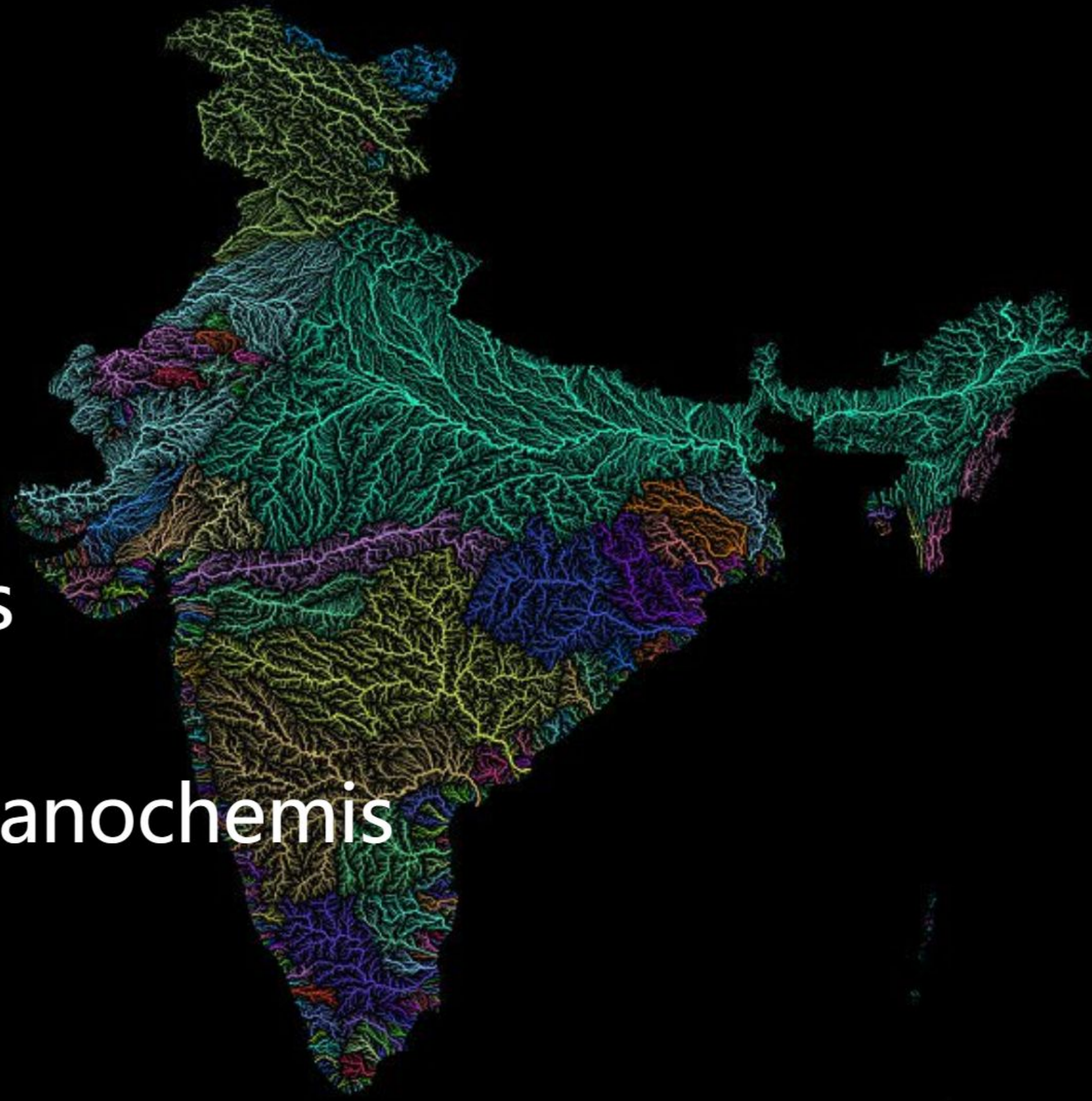
International Centre for Clean Water
ter

<https://iccw.world>
NISER Bhubaneswar, December 12, 20





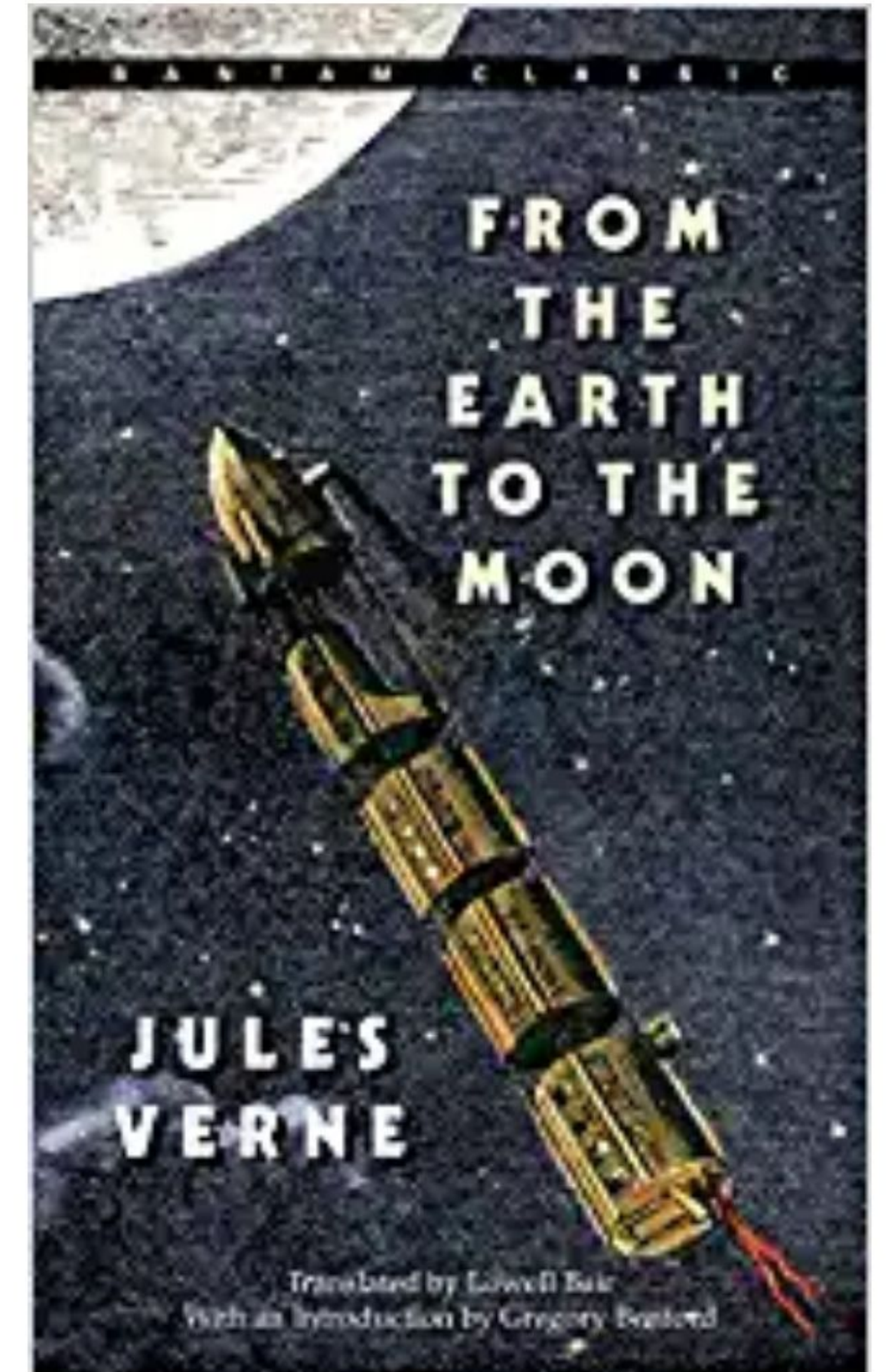
Advanced materials
Clean Water for all
Microdroplet mechanochemis-
try
Chemistry of ice



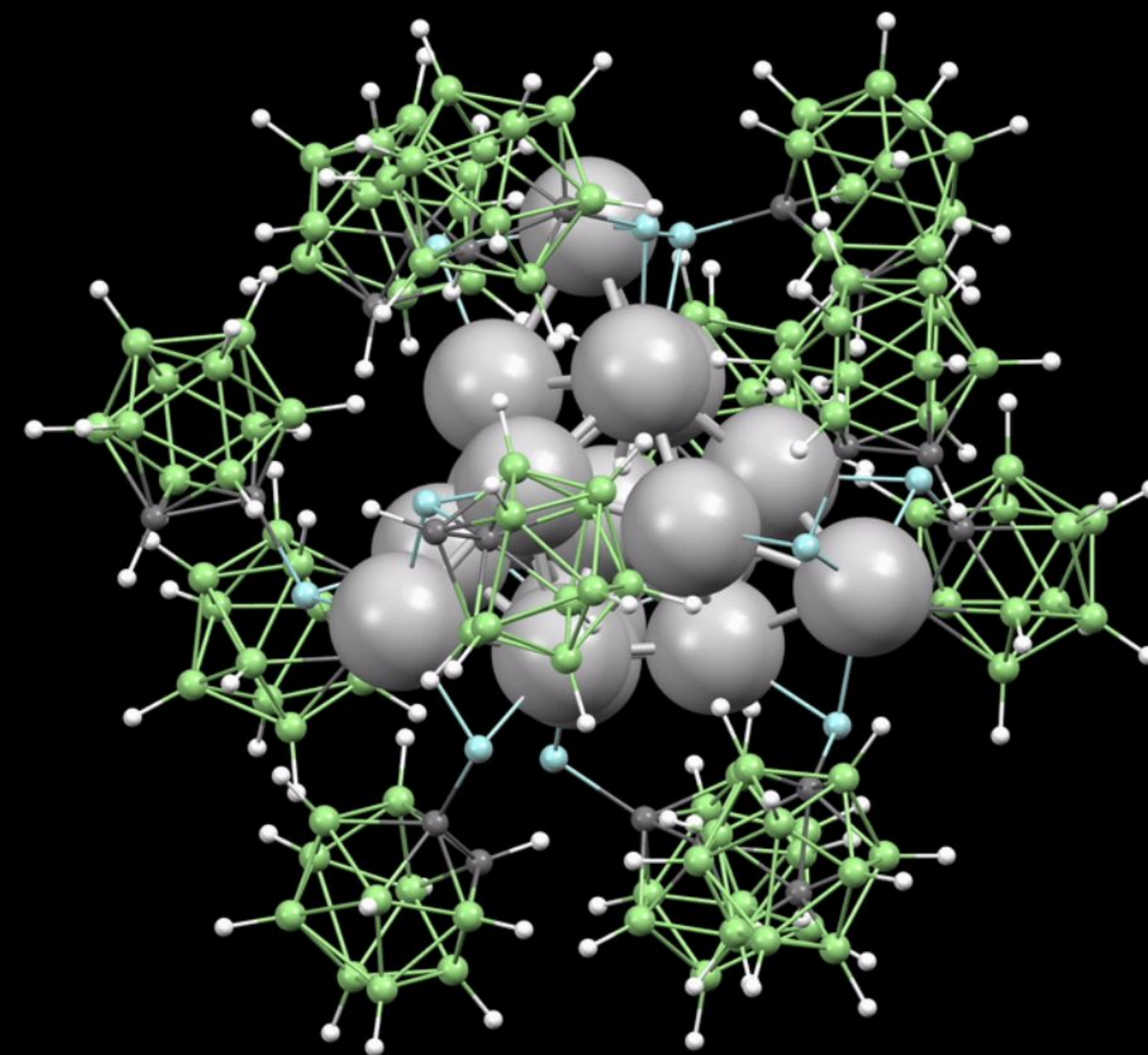
From S. Vishwanat
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© Robert Szucs/Grasshopper Geography

Our dreams become reality
with materials



But, matter is becoming
ATOMICALLY PRECISE



Vivek Yadav, et. al. *Nature Communications* 2025

Organic and inorganic matter too are becoming atomically precise



HSB 148

World's first nanochemistry-based water purifier

RSC | Advancing the
Chemical Sciences
Chemistry World

Pesticide filter debuts in India

20 April 2007

Kilugudi Jayaraman/Bangalore, India

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

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

'Our pesticide filter is an offshoot of basic research on the chemistry of nanoparticles,' Thirupathi Pradeep who led the team at IIT Chennai told Chemistry World. He and his student Suresh Kumar Han 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,



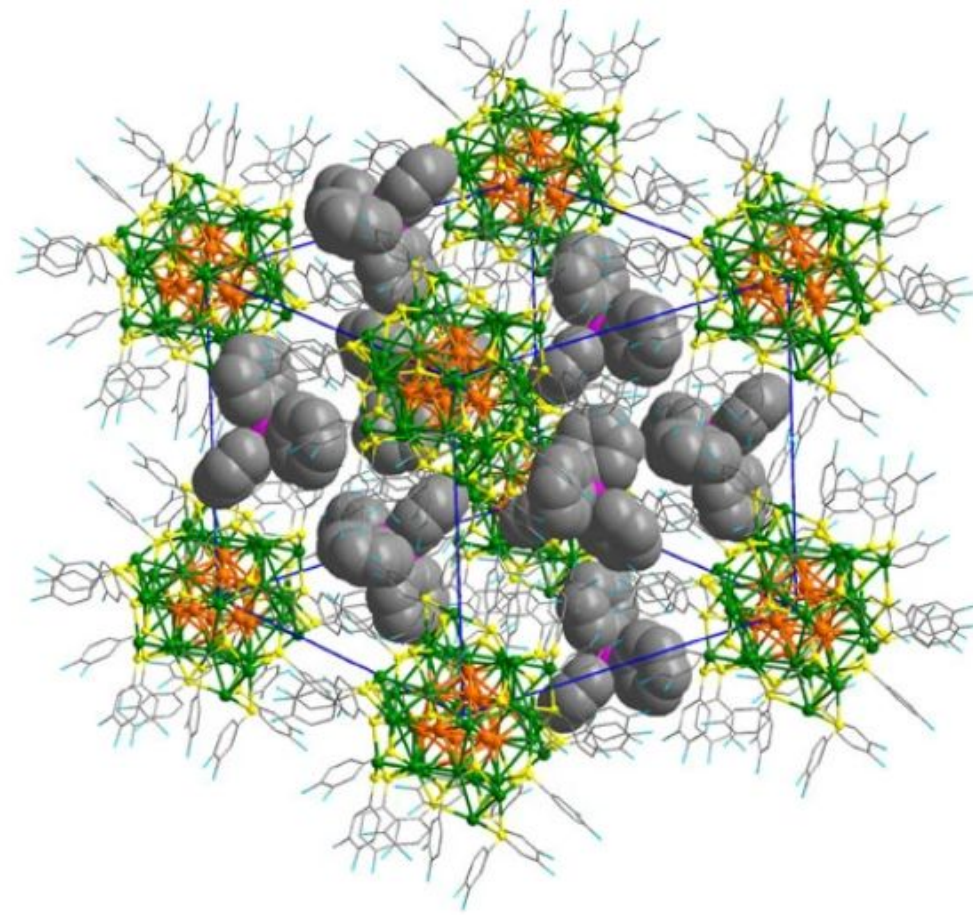
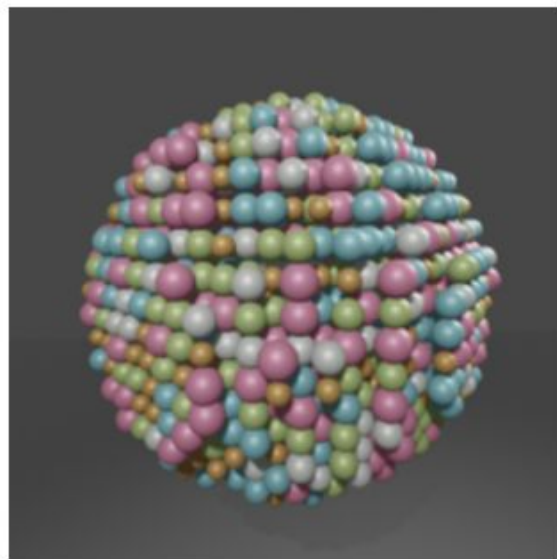
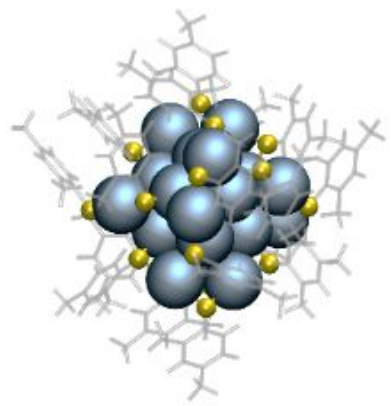
Indian patent 200767

US 7,968,493

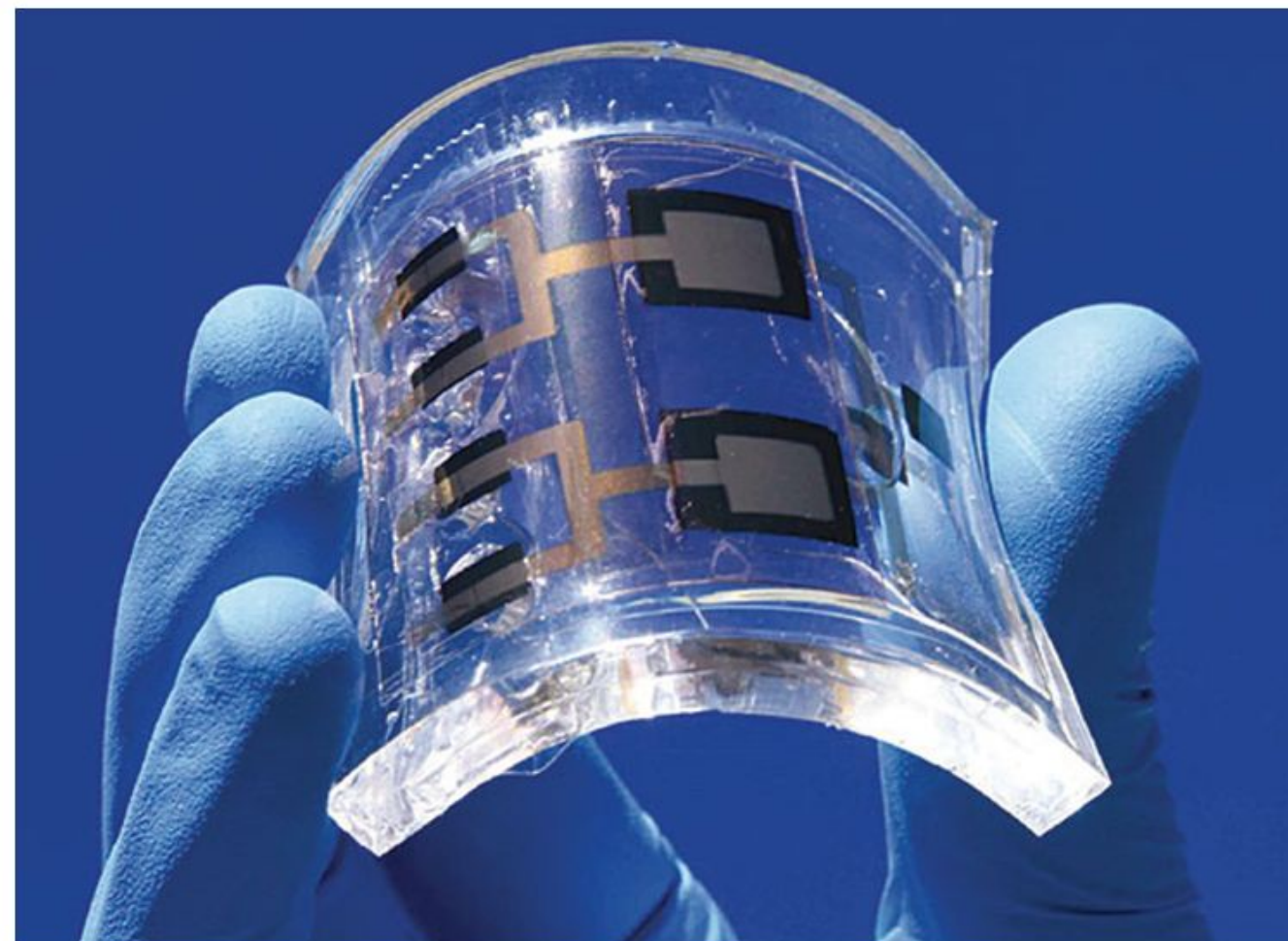
EP 17,15,947

Product is marketed now by a Eureka Forbes Ltd

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

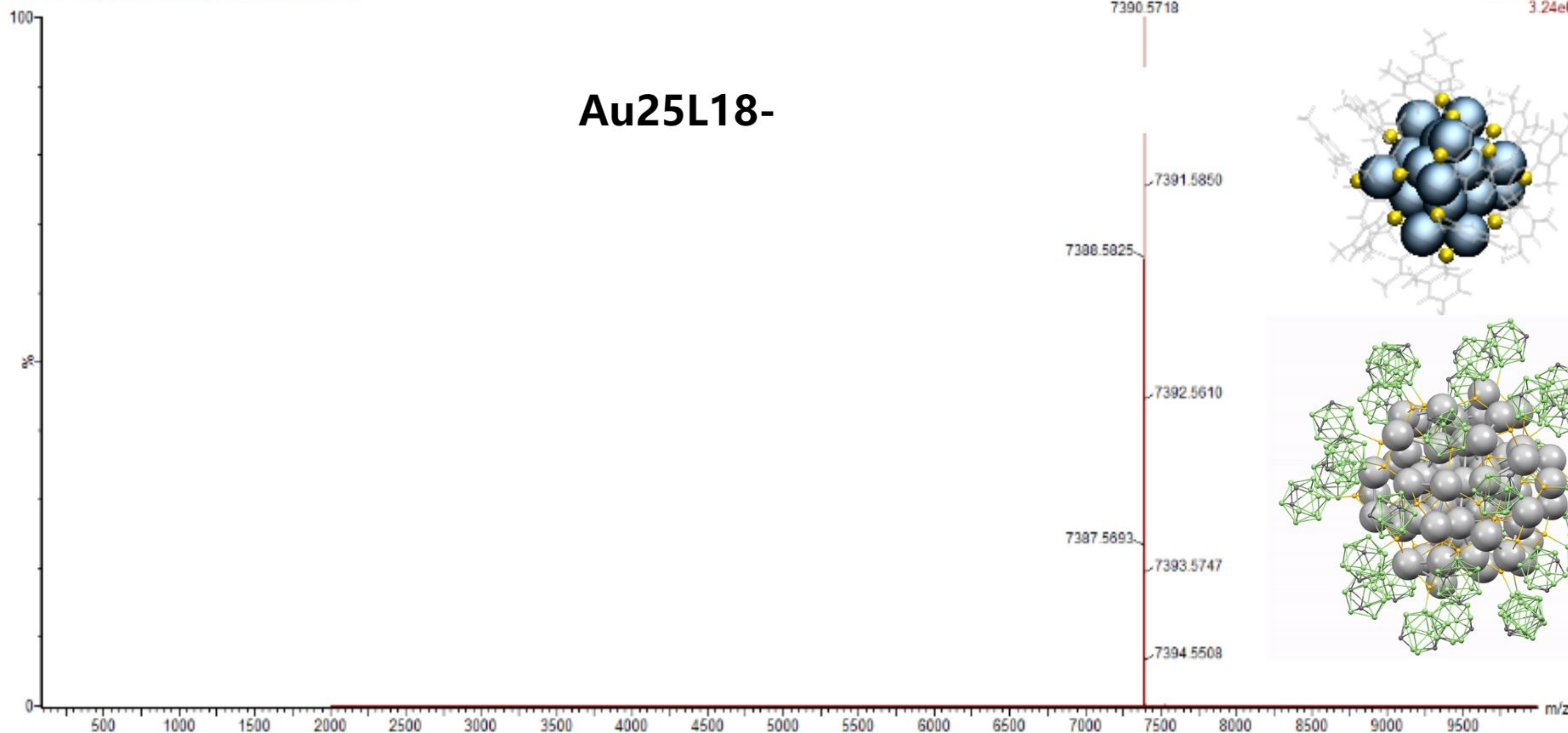


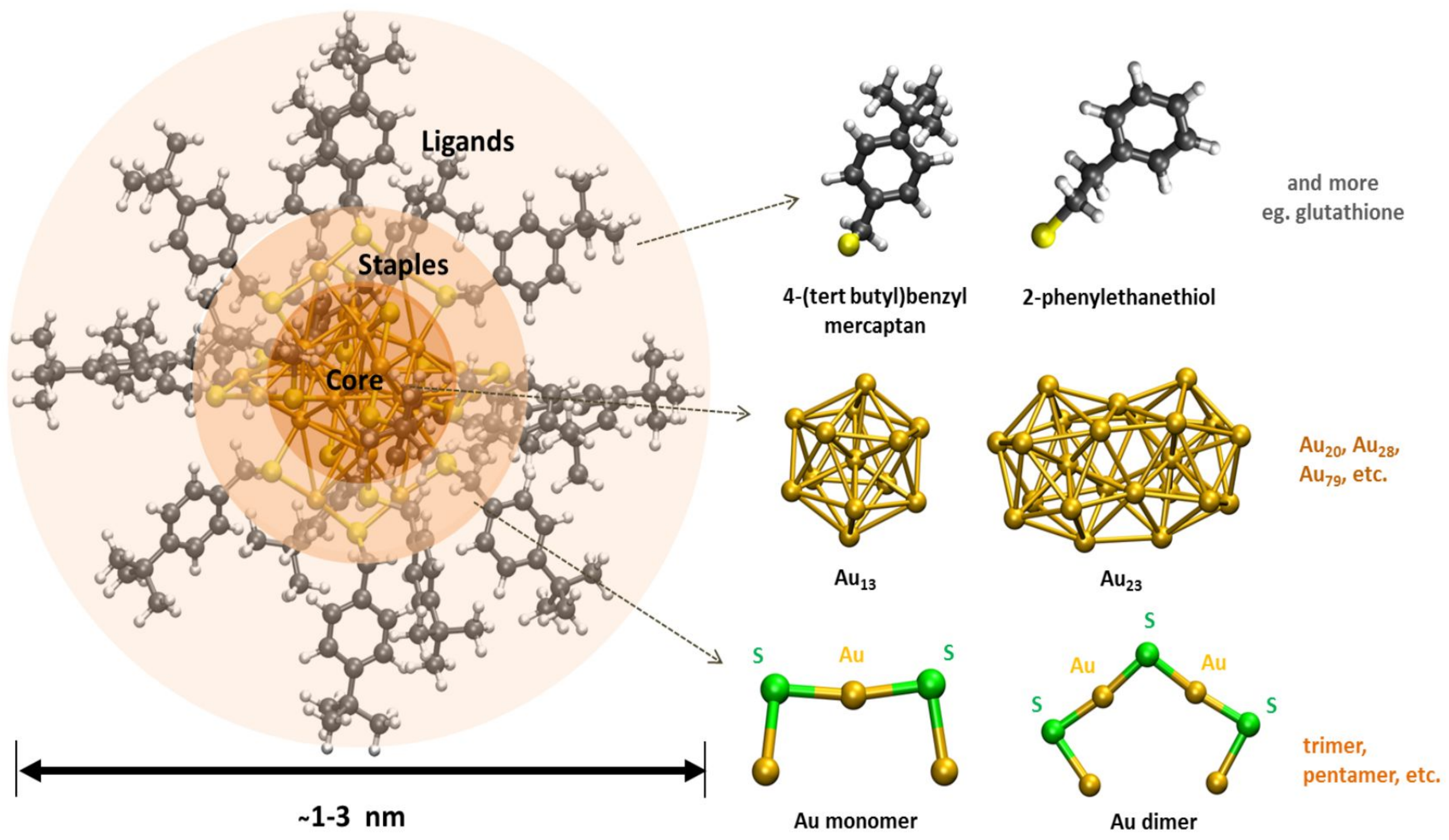
Chasing the 'Cluster' Dreams



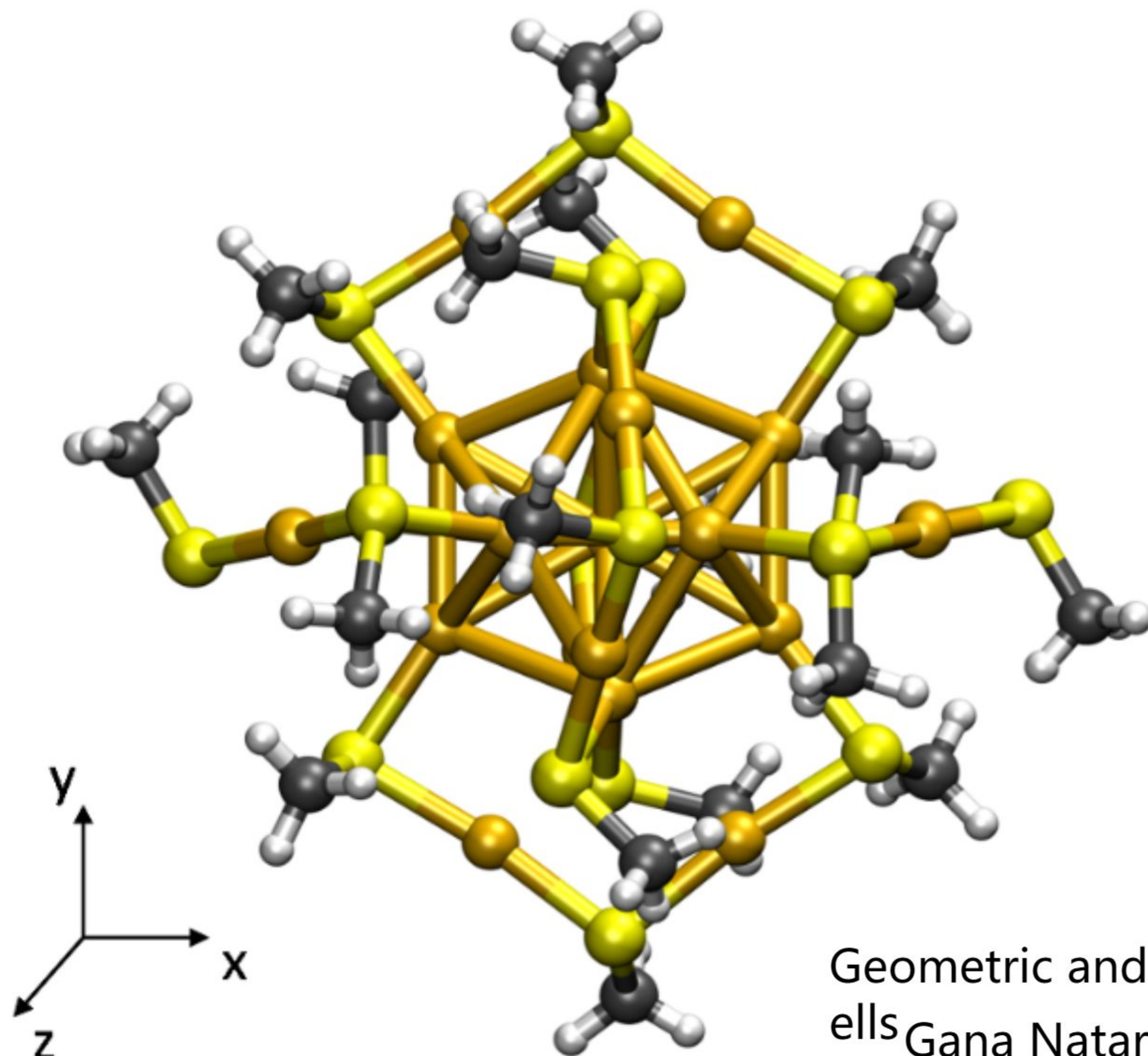
Molecular formula, Molecular weight

AU25PET18_RES_NEG_MS_3 32 (0.558) Cm (5:80)

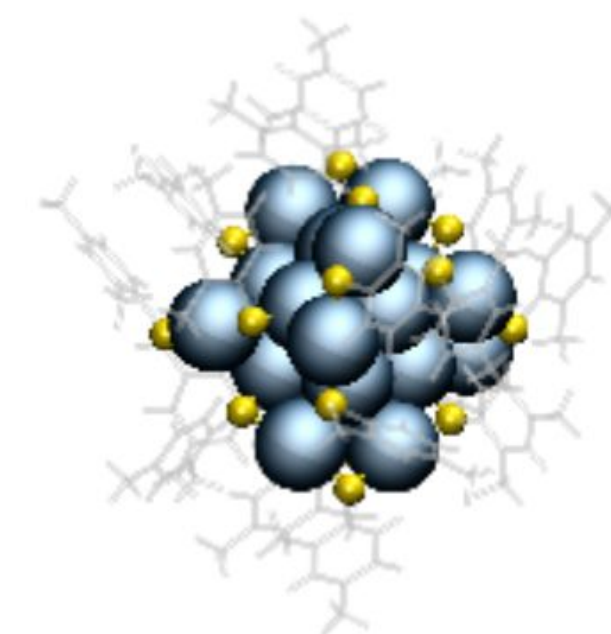
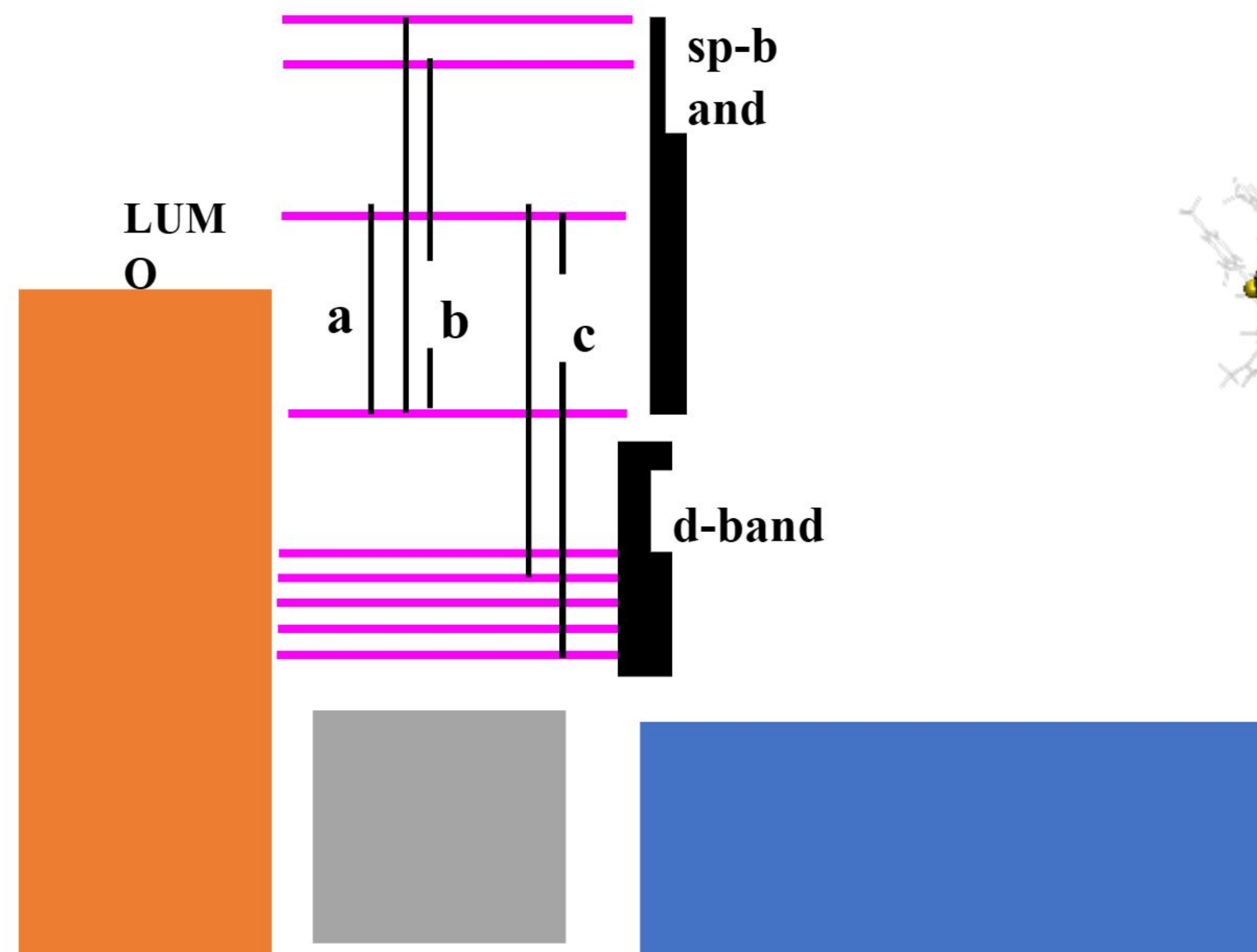




Molecular structure



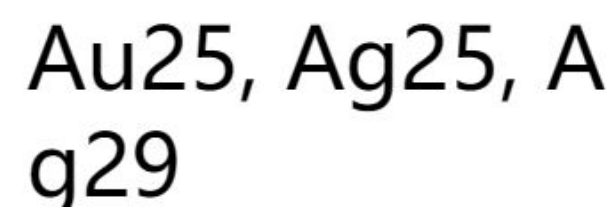
Geometric and electronic shells
Gana Nataraja
n



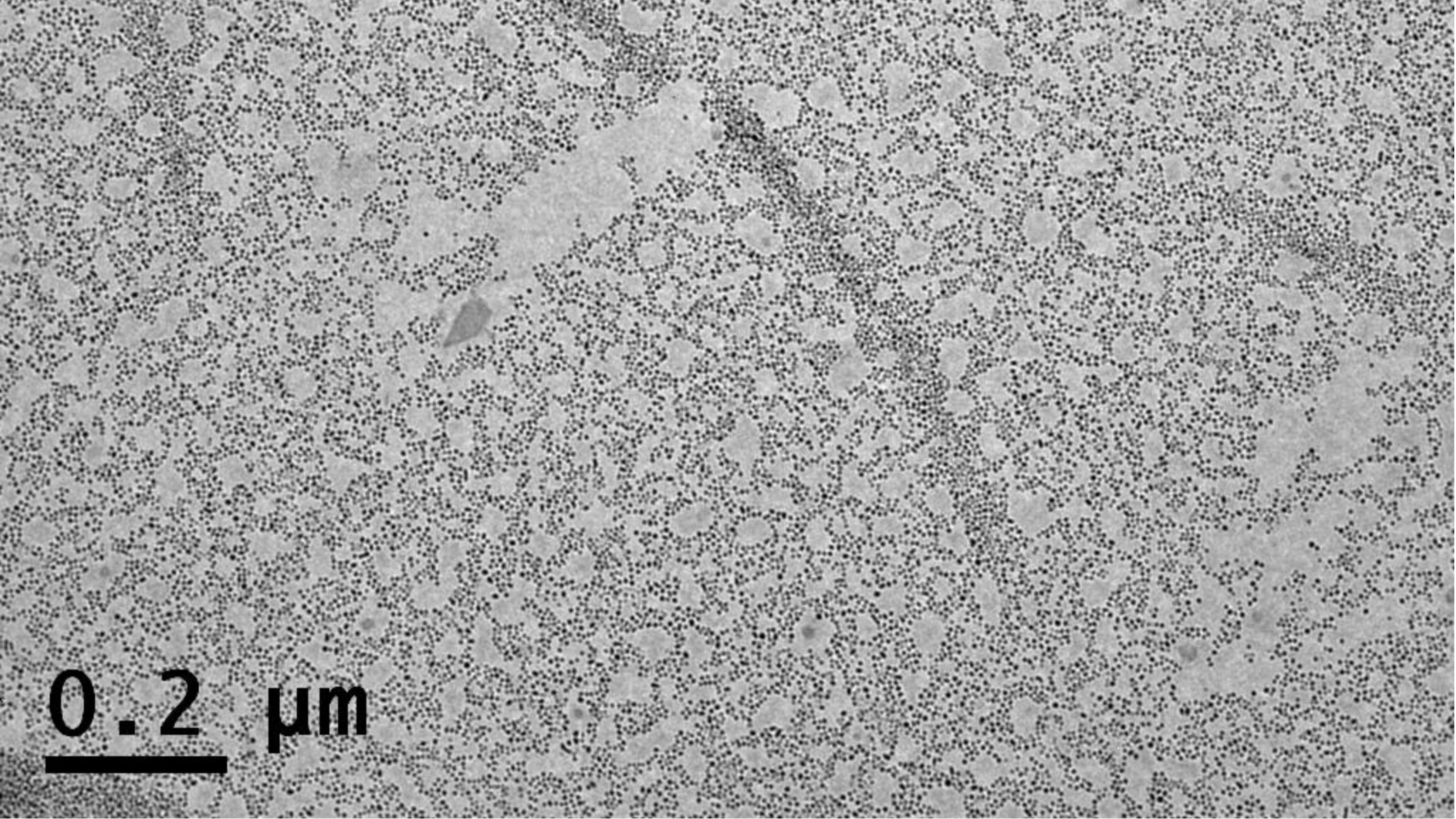
Jobin et. al. CPL, 2004

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

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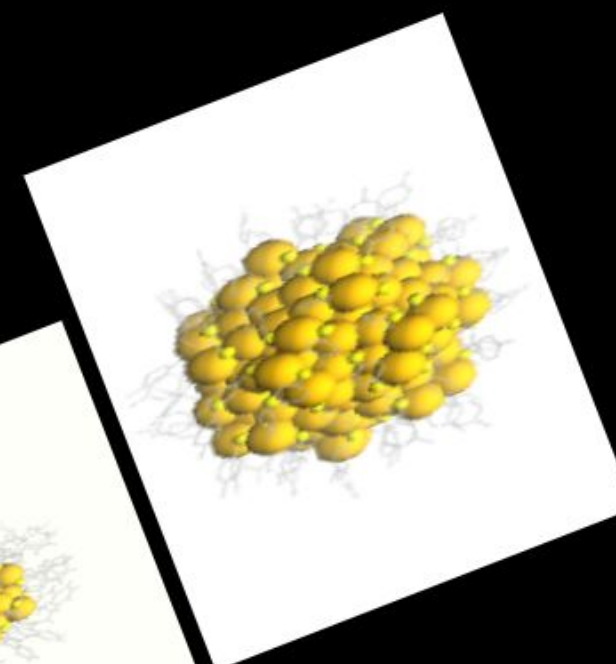
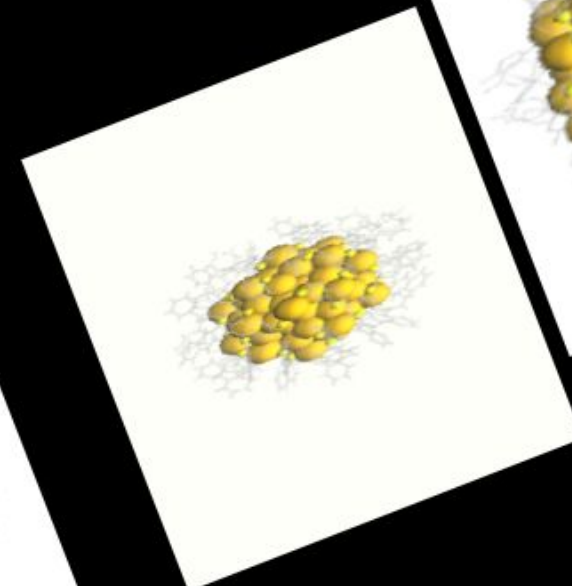
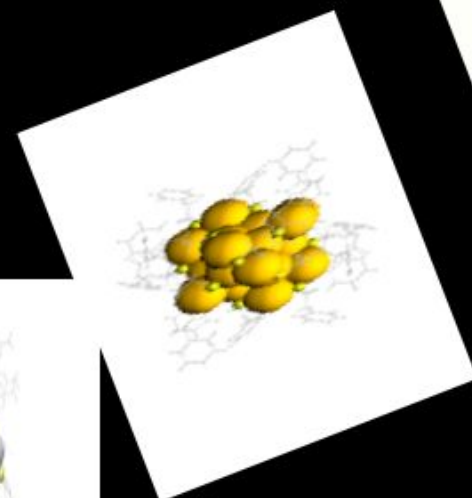
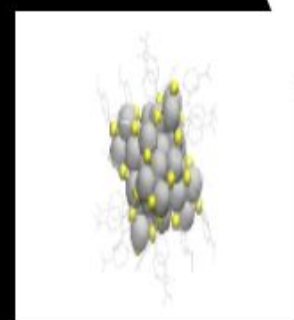


Terry Bigioni et al. *Nature* 2013



0.2 μm

Ag₂₉(BDT)₁₂₃⁸⁻ Ag₂₅(DMBT)₁⁻ 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

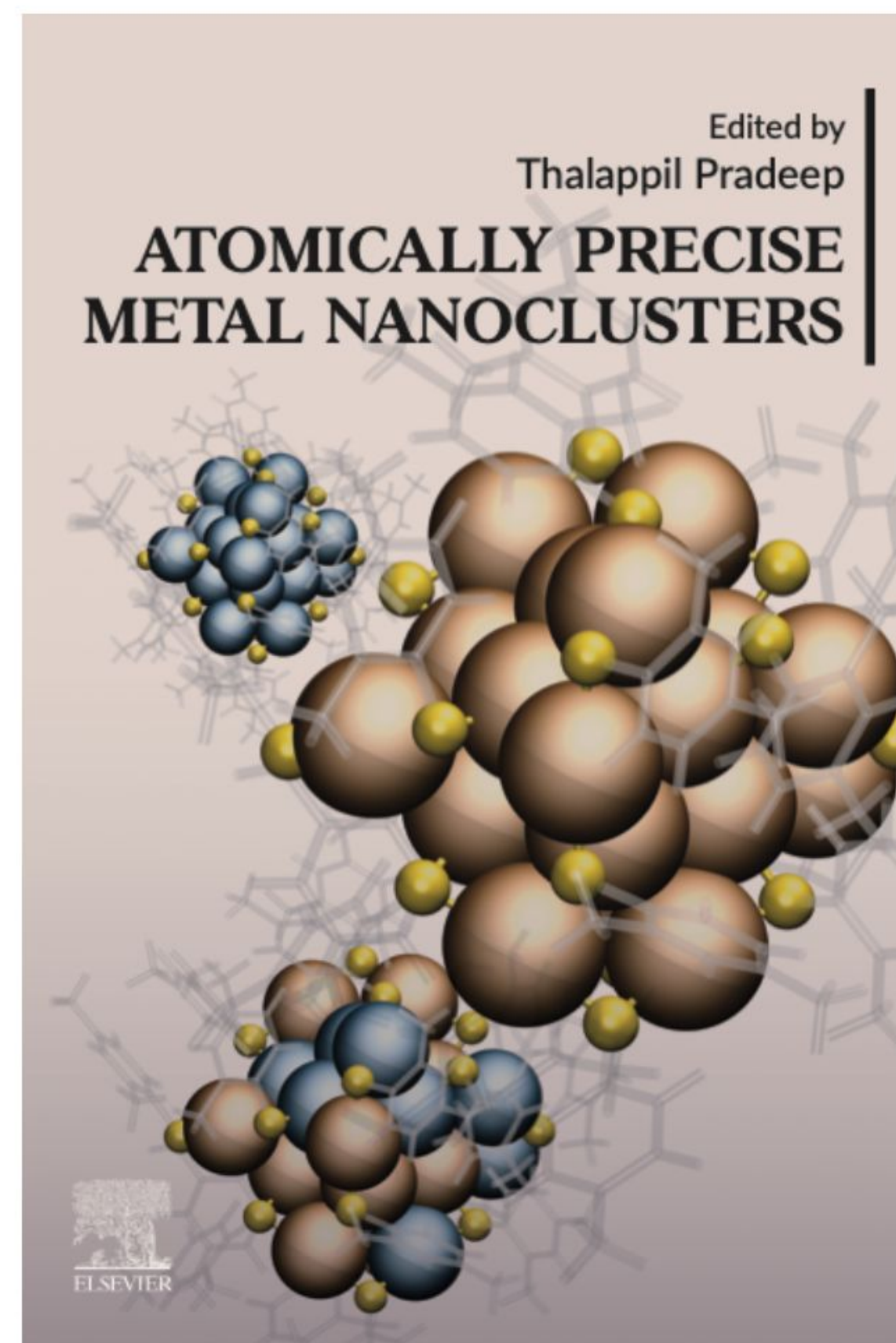
Physical properties

Electrical, magnetic

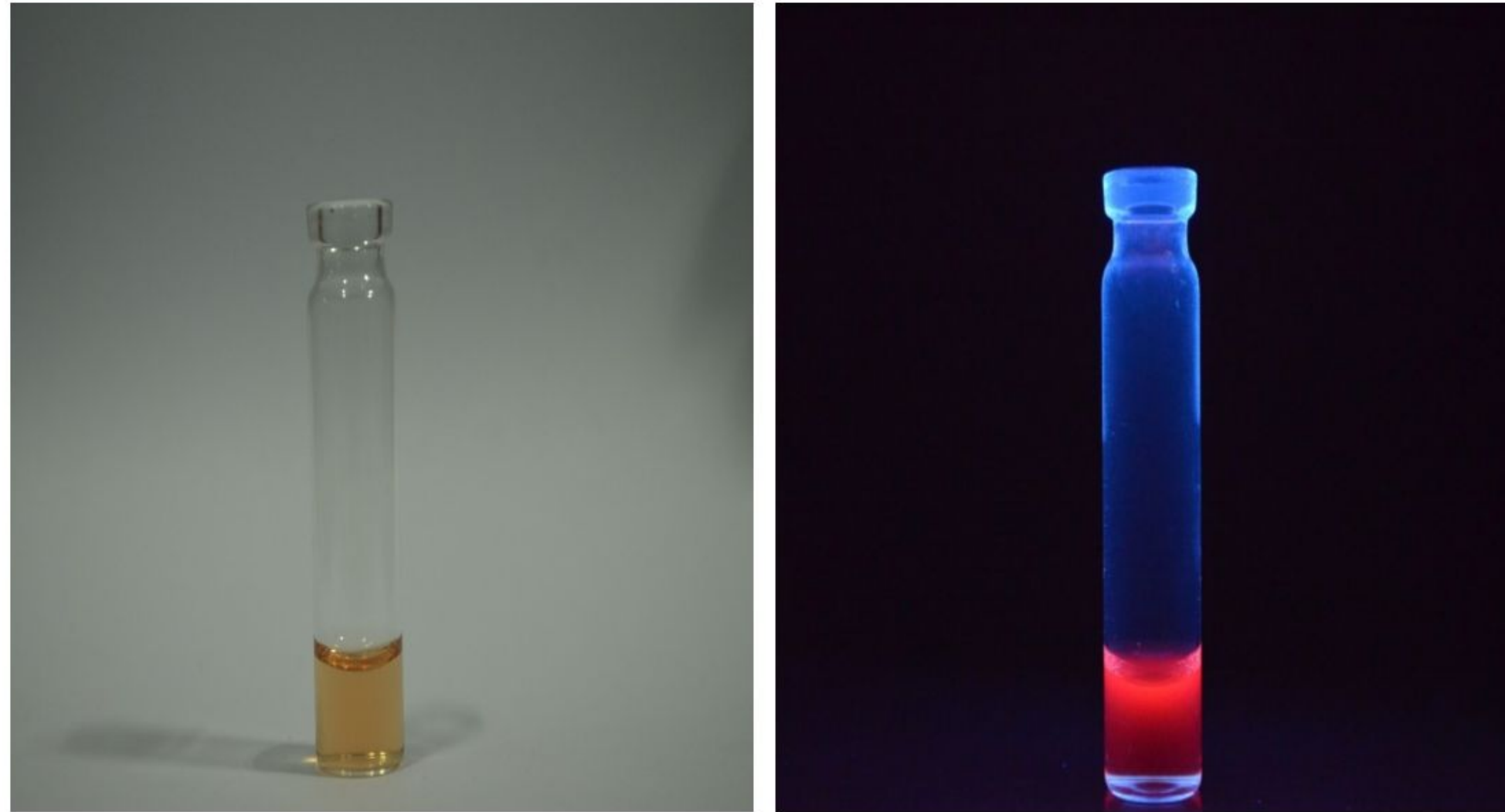
Mechanical properties

Electrochemical properties

Future?



Molecular reactions



Reactions on clusters

Reactions between clusters

Inter-cluster reactions



Article

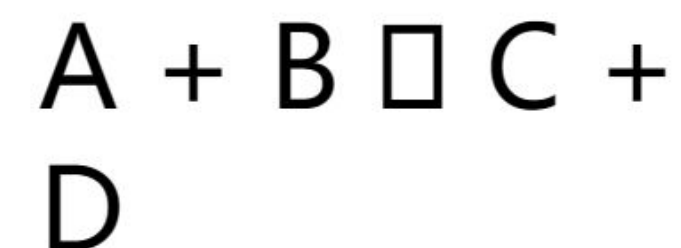
pubs.acs.org/JACS

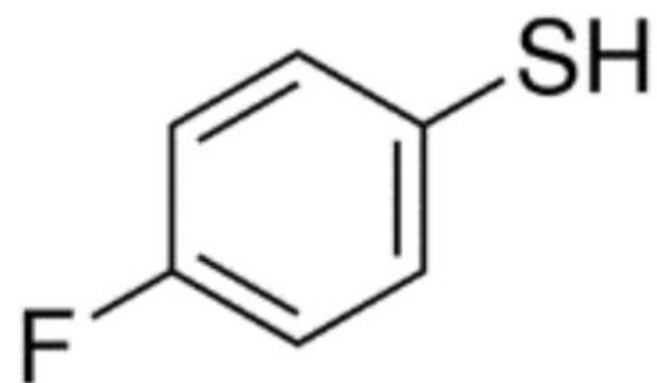
Intercluster Reactions between $\text{Au}_{25}(\text{SR})_{18}$ and $\text{Ag}_{44}(\text{SR})_{30}$

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

[Ag₂₅(DMBT)₁₈+Au₂₅(PET)₁₈]²⁻

DMBT

**PE
T**

**Ag₂₅(DMBT)
18**

[Ag₂₅(DMBT)₁₈+Au₂₅(PET)₁₈]²⁻

**Au₂₅(PET)
18**

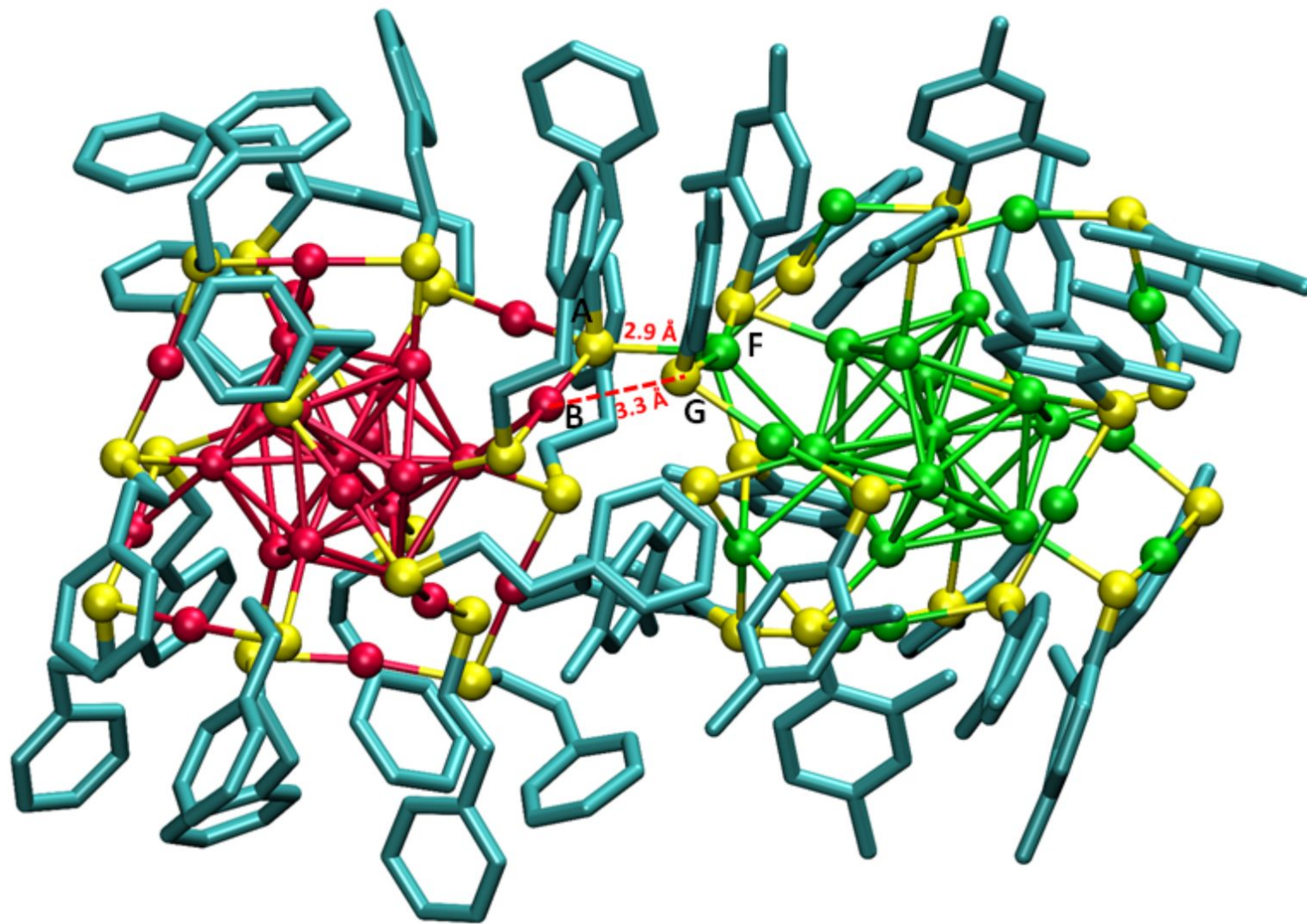
Evolution of alloy clusters from the dianionic adduct, [Ag₂₅Au₂₅(DMBT)₁₈(PET)₁₈]²⁻

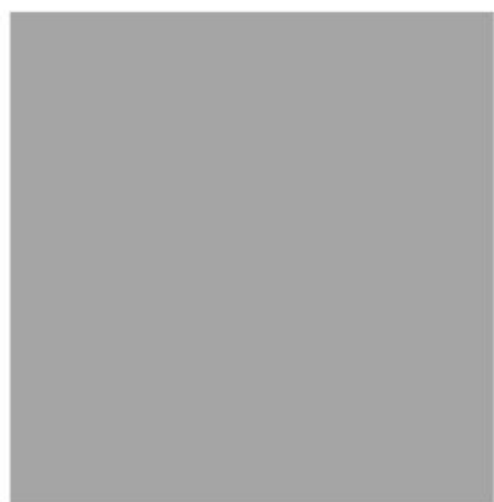
within 5 min

Ag₂₅(DMBT)₁₈:Au₂₅(PET)₁₈
0.3:1.0

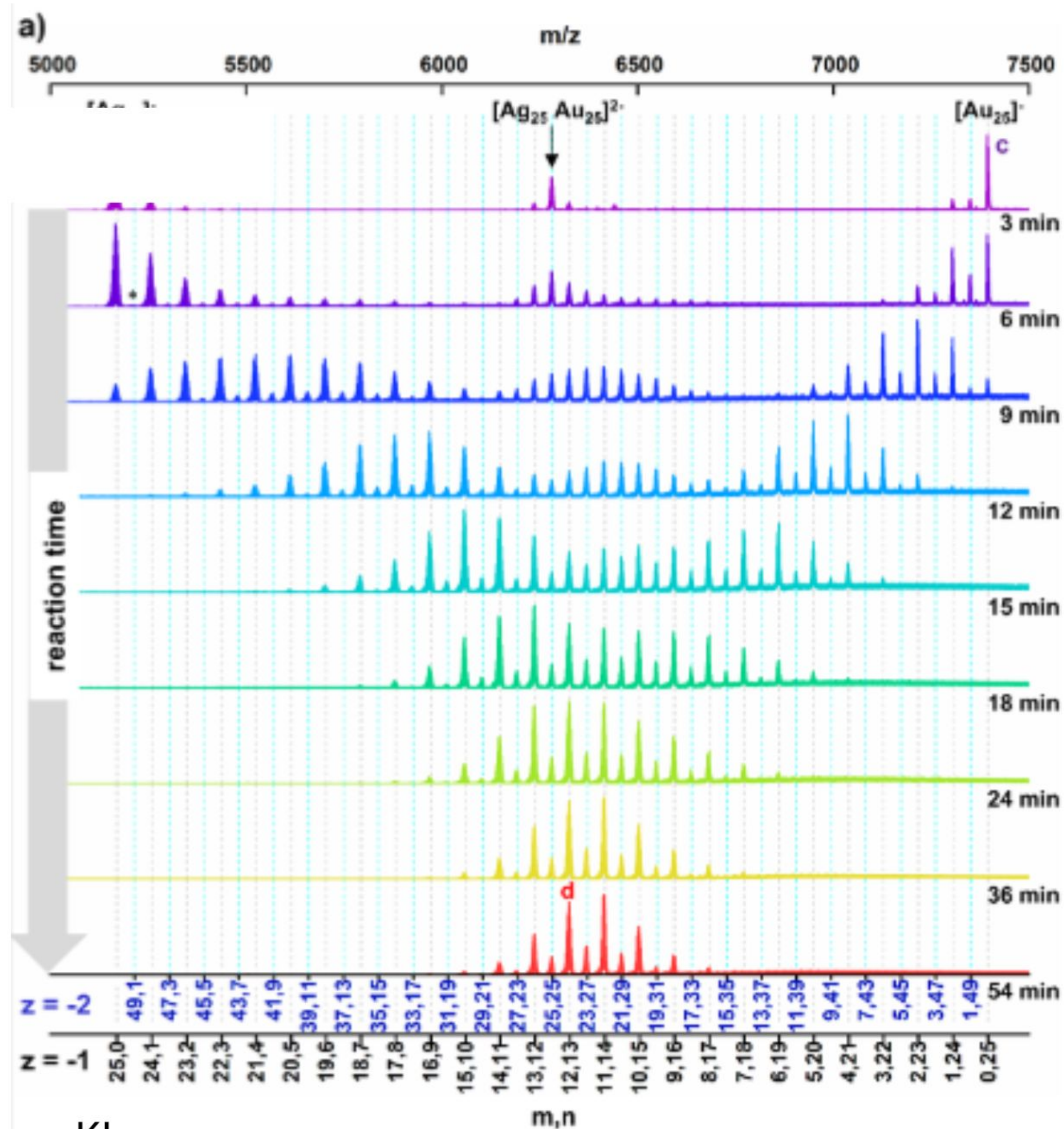
within 2 min

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





Complexities



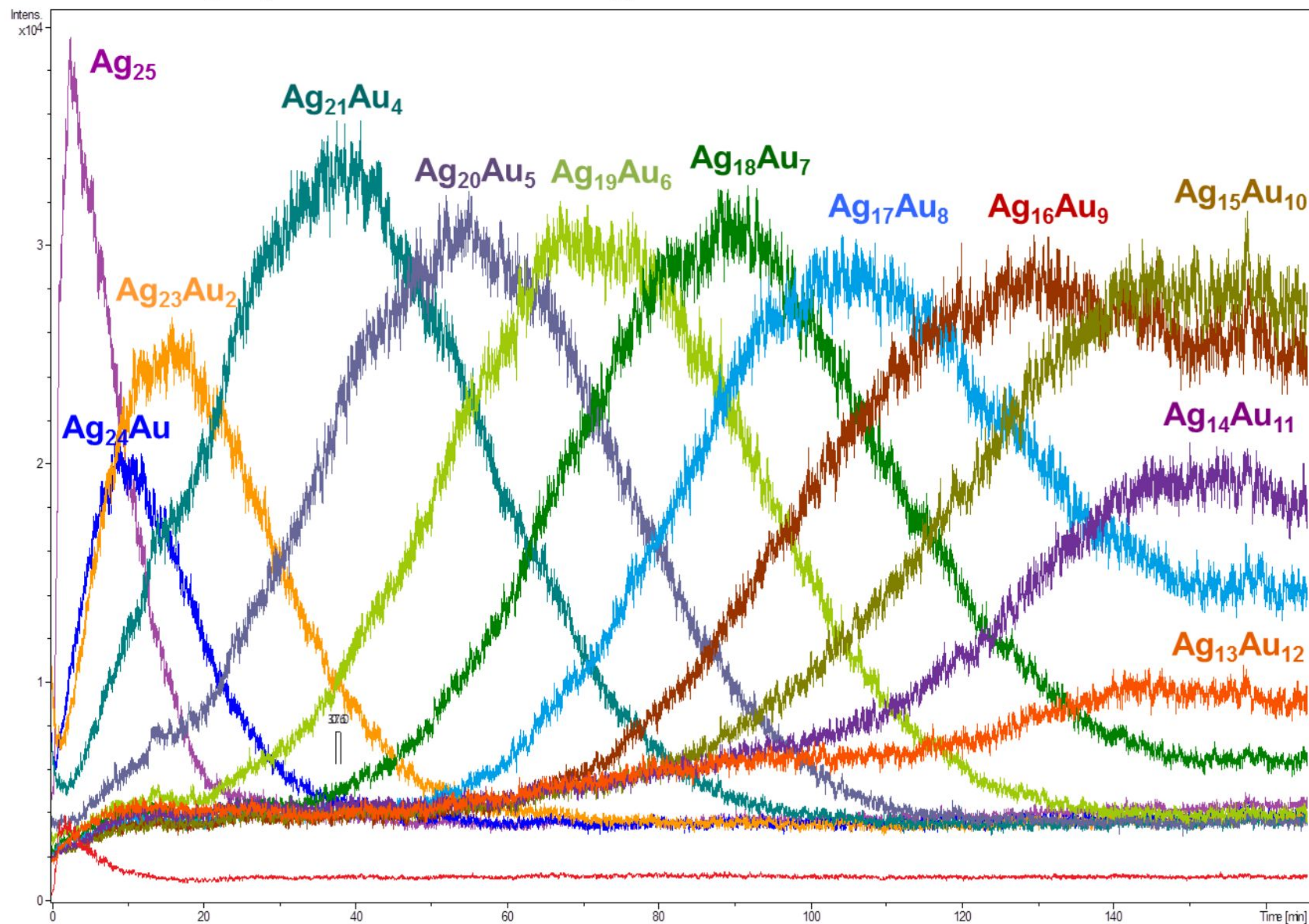
Manfred Kappes, KI
T

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

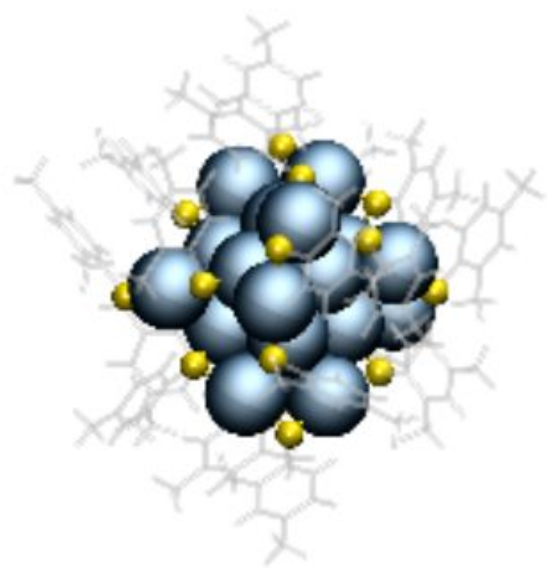
21

Kinetics of the exchange (monitored on the Ag25 sid

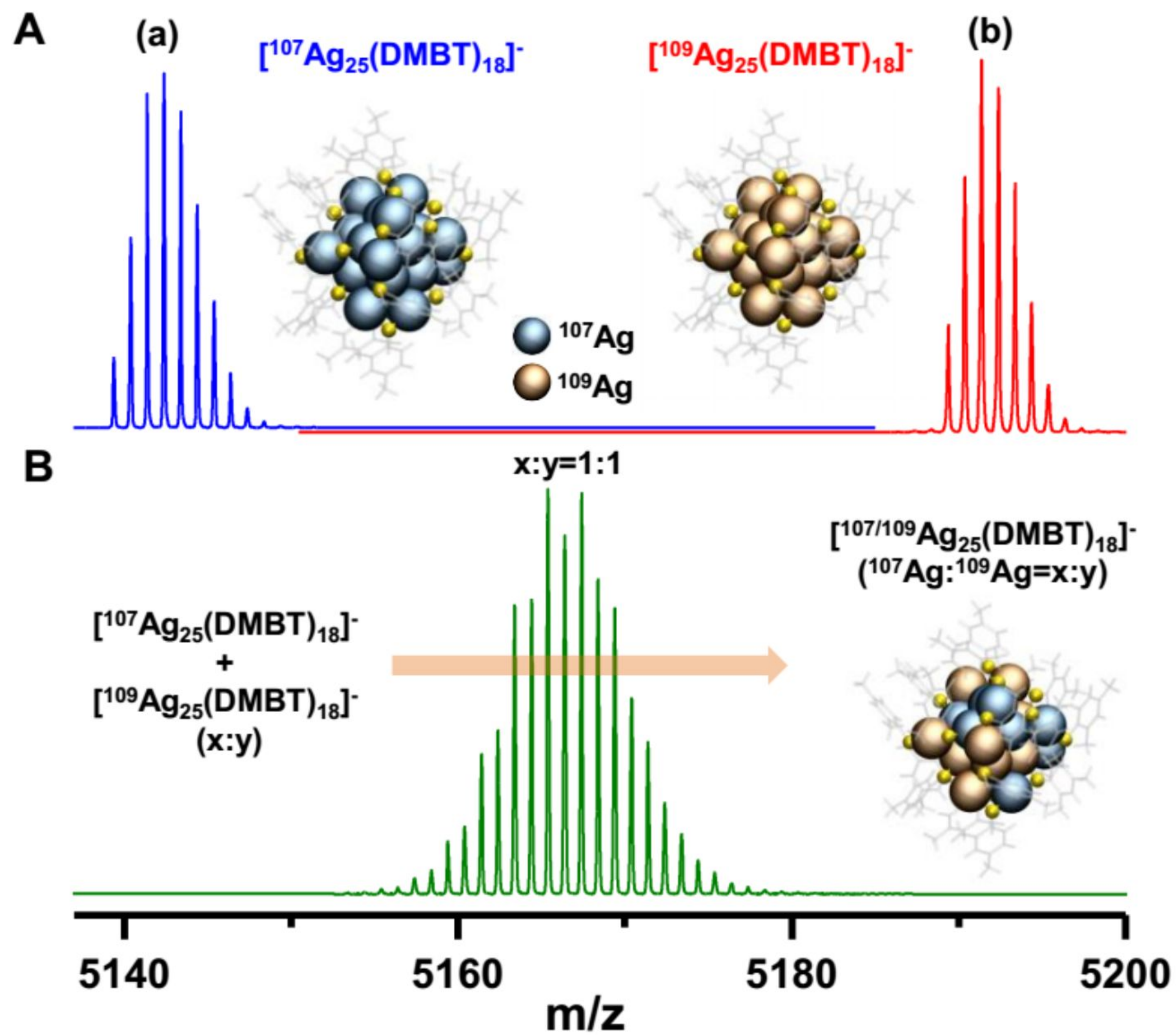
e)

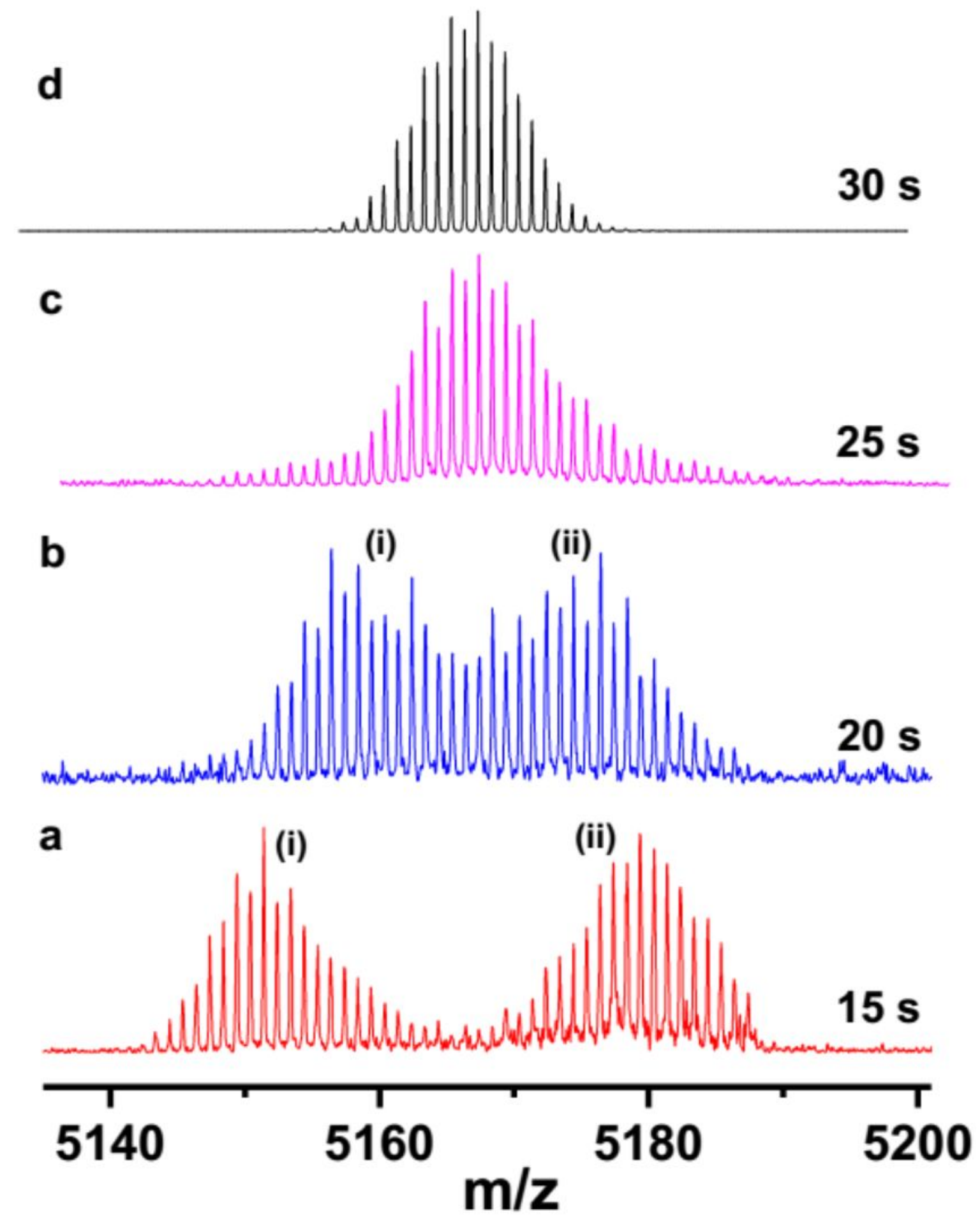


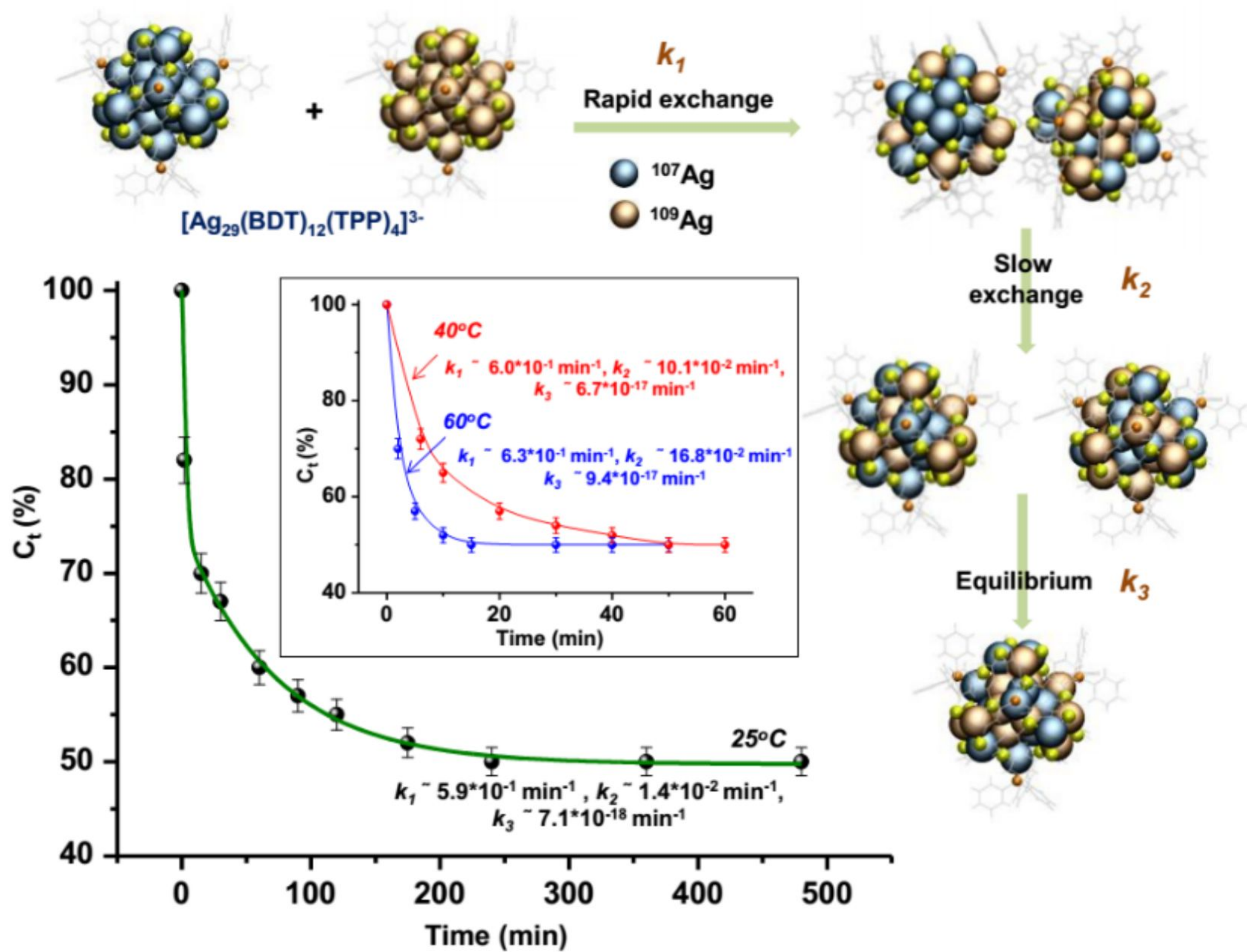
Coulomb adduc



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.





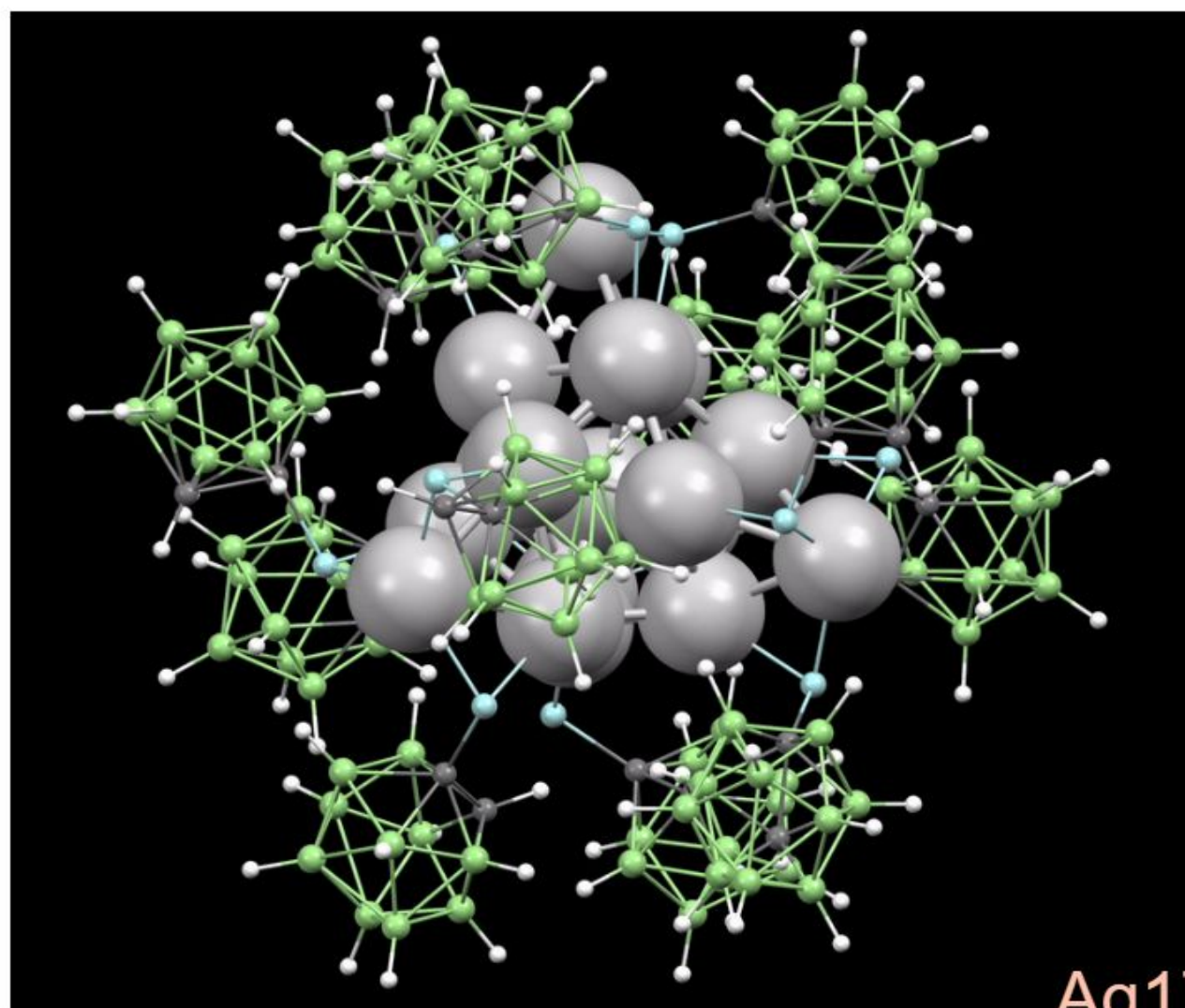


New materials and new properties

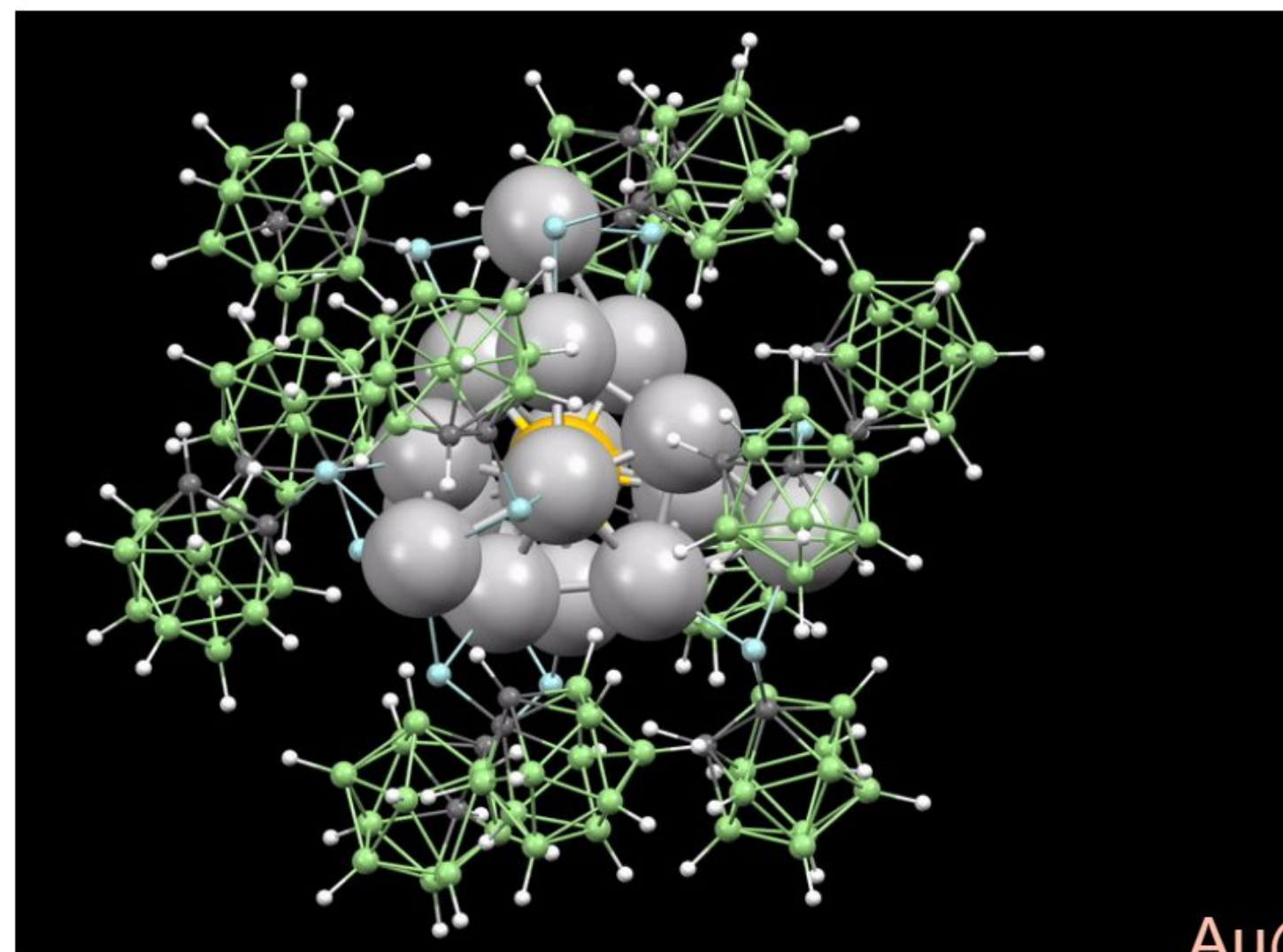
Ag₁₇ **AuAg₁₆** **Ag₁₃Cu₄** **AuAg**
12Cu₄

Vivek Yadav, et. al., *Nature Communications*, 2025

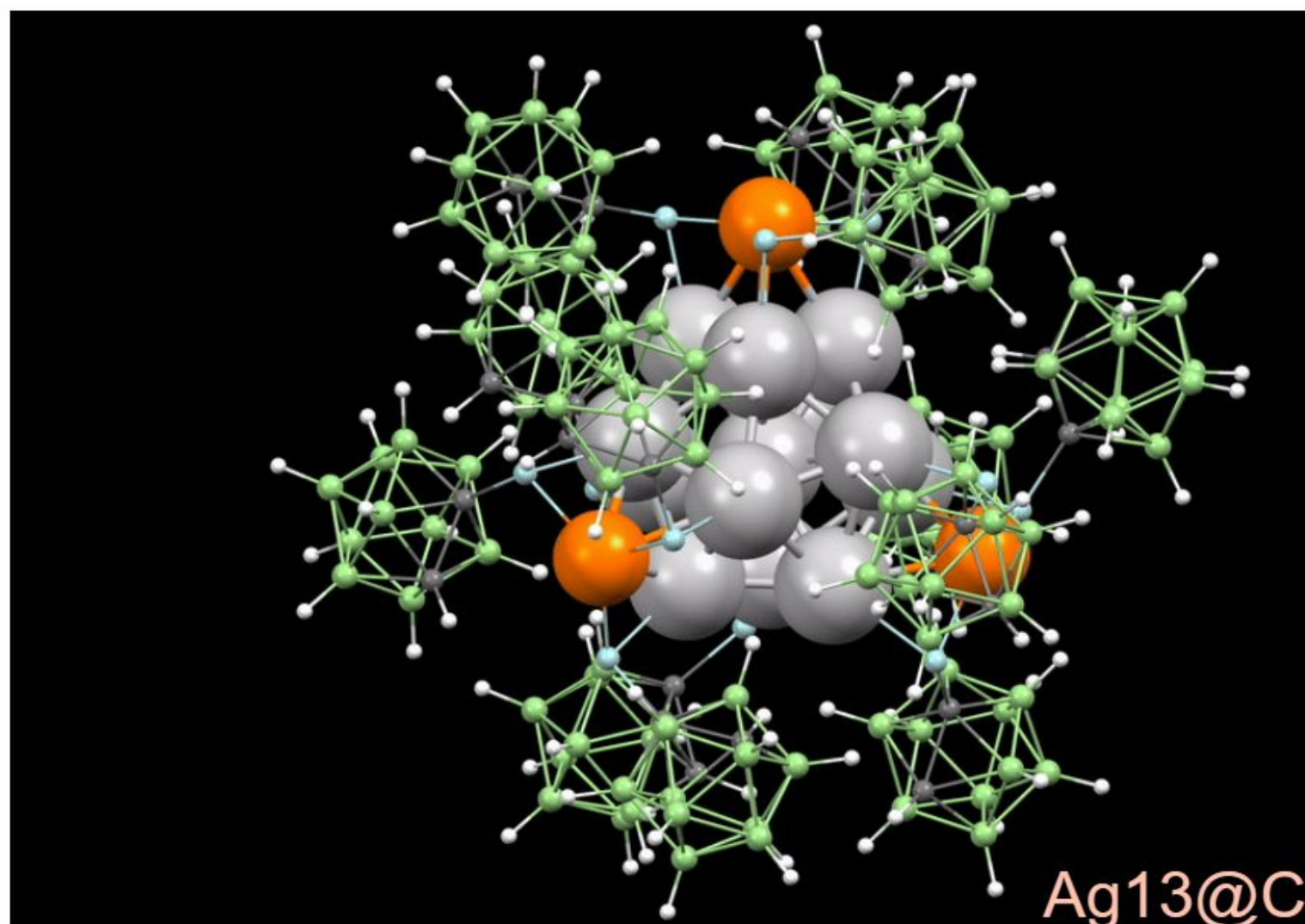
Structure of M17 Nanoclusters



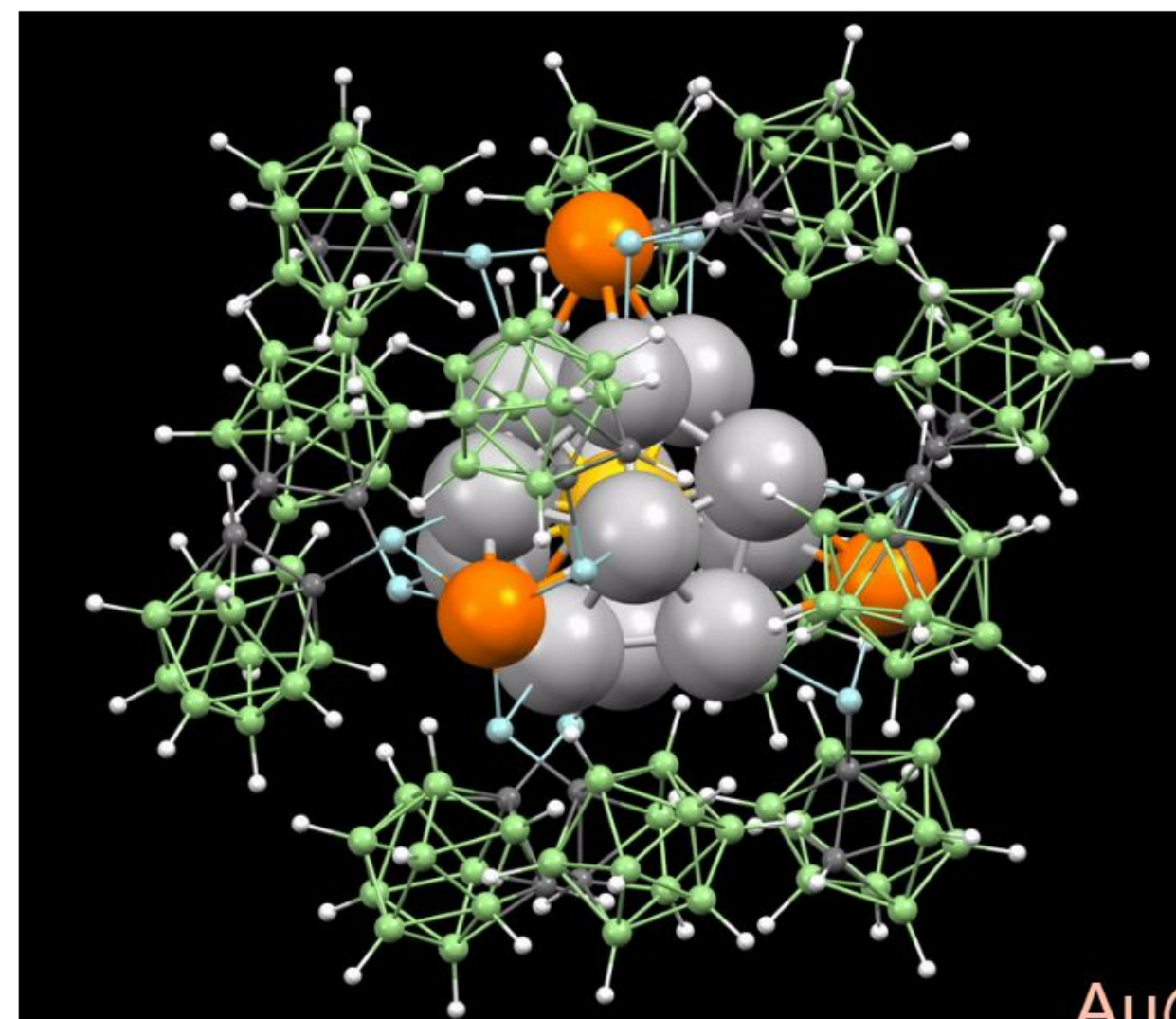
Ag₁₇



Au@Ag₁₆



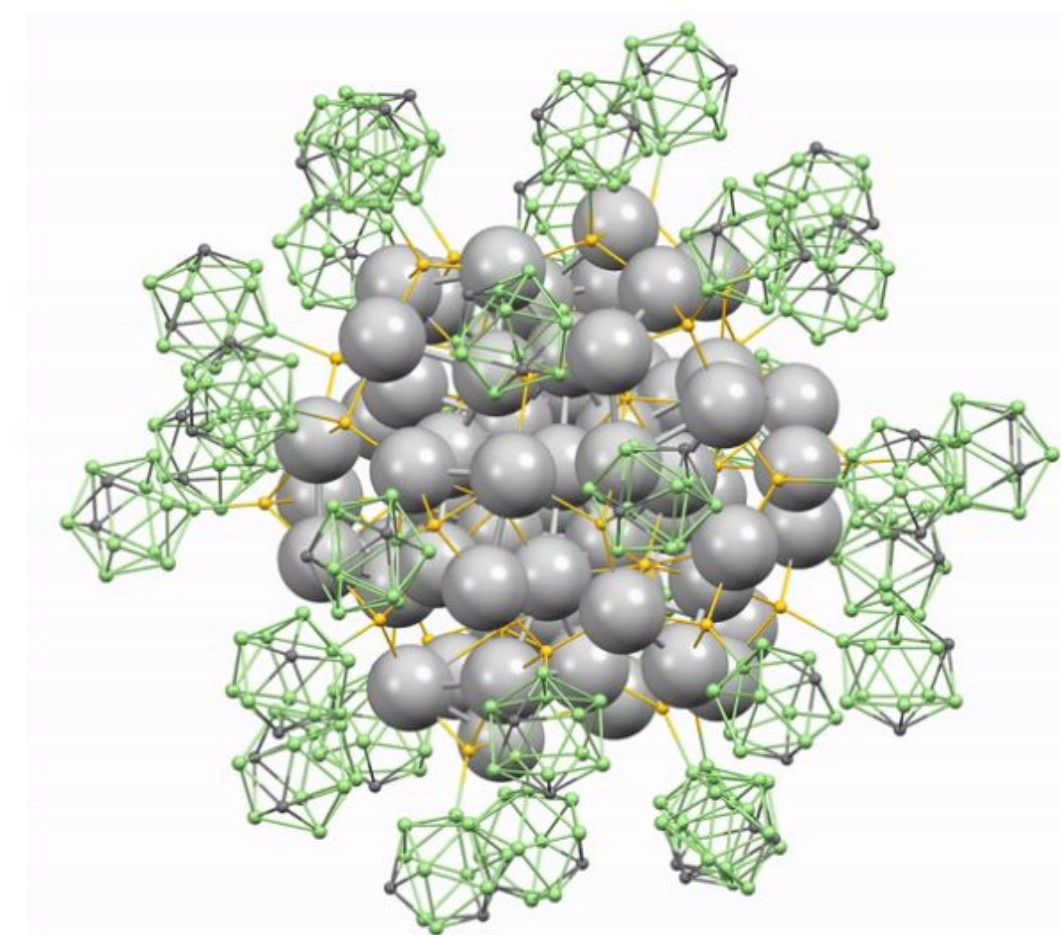
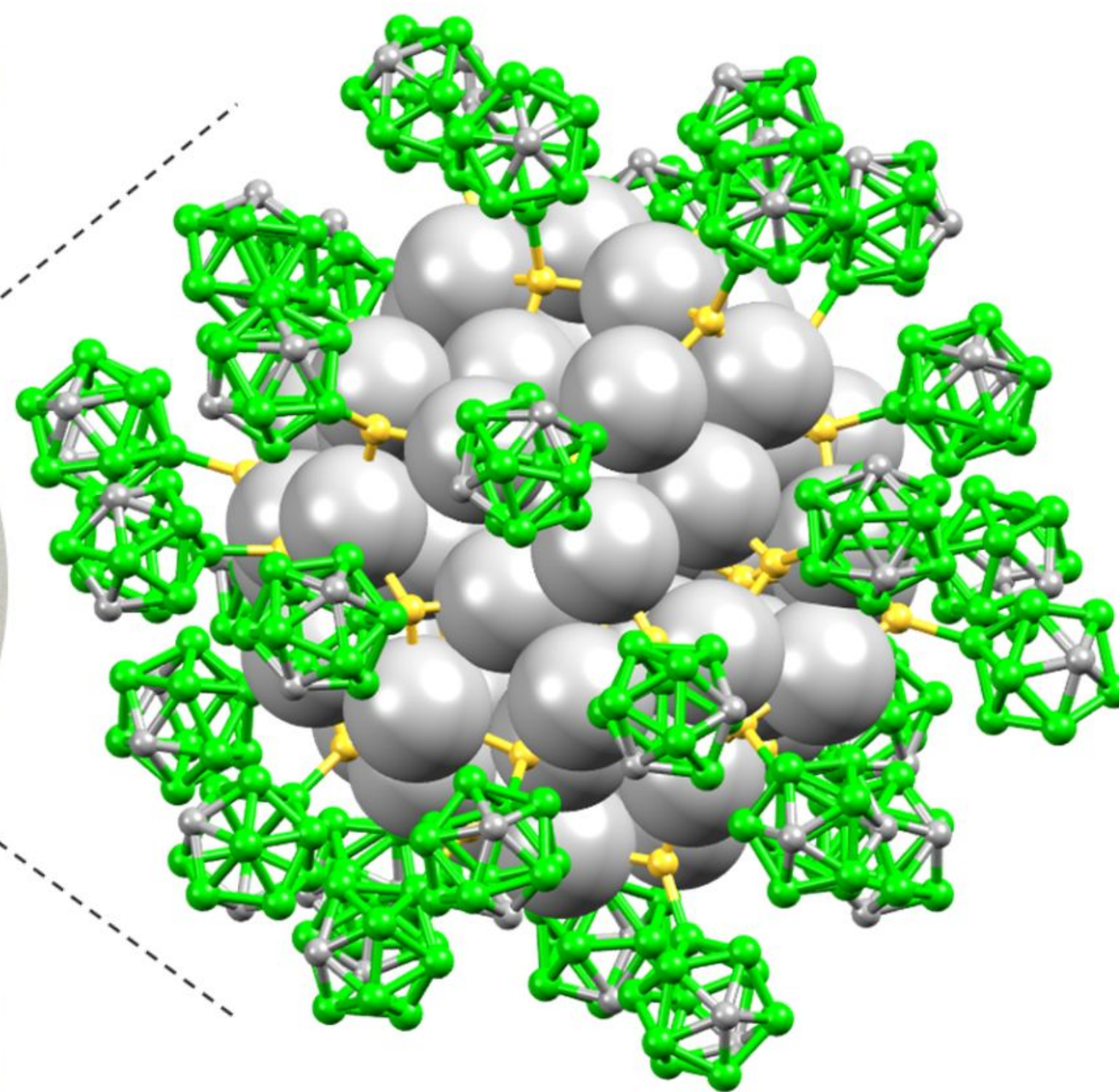
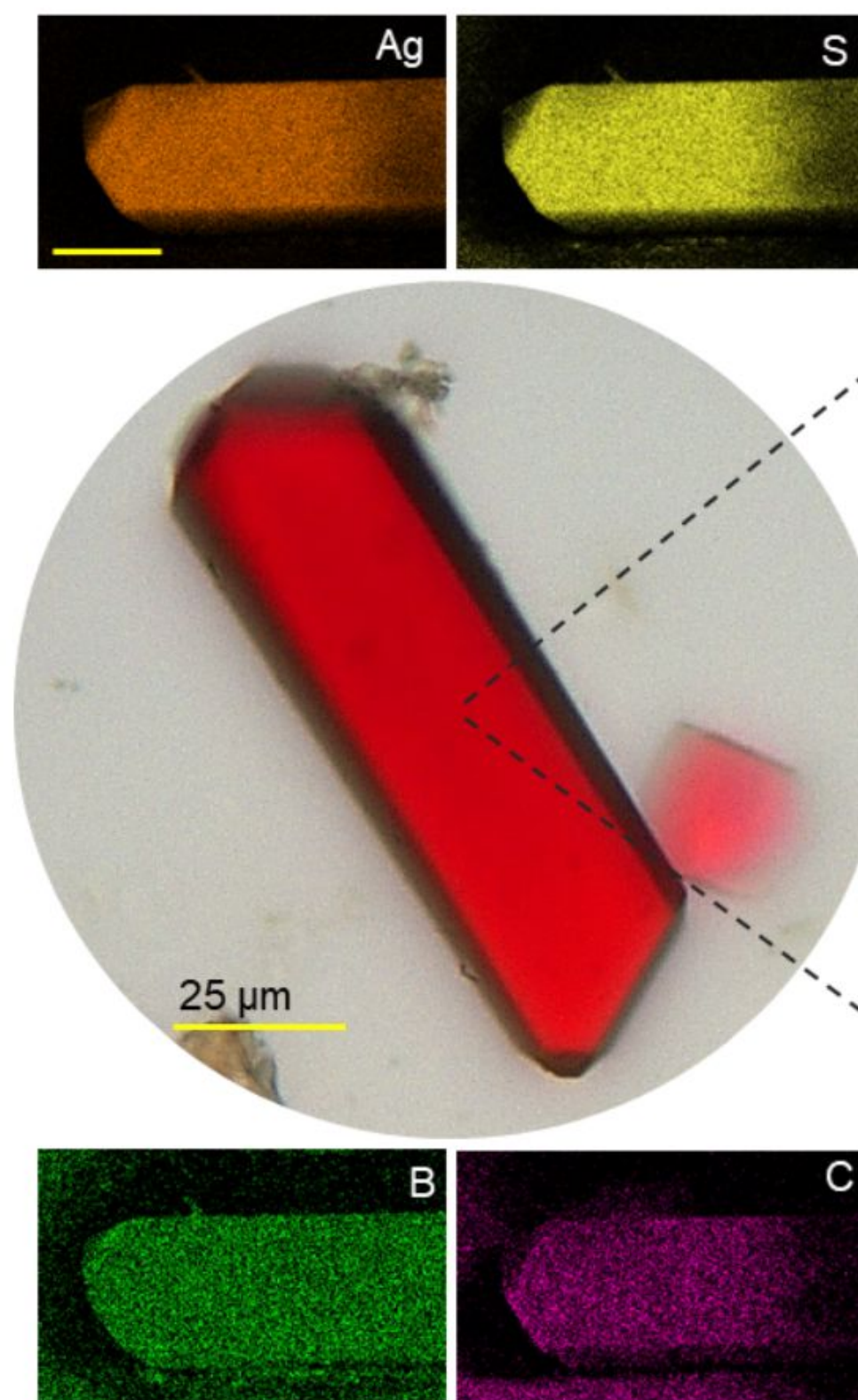
Ag₁₃@Cu



Au@Ag₁₂@Cu

Catalysis

[Ag₆₂S₁₂(CBT)₃₂] Nanocluster



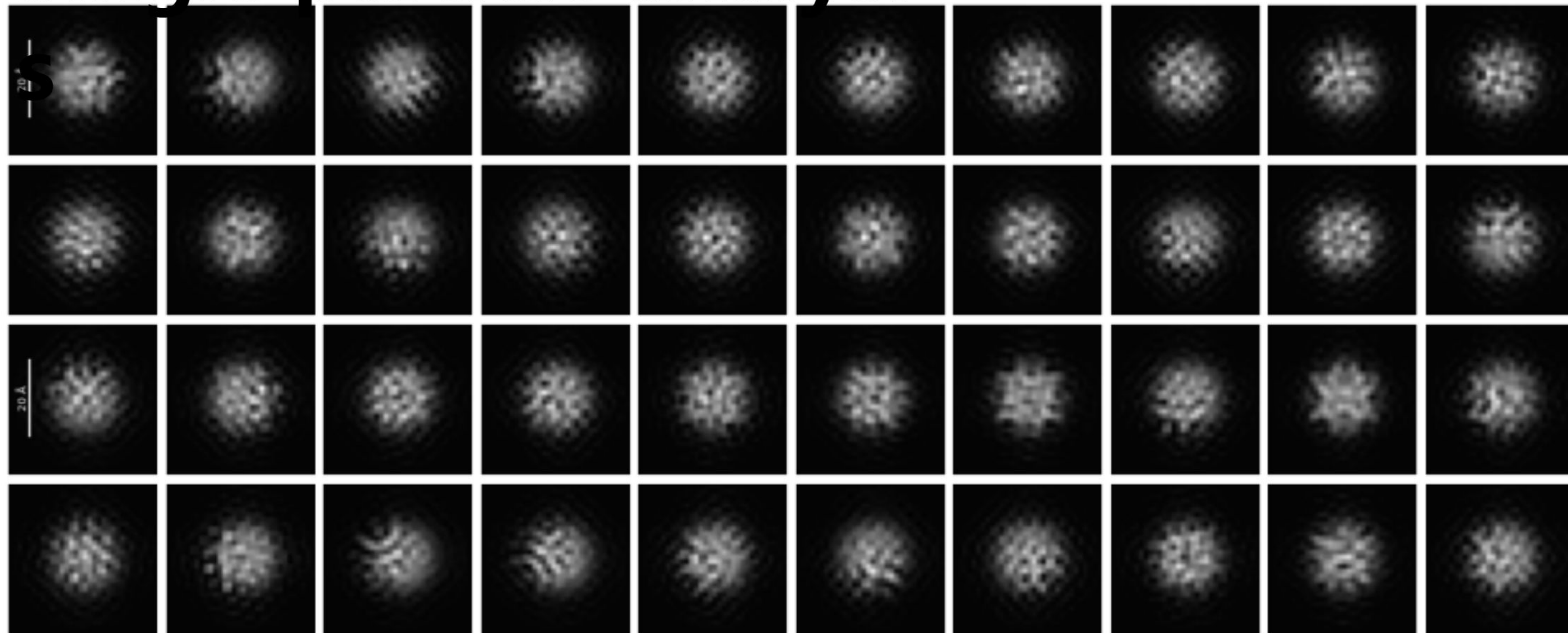
Largest molecule with carboranes so far

.....

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



Single particle analysis

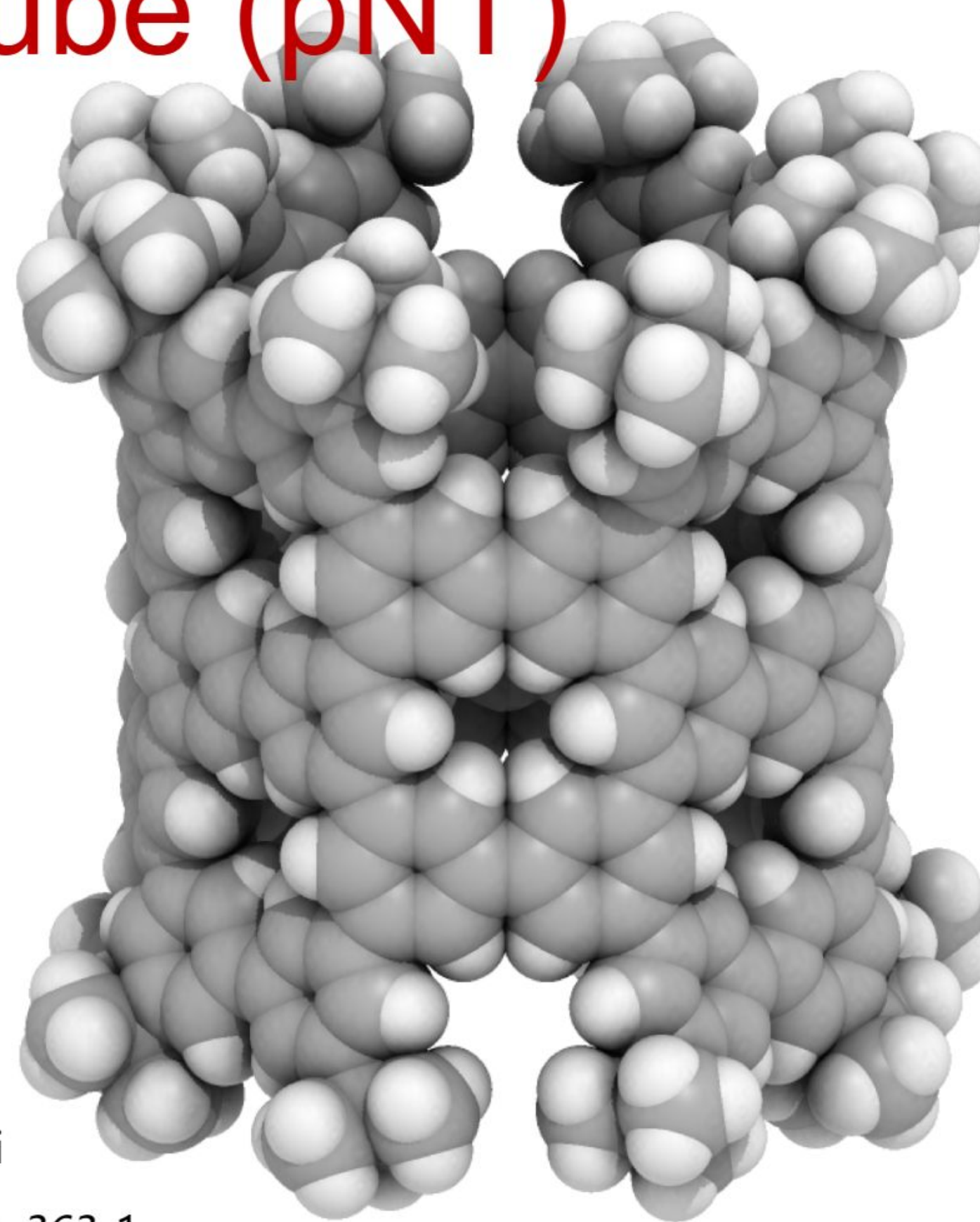
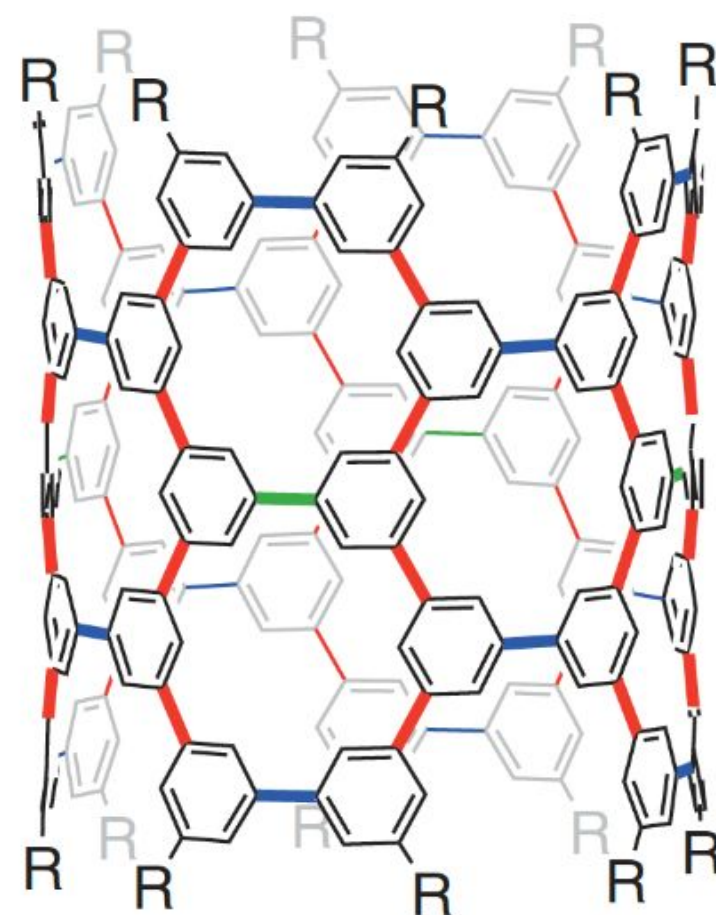
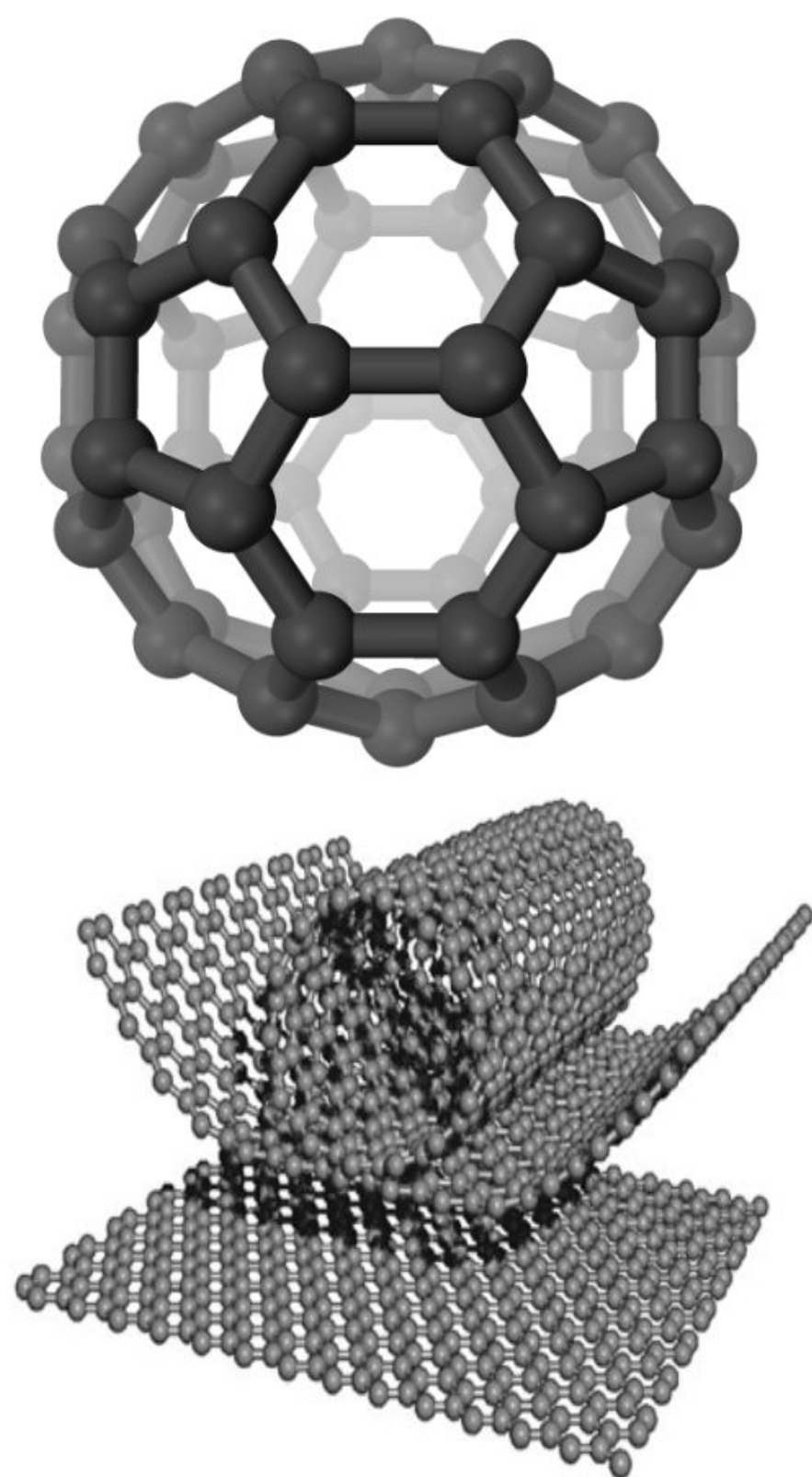


B. S. Sooraj, et. al. Unpublished

Power of chemistry - Anything can be made

Phenine nanotube (pNT)

Precision is at another level



— Yamamoto coupling
— Suzuki-Miyaura coupling
— Bäurle/Yamago/Isobe coupling
ng H. Isobe *et al. Science* **2019**, 363, 1
51

Clean water for all



ACS Sustainable Chemistry & Engineering Editorial, December 2016

Water positive materials

PNAS PNAS PNAS

Biopolymer-reinforced synthetic granular nanocomposites for affordable water purification

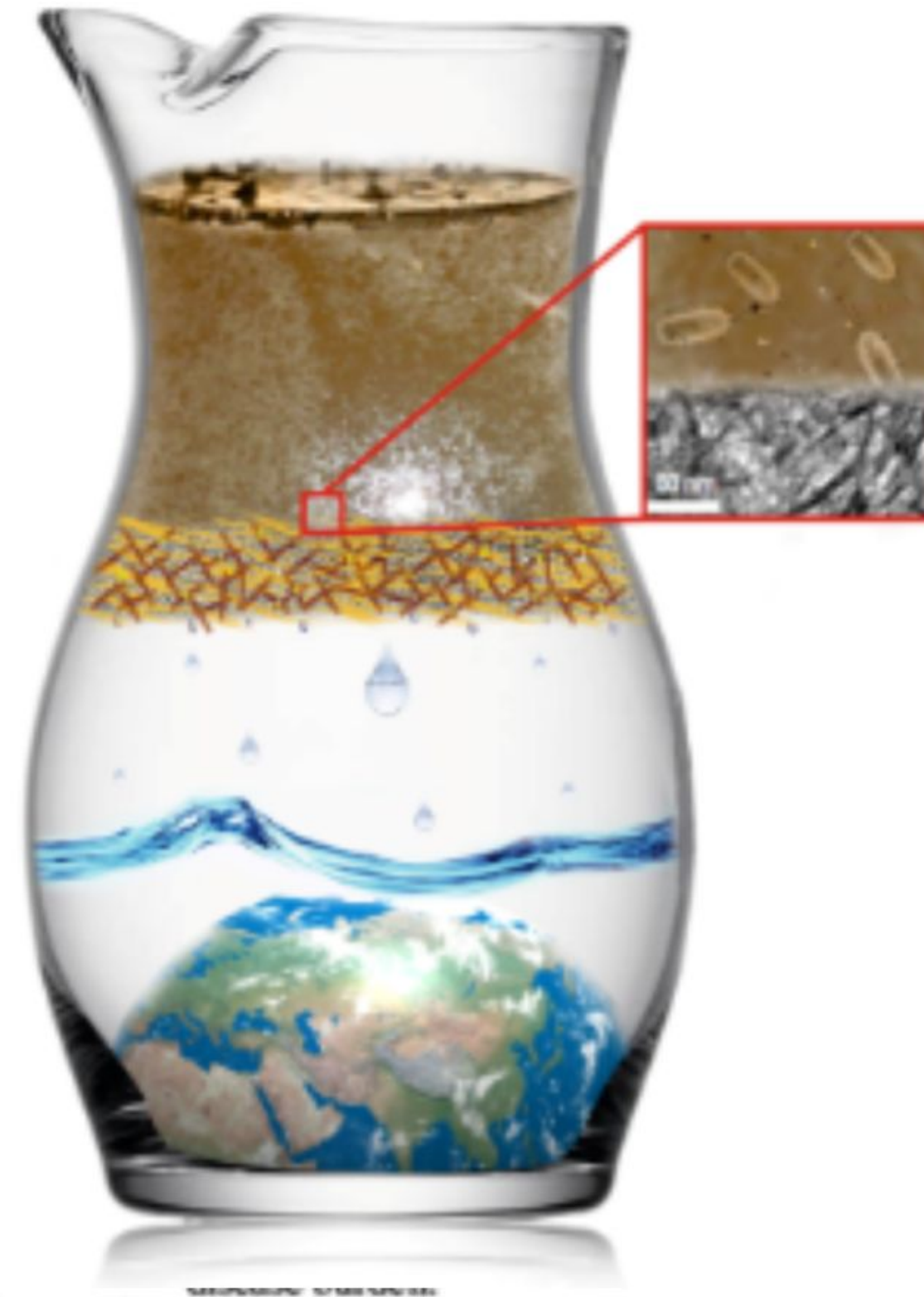
Mohan Udhaya Sankar¹, Sahaja Aigal, Kamalesh Chaudhari, and Thalappil Pradeep

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 materials can be synthesized in a simple and effective fashion without the use of electrical power. The nanocomposites exhibit 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 helped in the crystallization of strong covalent bonds. X-ray photoelectron spectroscopy confirmed the composition is rich in oxygen. Further, the high-resolution transmission electron microscopy confirmed the presence of nanoparticles. The water purifier developed that can demonstrate an affordable water purifier for rural areas in India, as the waterborne

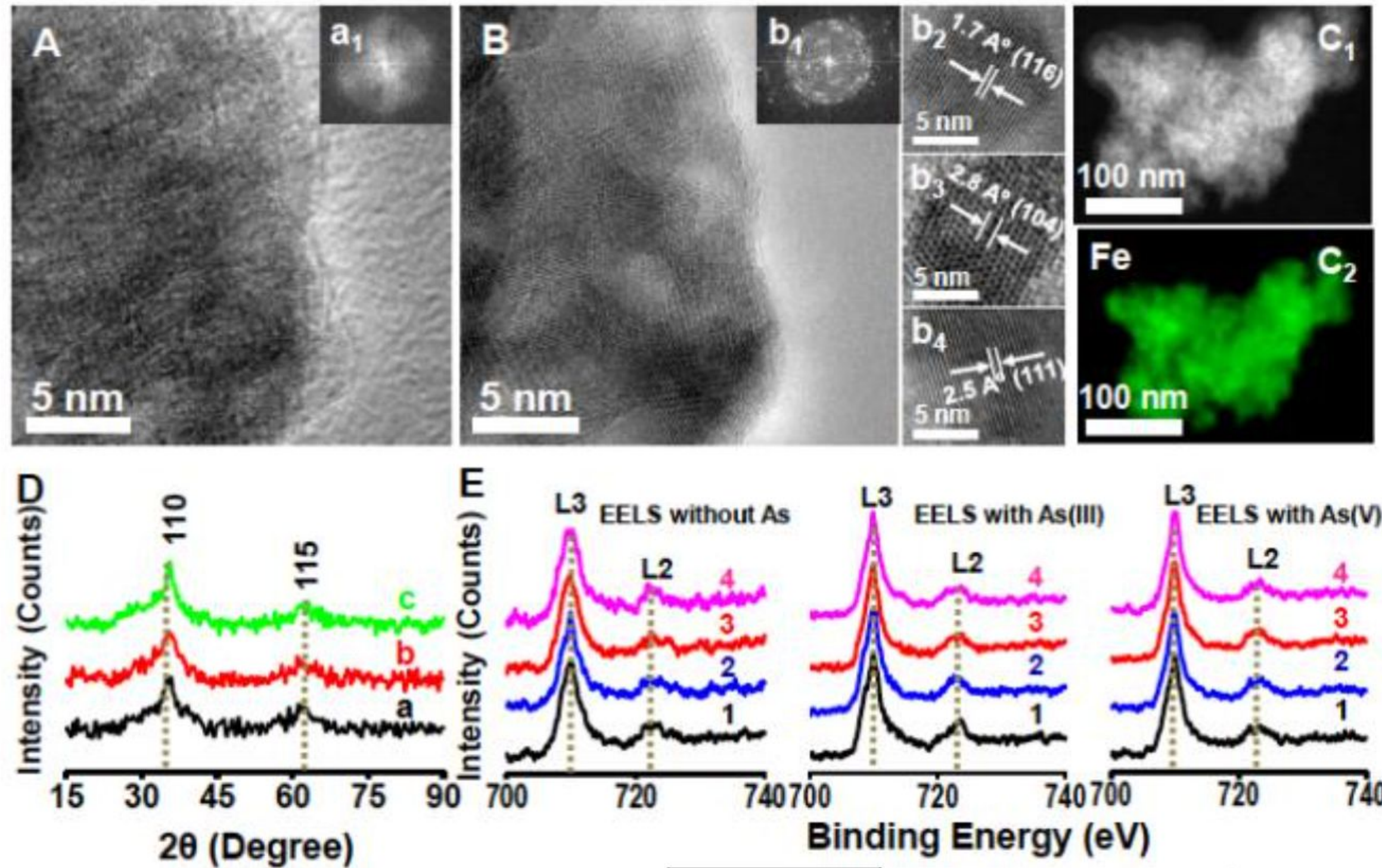
How to make?

What is special?

Live/dead staining experiments

No nanotoxicity

Variety of materials



www.advmat.de

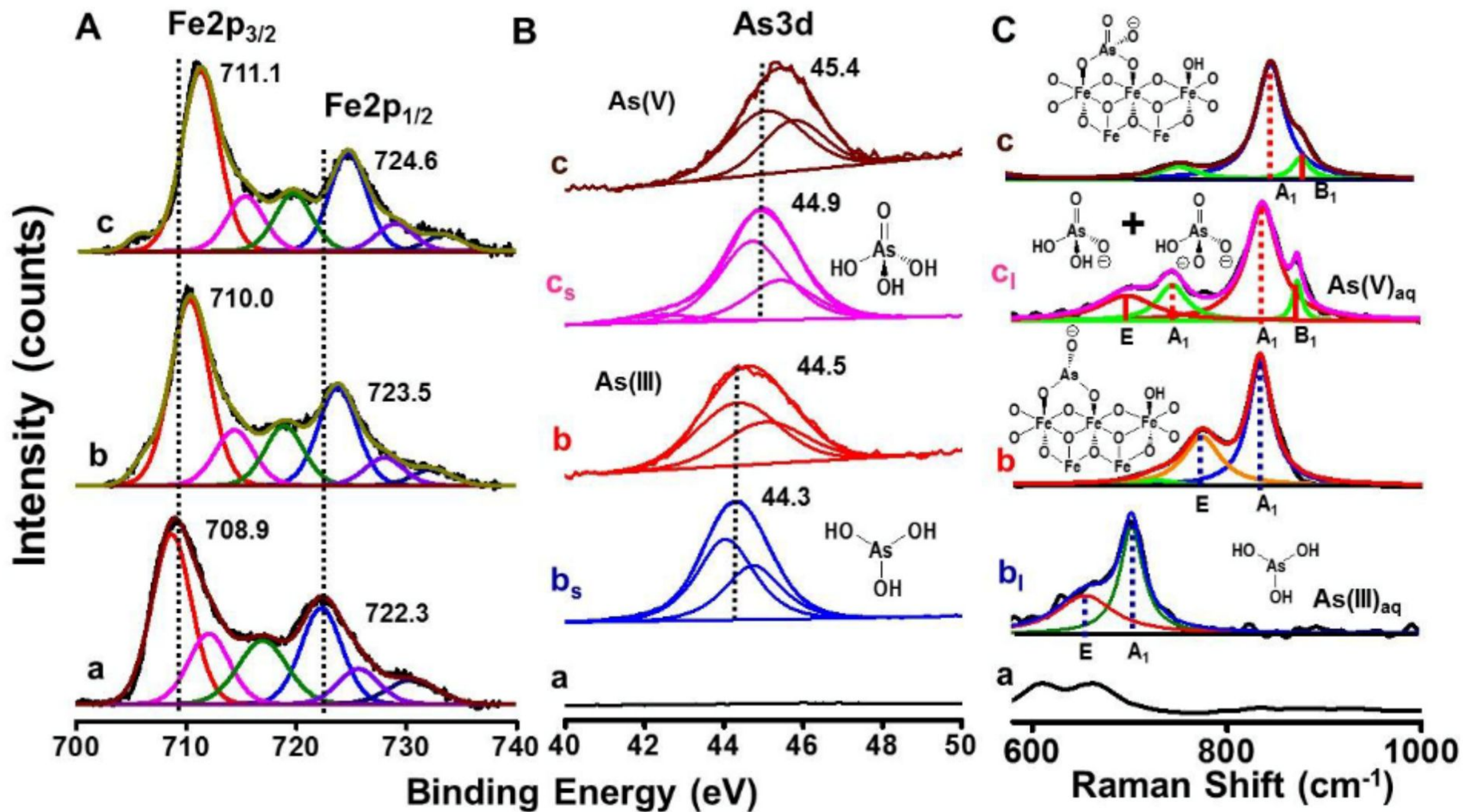
Author Pr ⁶ ADVANCED MATERIALS

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

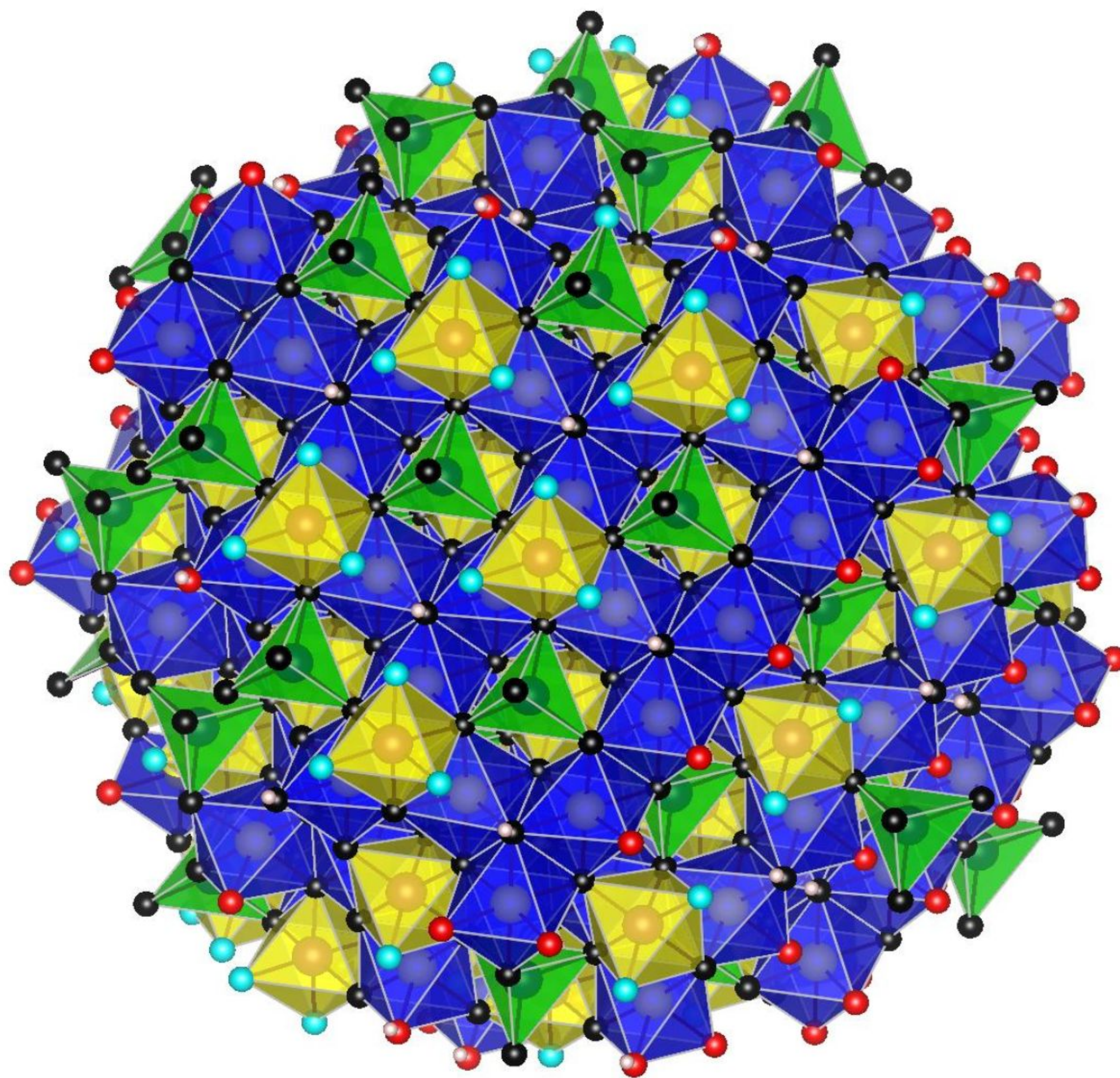
By Avula Anil Kumar, Anirban Som, Paolo Longo, Chennu Sudhakar, Radha Gobinda Bhuin, Soujit Sen Gupta, Anshup, Mohan Udhaya Sankar, Amrita Chaudhary, Ramesh Kumar, and T. Pradeep*

Communication

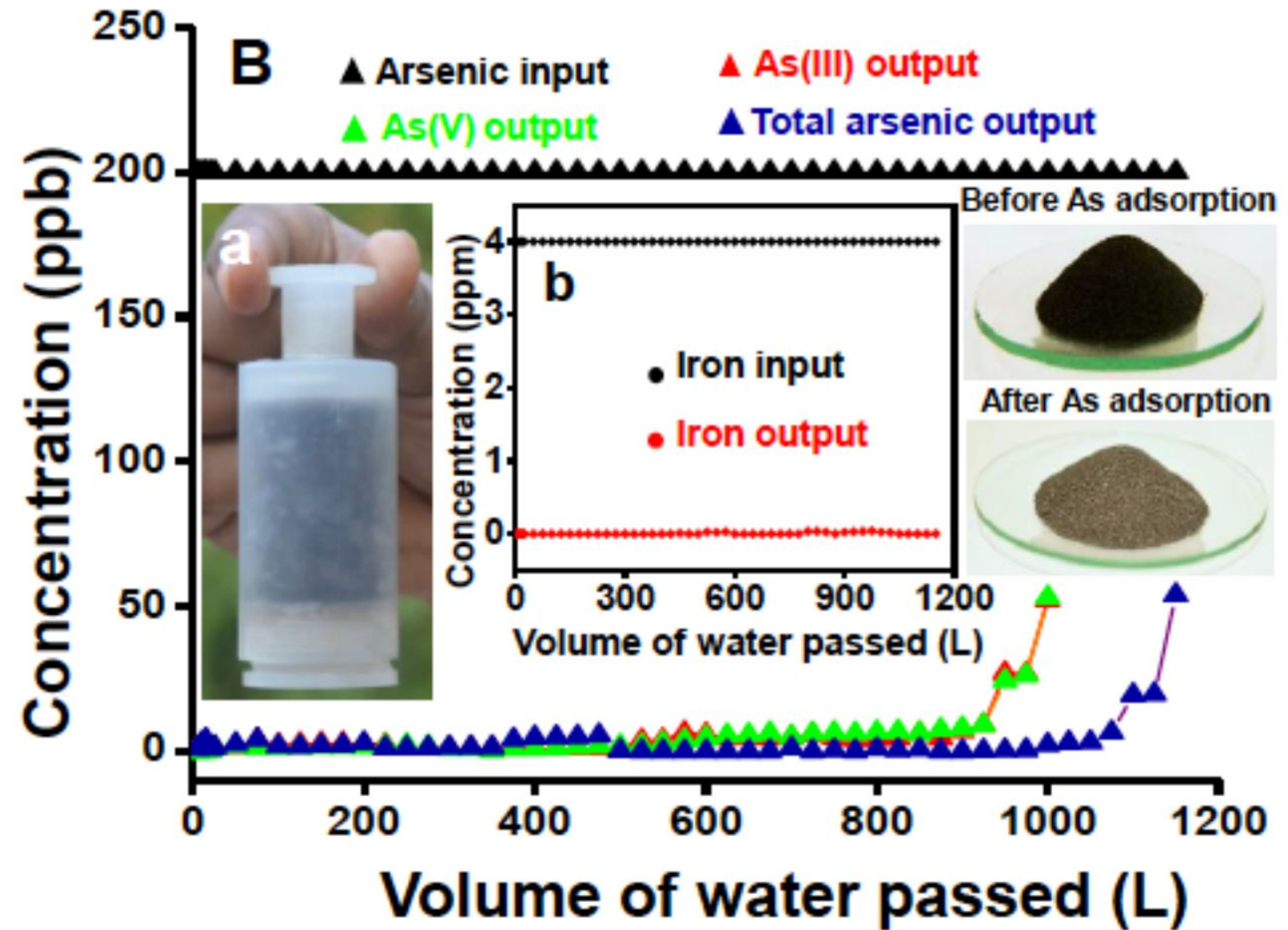
Mechanism – molecular tools



Modeling surfaces



Lab studies



Initial pilot studies



Implementation - From 25 KLD to 1 MLD



Large water supply schemes
Capacity: above 1 MLD

5 schemes in use across India



Retrofitted Water Purification Plant
Capacity: 0.1-1 MLD

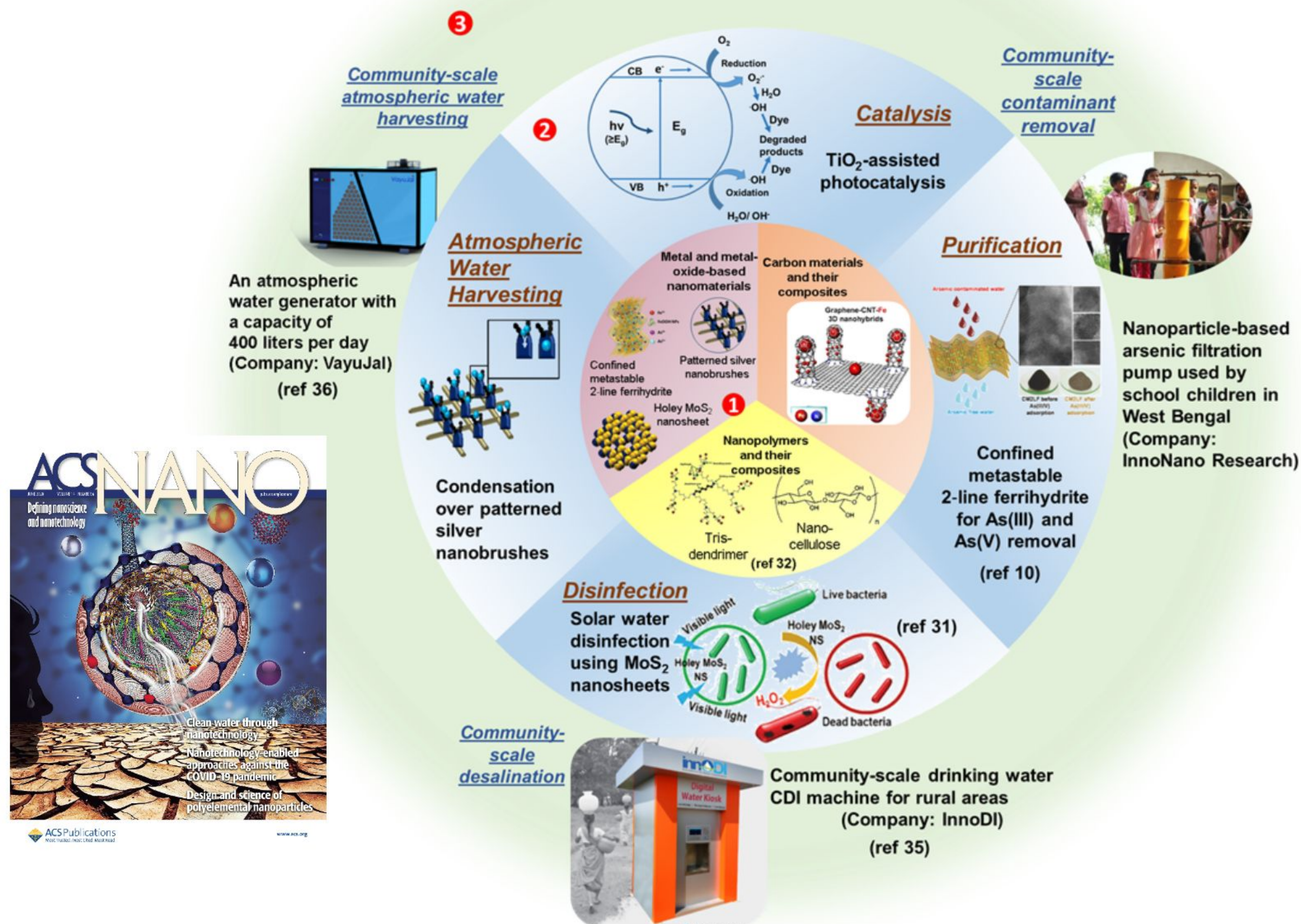
Over 180 units in use across India

Now they are across the countr



Smart water purifiers and big data

Evolution of materials to products





Water that Heals

A TRAVELOGUE



a SURESH MENON film

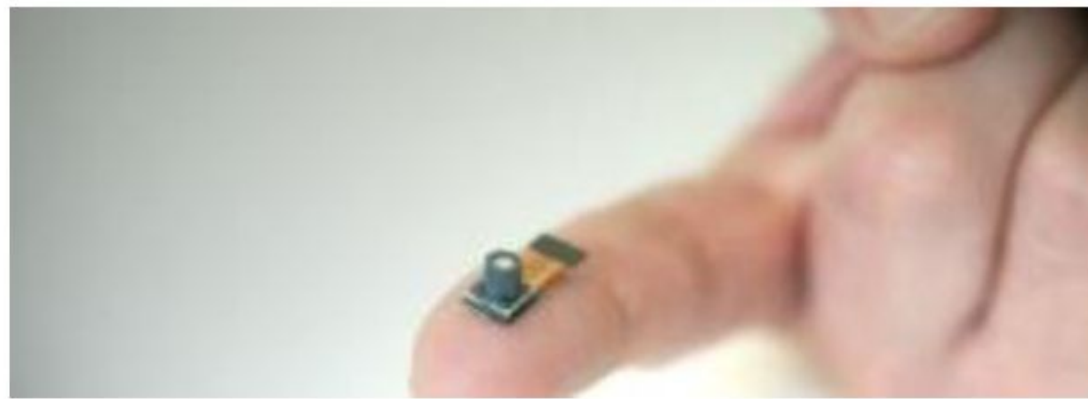
Full video at <https://www.youtube.com/watch?v=fiJyptbXBtM>



Clean water for all

<https://www.peopleswaterdata.org>

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

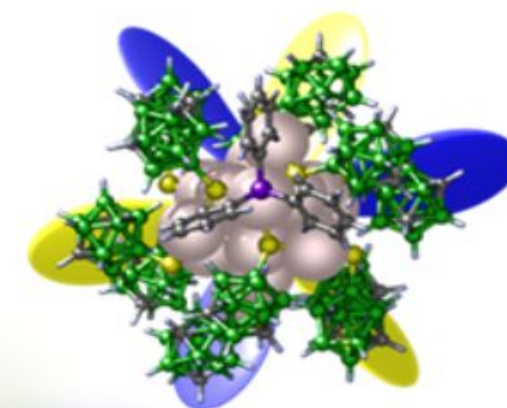
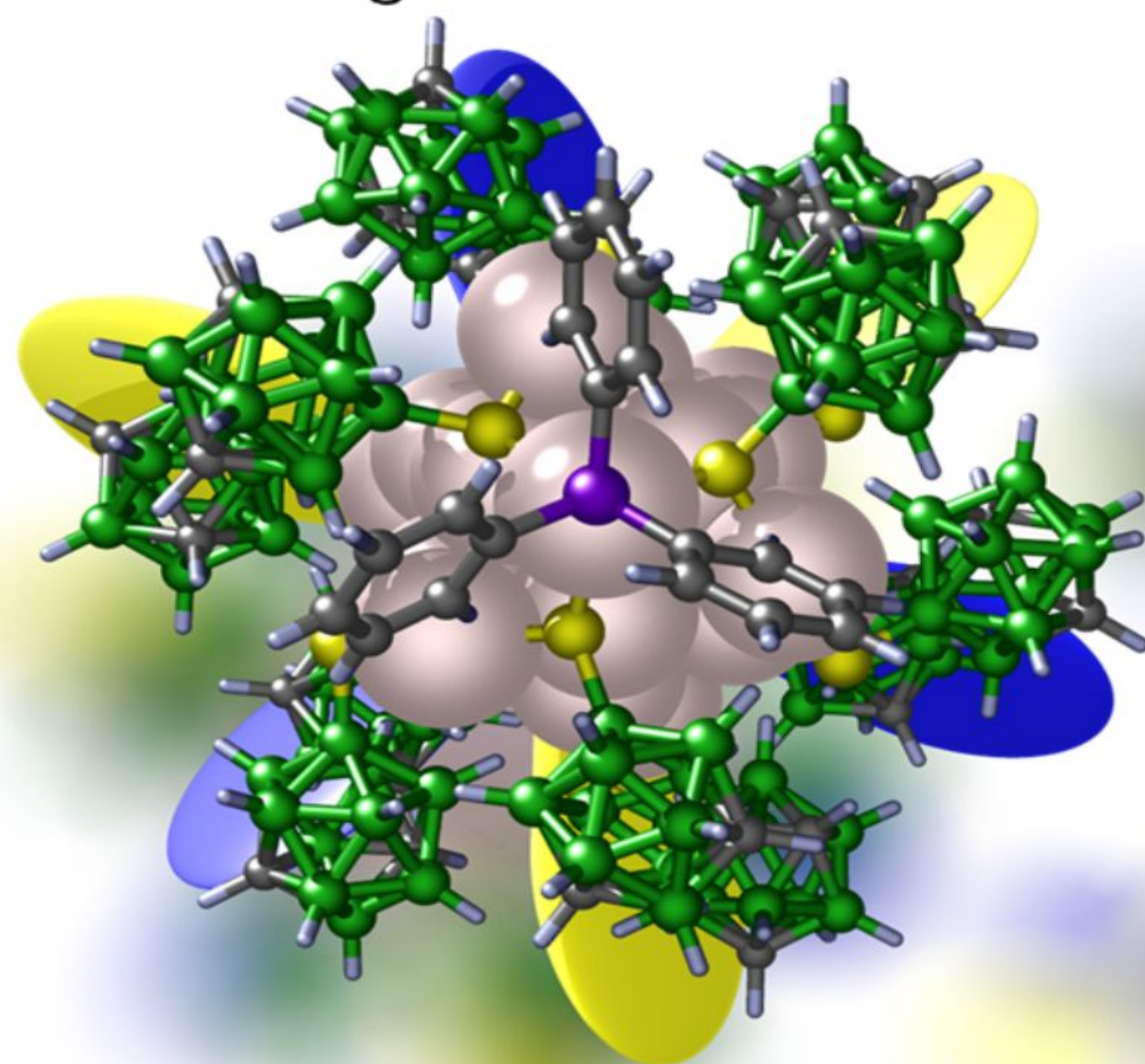
+

Mercury quenching experiment using nanofiber

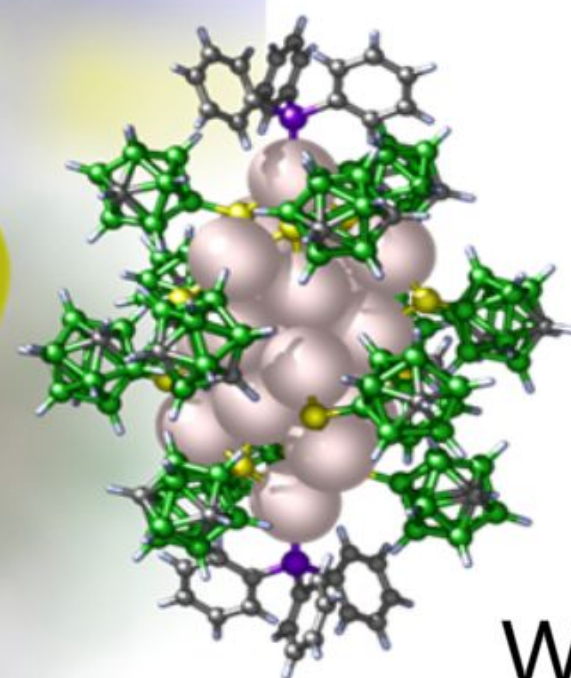
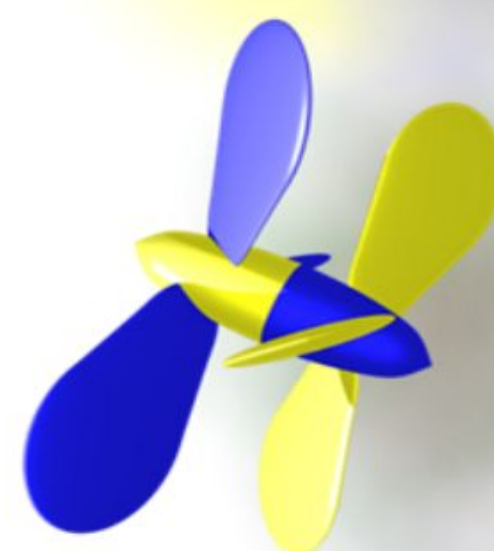


Carborane-thiol protected silver nanomolecule

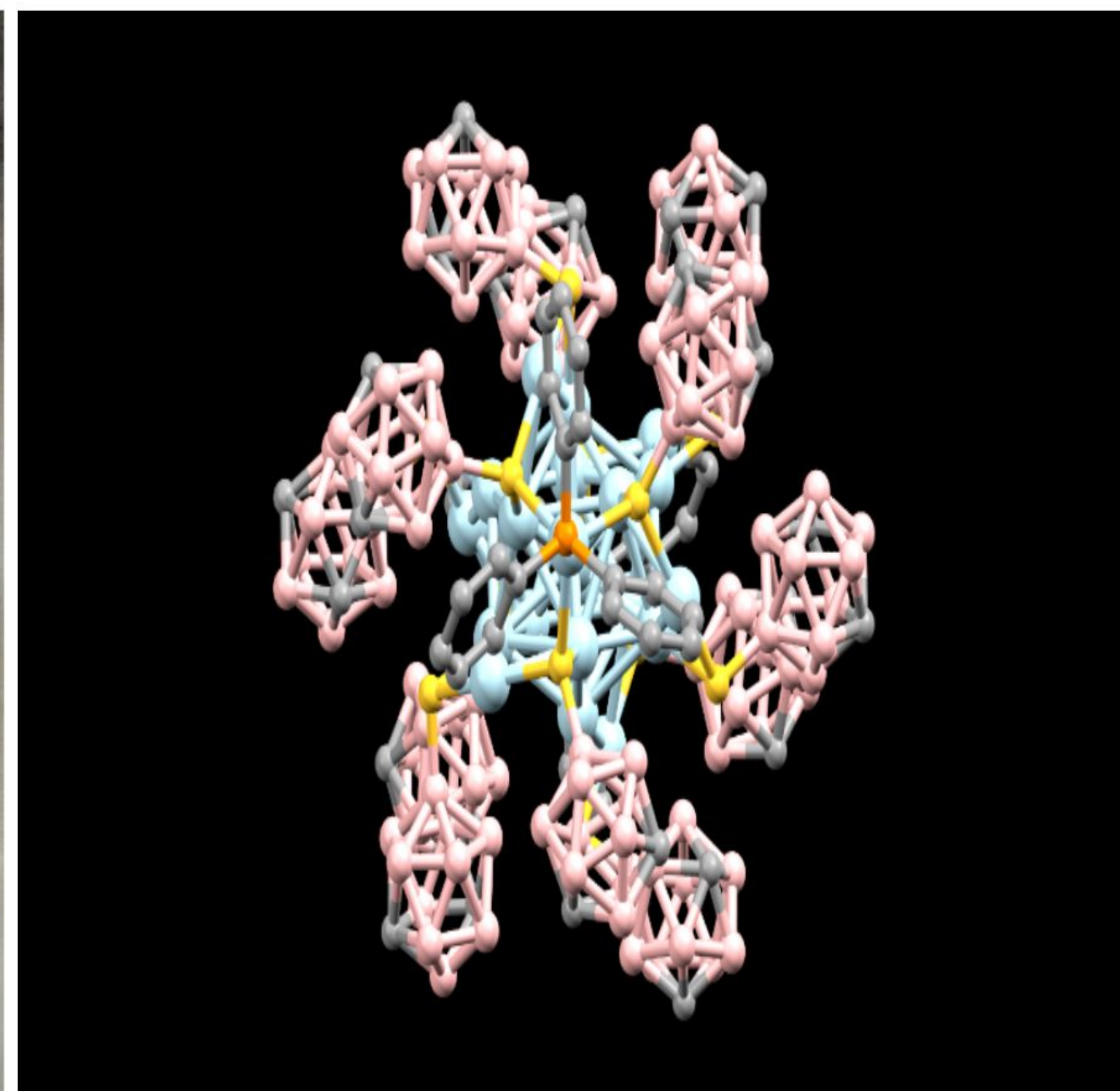
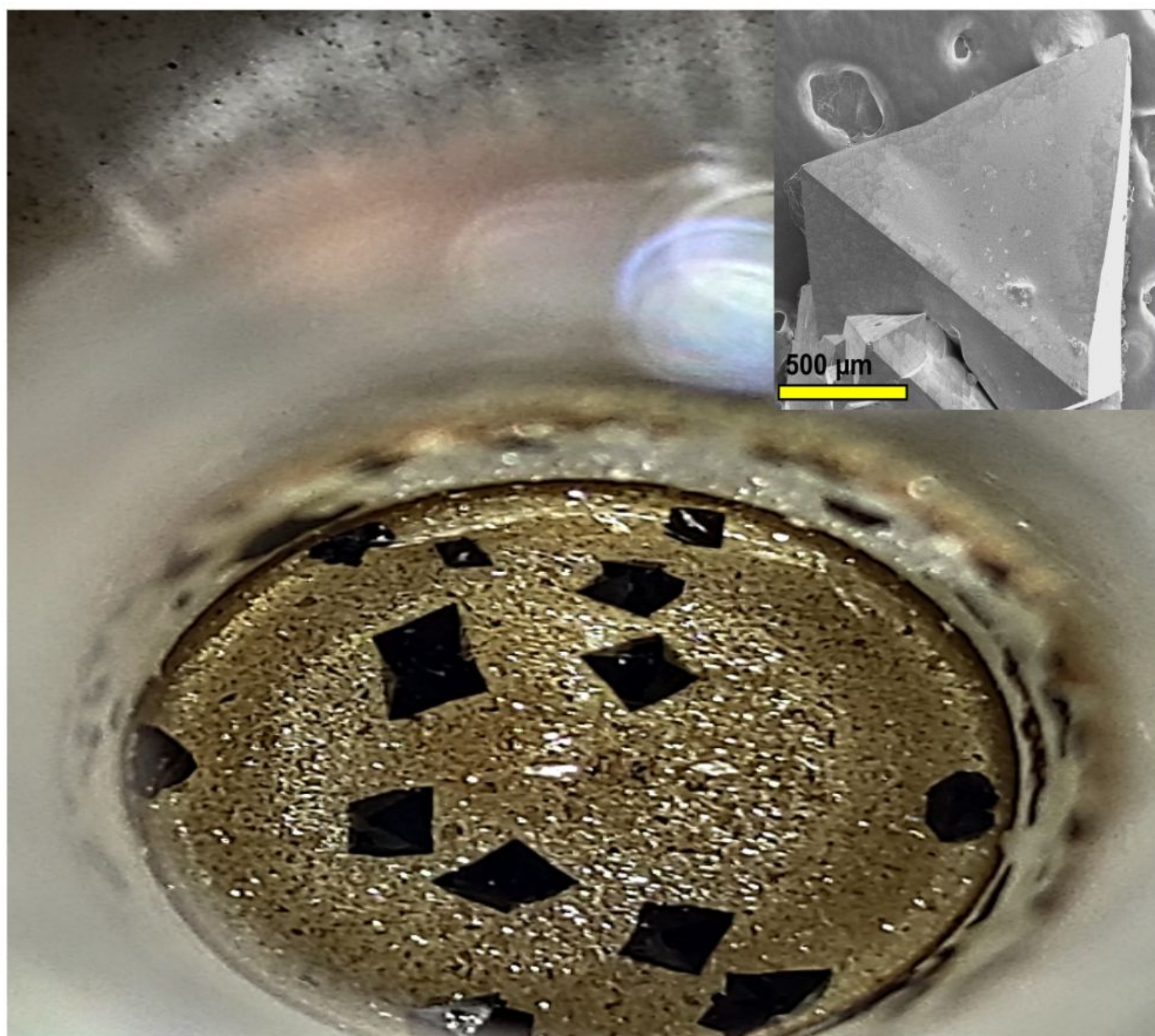
Rotary nanomolecule



Double rotors

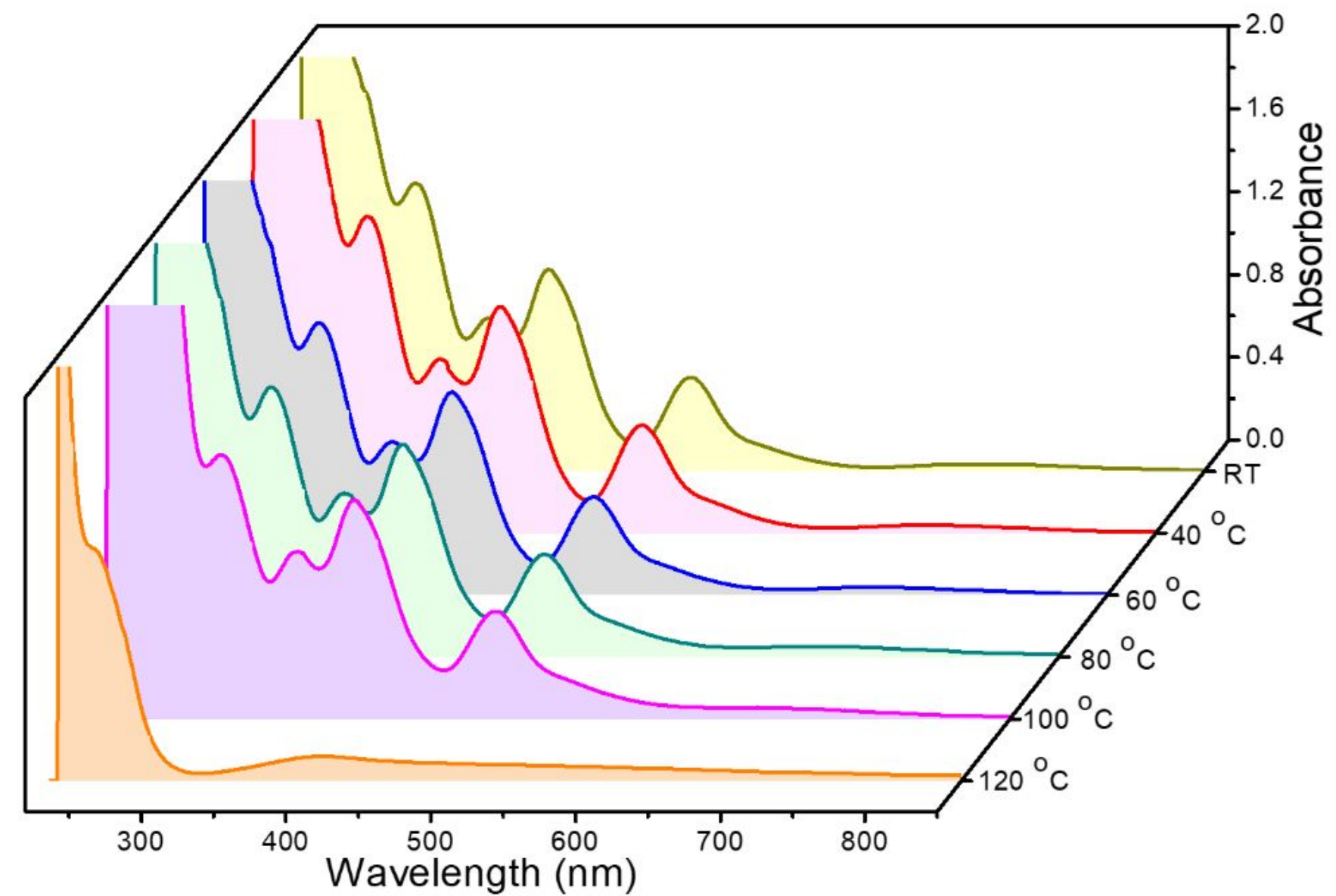
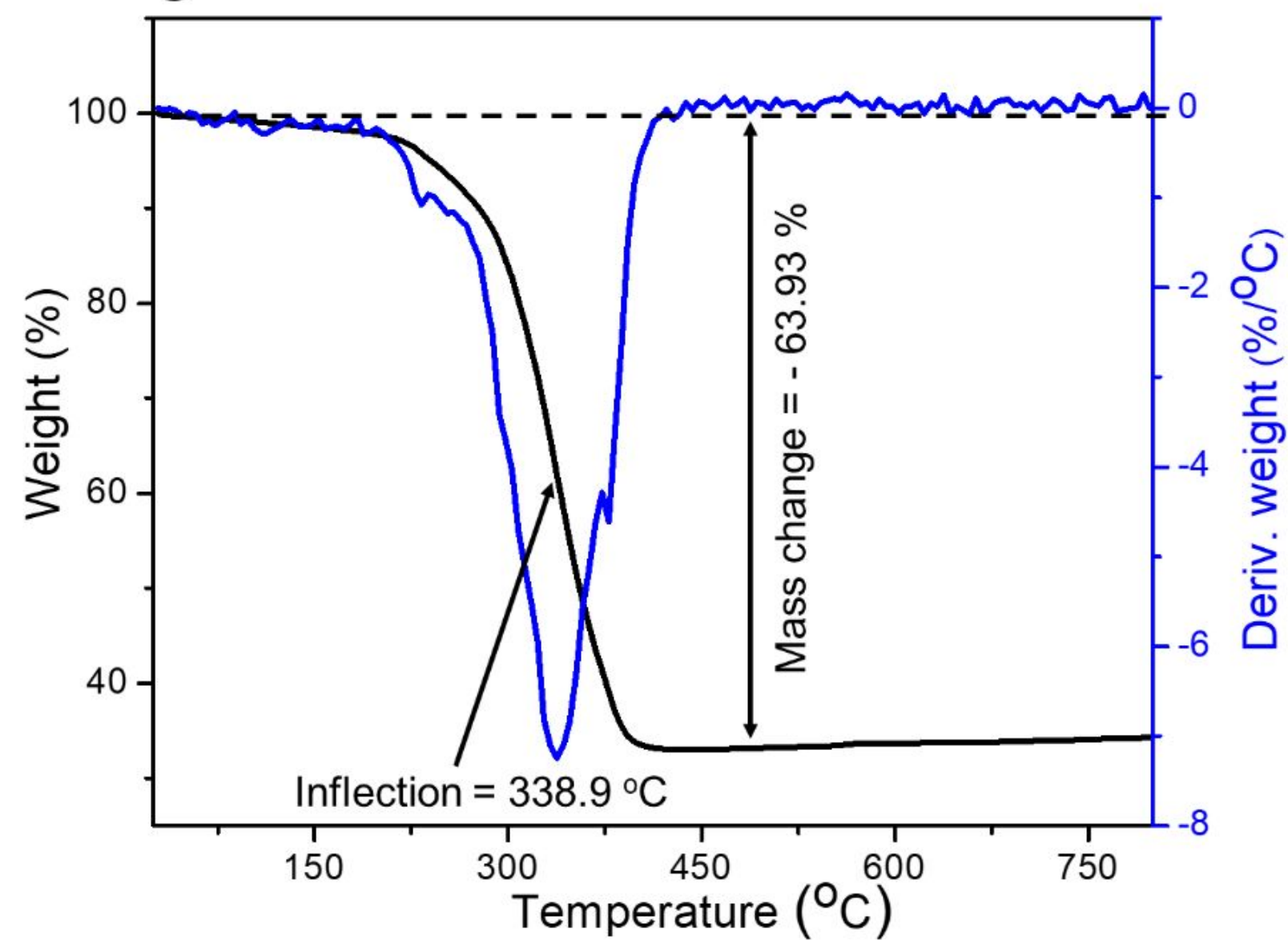


With Tomas Bas
e



Thermal stability

y

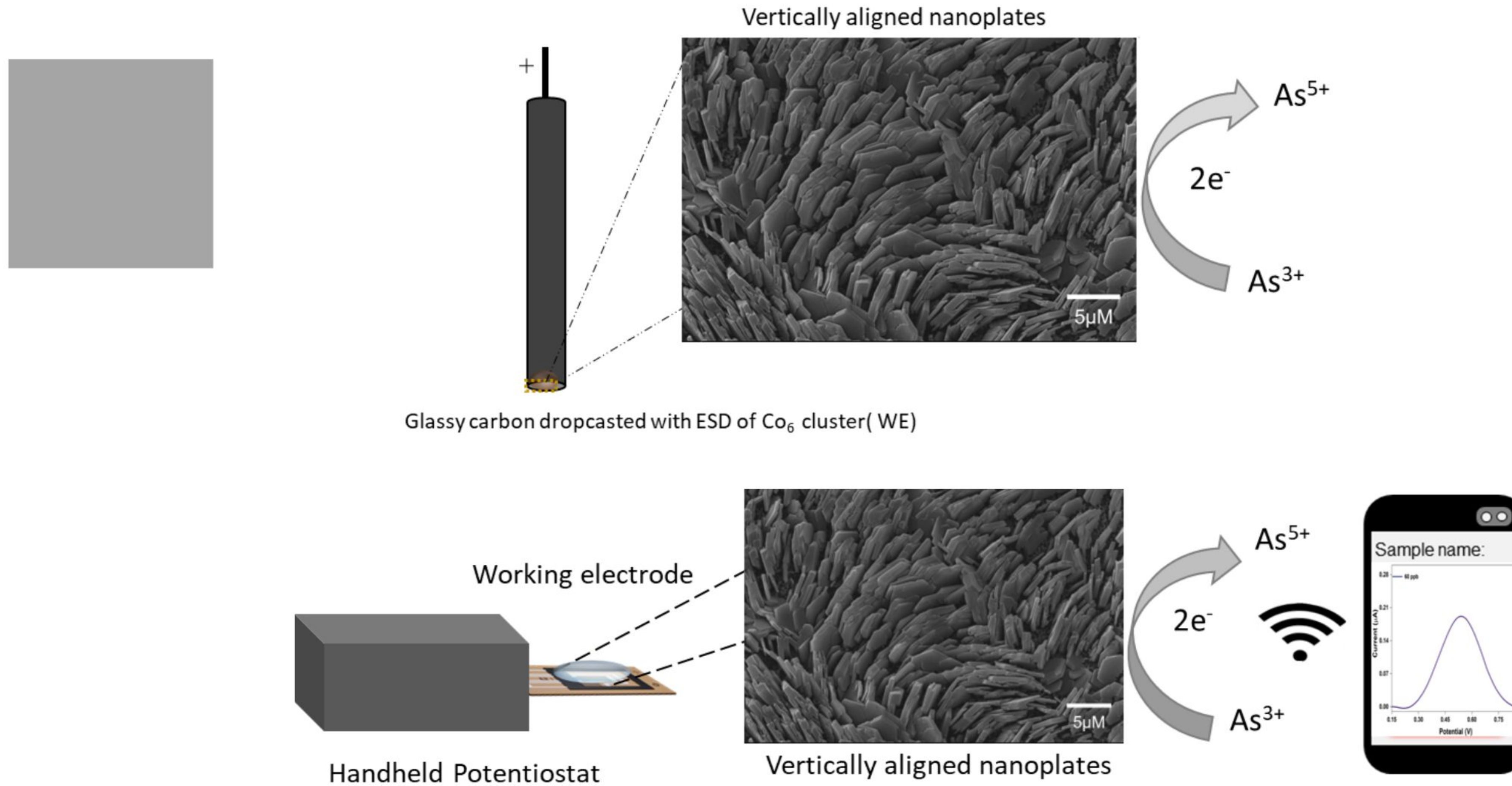


New electrodes - Aligned nanoplates of Co₆S

8

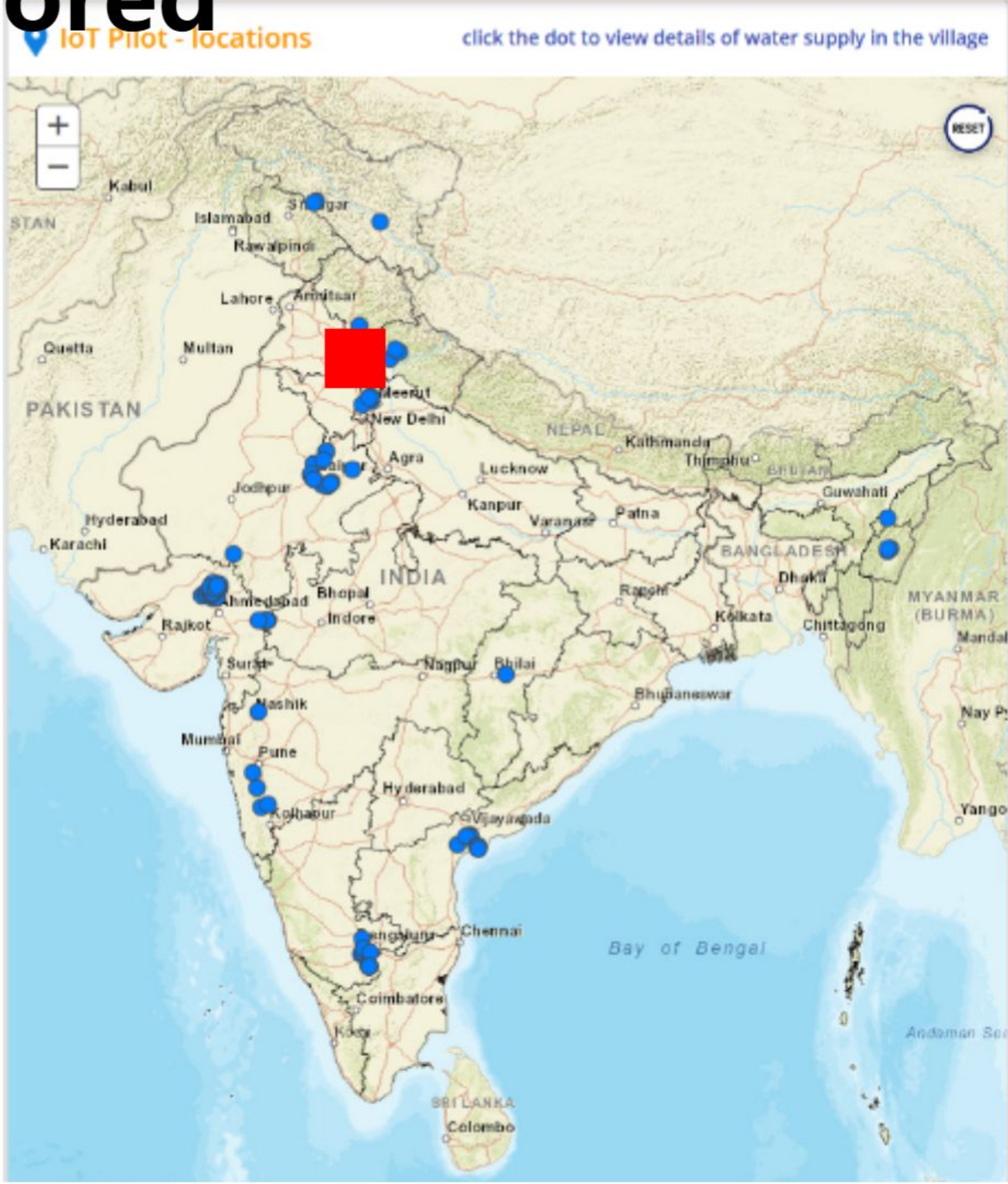
1,2-bis(diphenylphosphino)ethane (DPPE)

Sensing



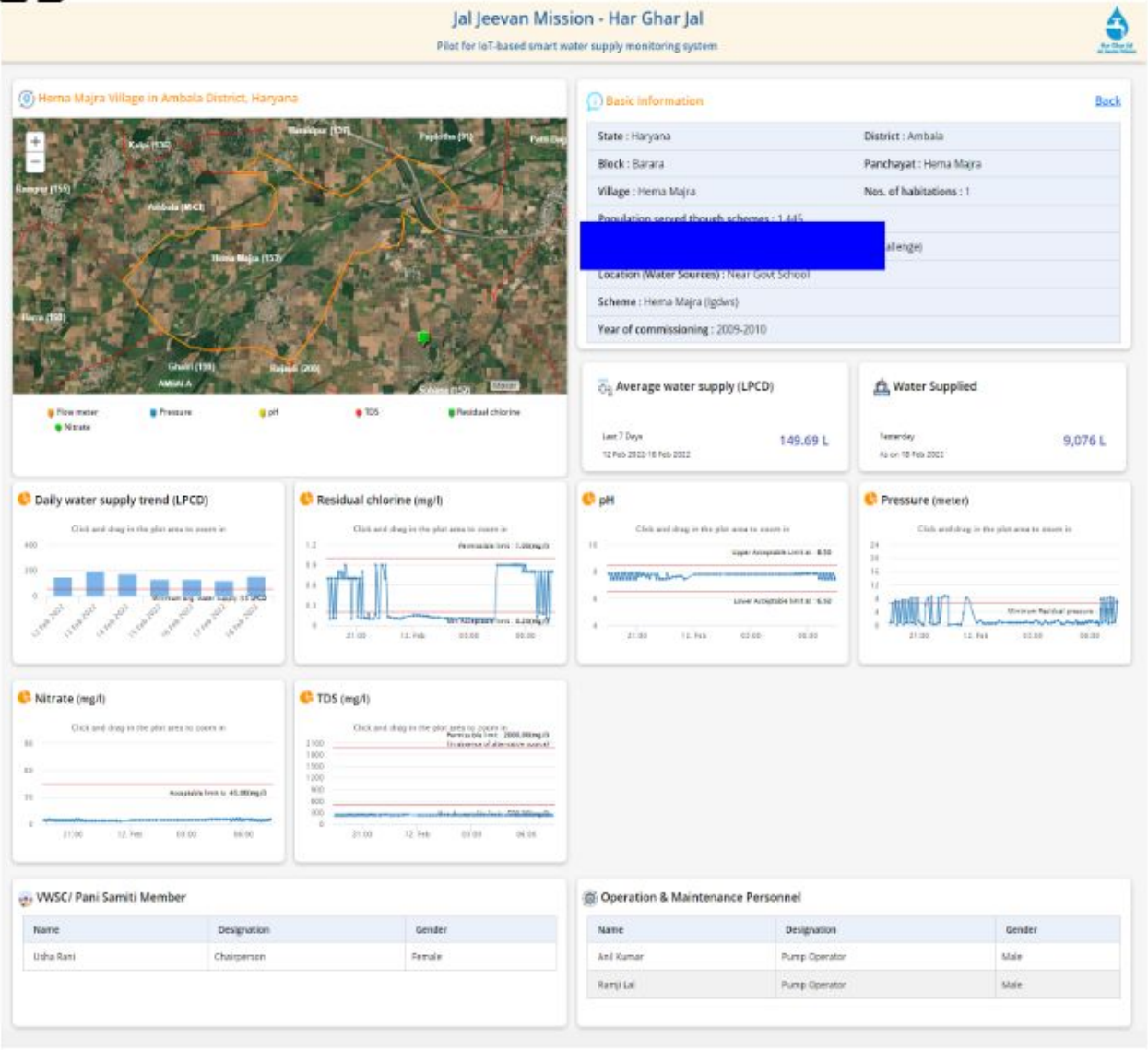


India's water is being monitored

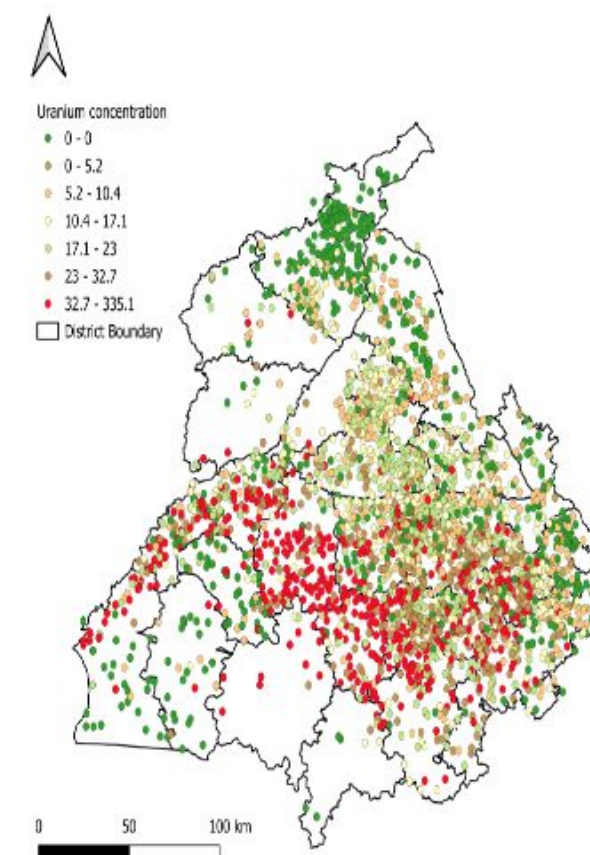


IITM/IIS

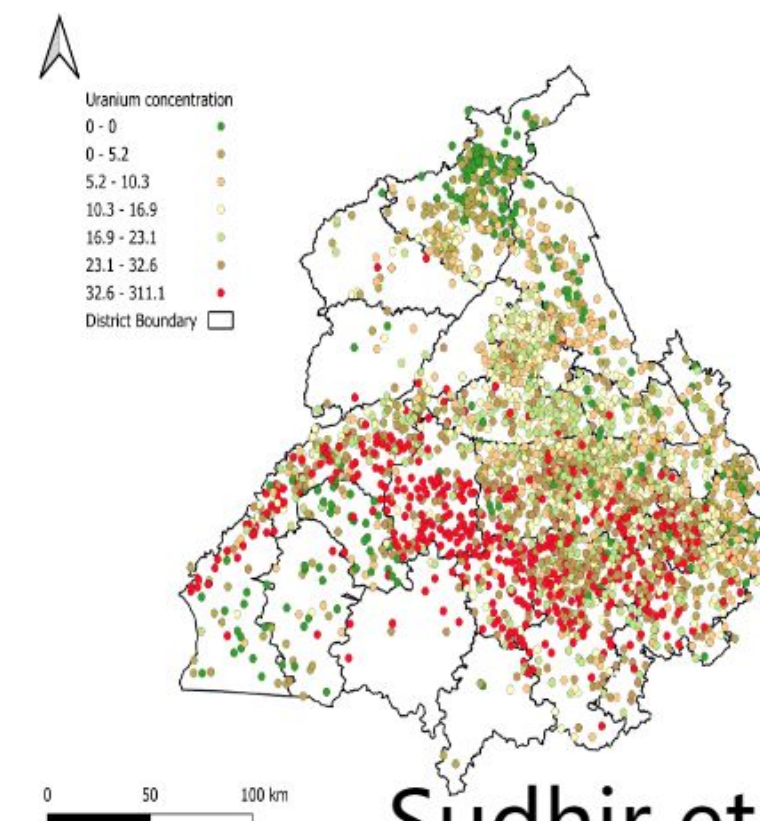
Installations made by four companies



Arsenic poisoning across the world



[1]



Sudhir et. al. Unpublish

ed

scale has been added like figure 1

Can Water Microdroplets Make Soil?

A path to sustainable nanotechnology



Science

**A scale of 100
0**

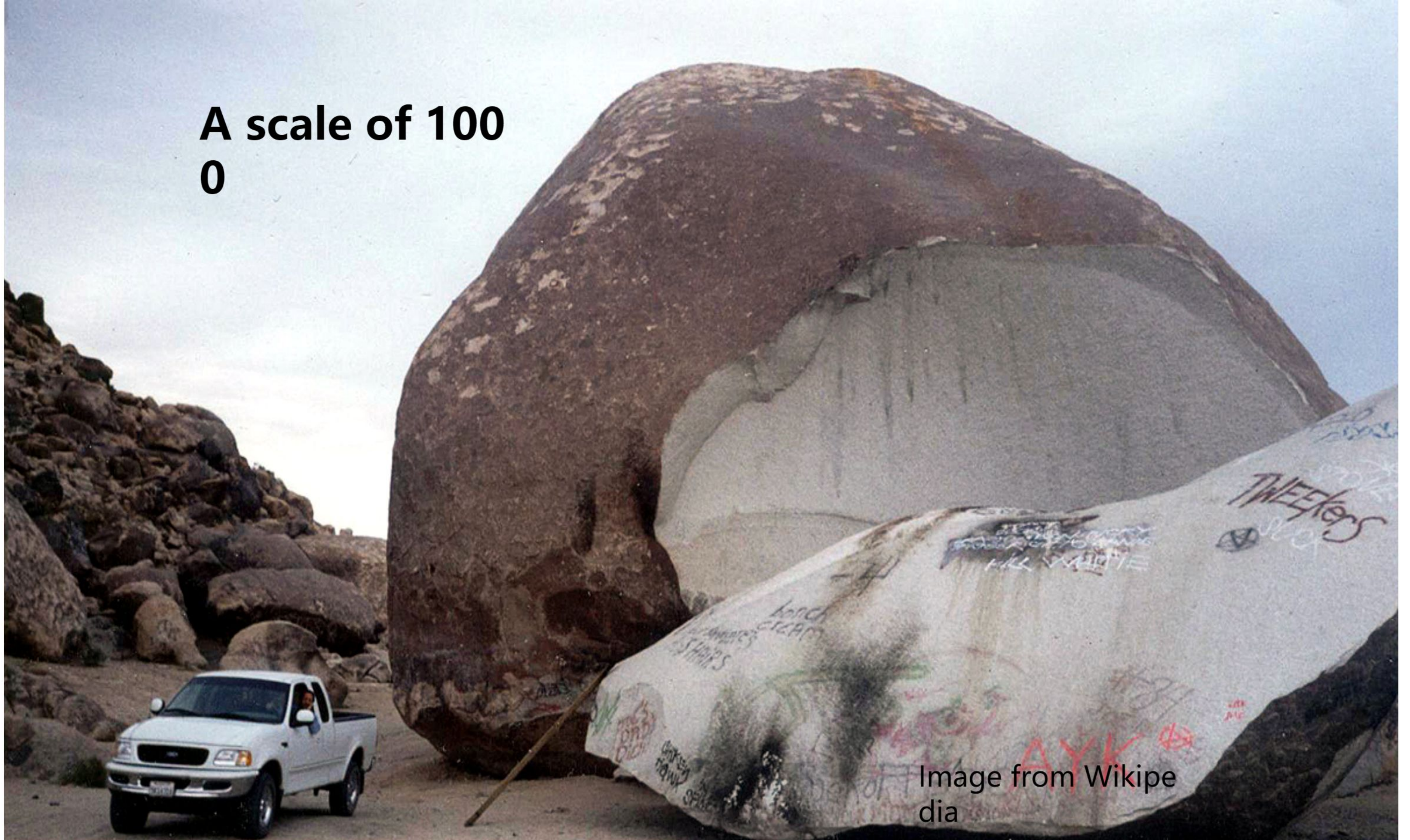


Image from Wikiped
ia



Thanks to ChatGP

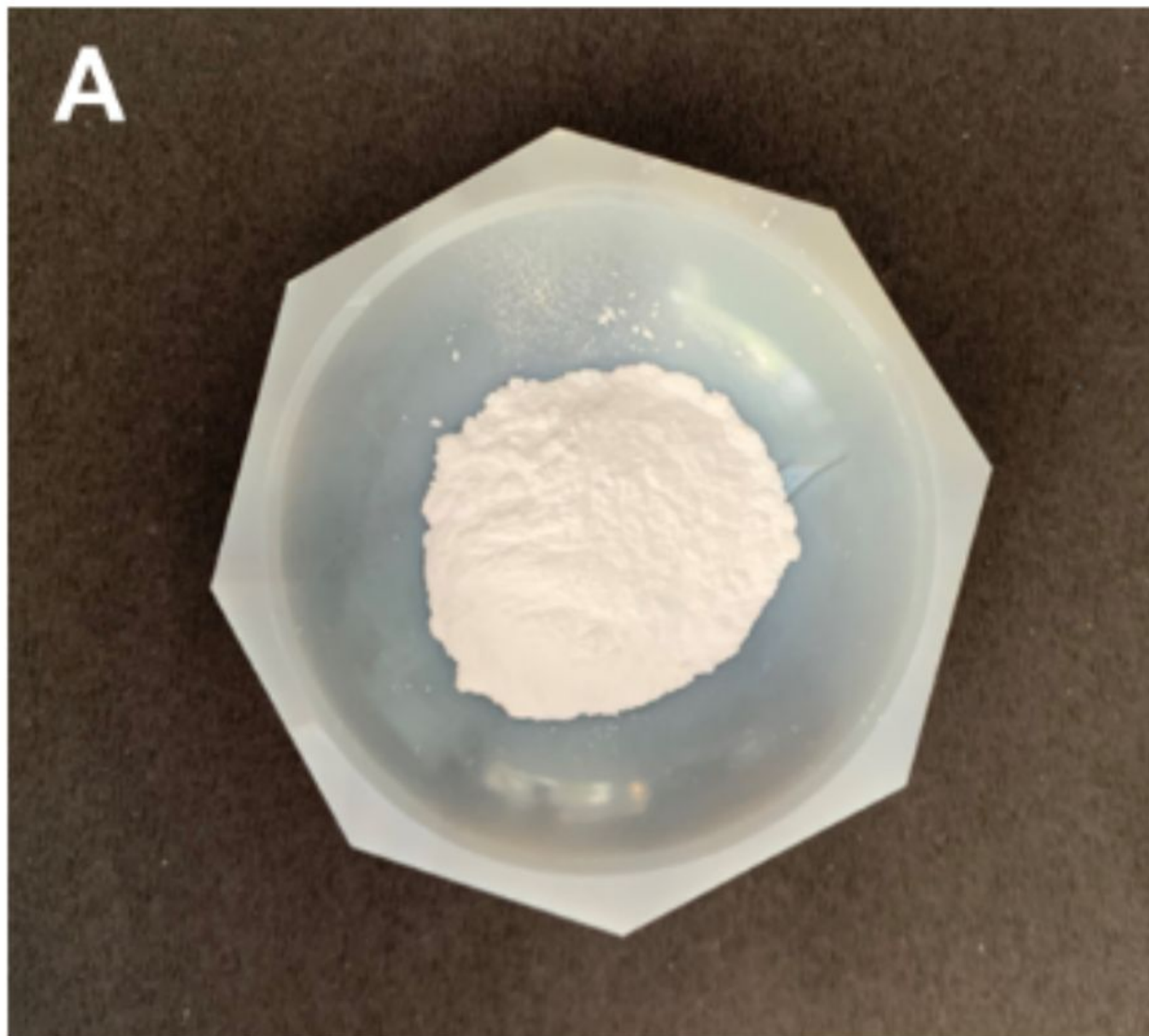
T

Sand, the Ubiquitous Material

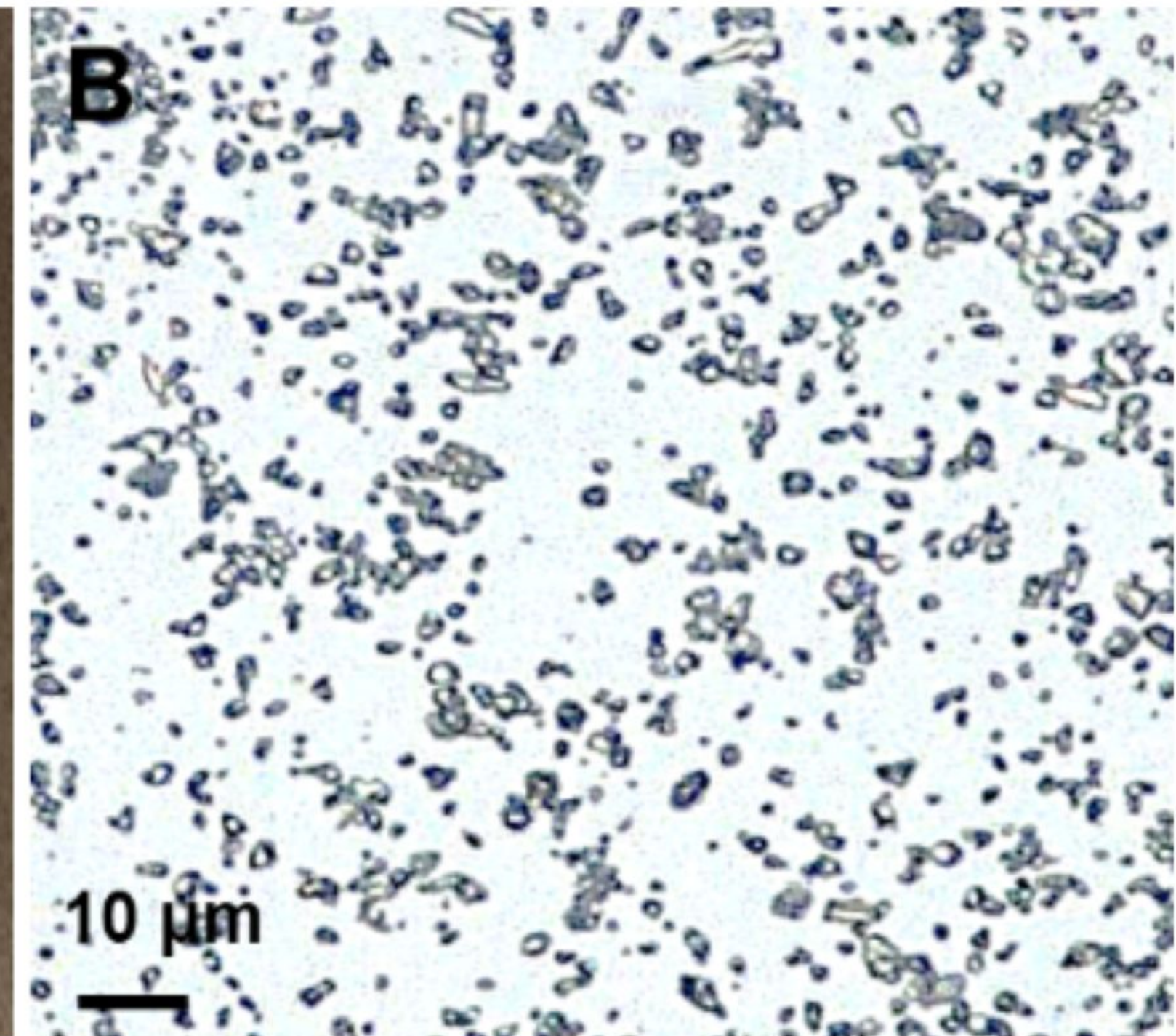


Images from Wikipedia
dia



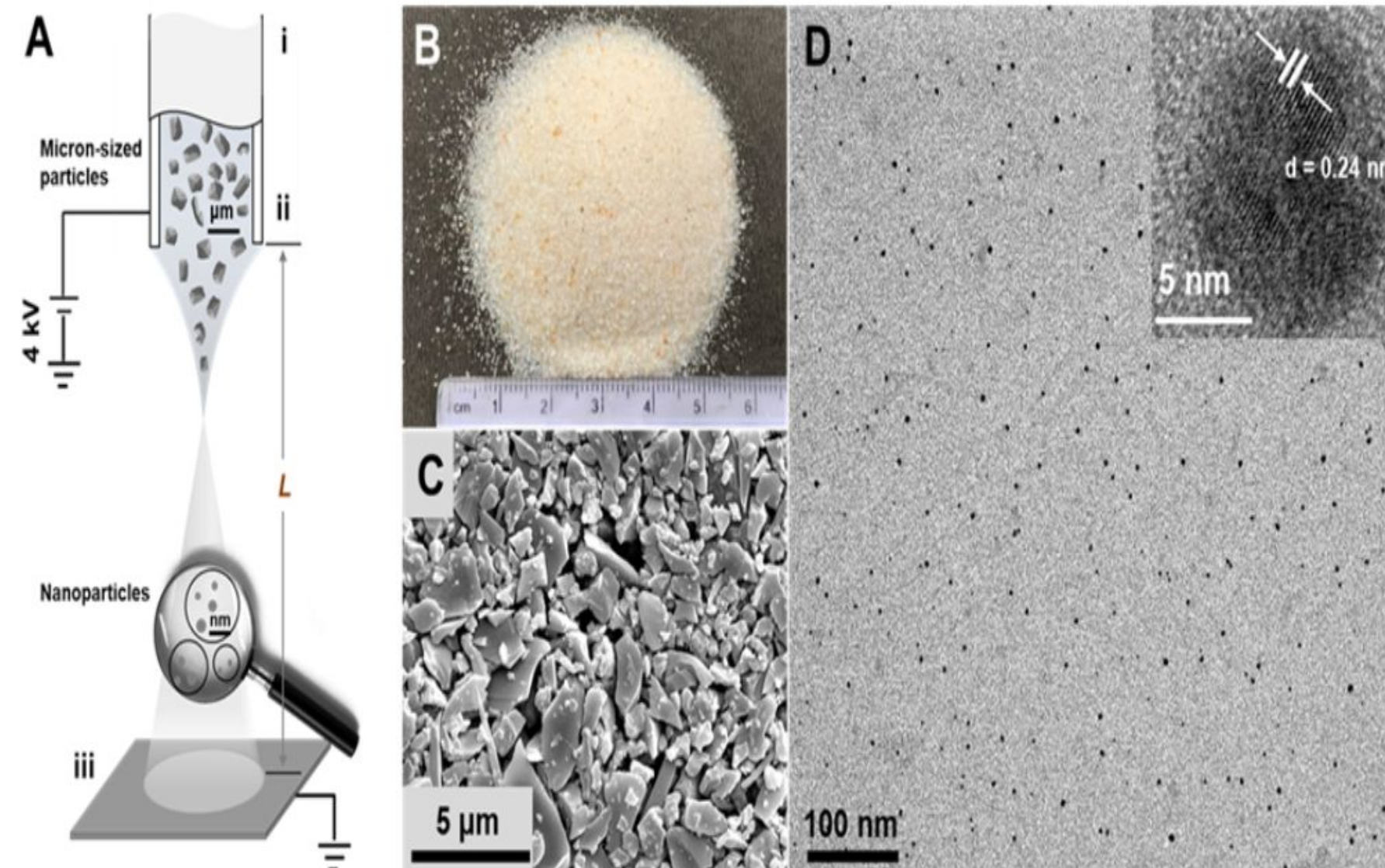
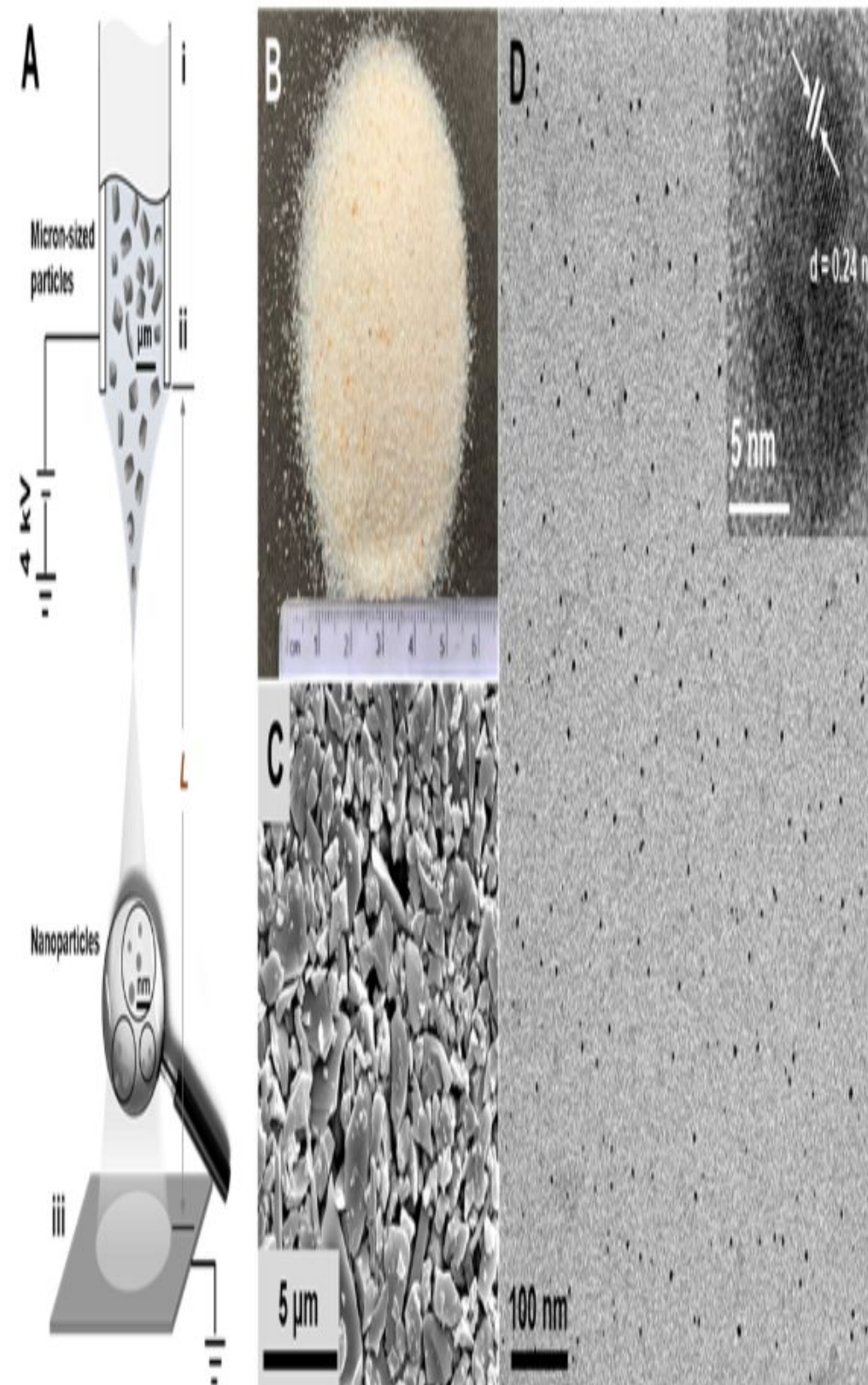


Ground silica



Optical image of silica

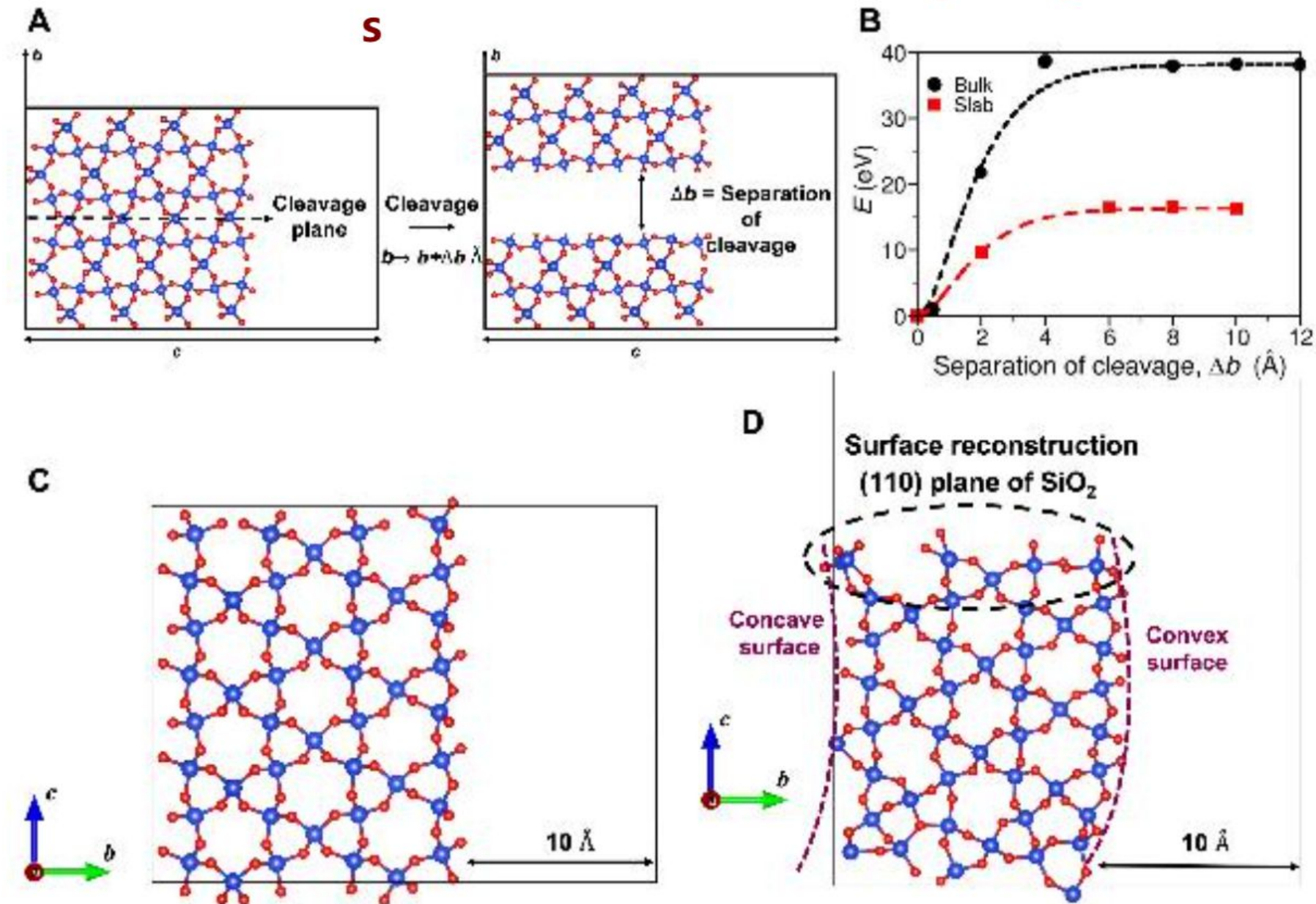
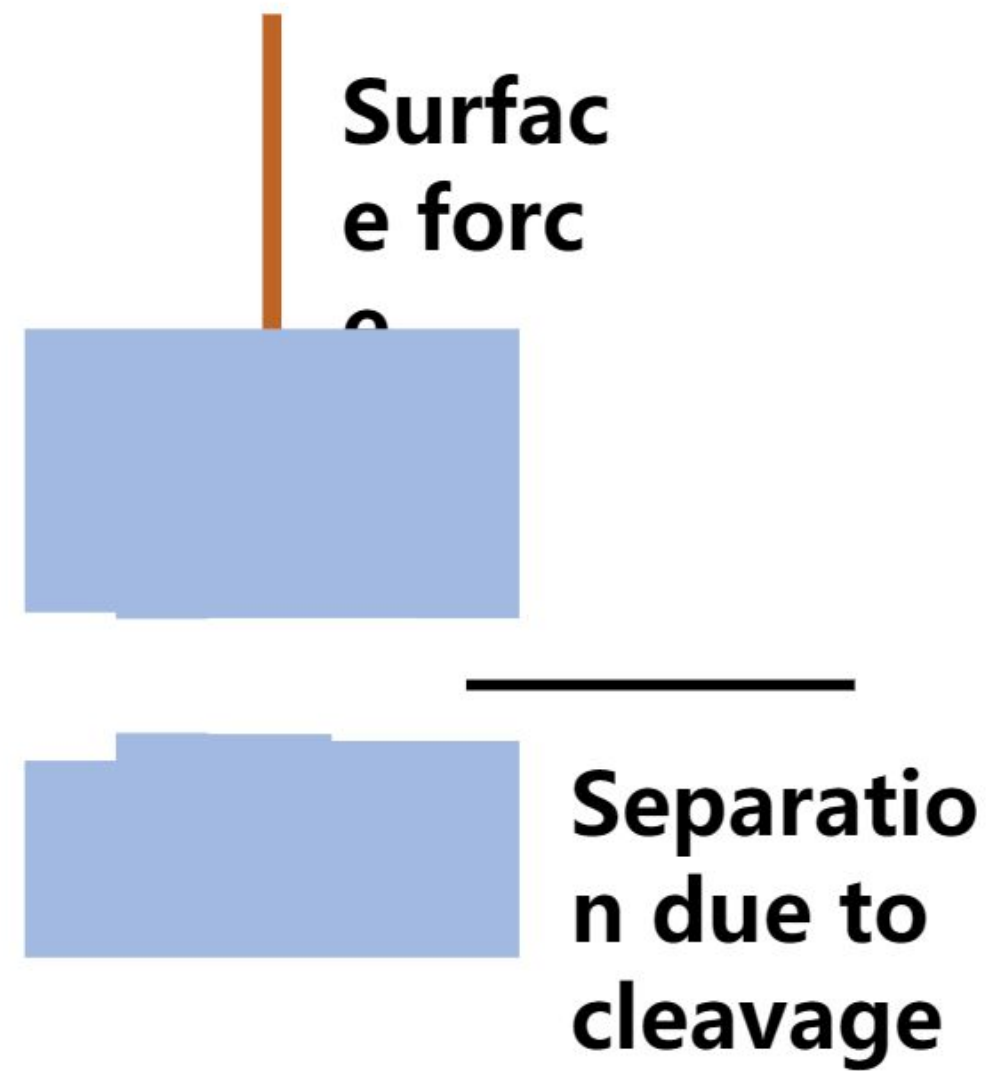
Weathering of Minerals in Microdroplets



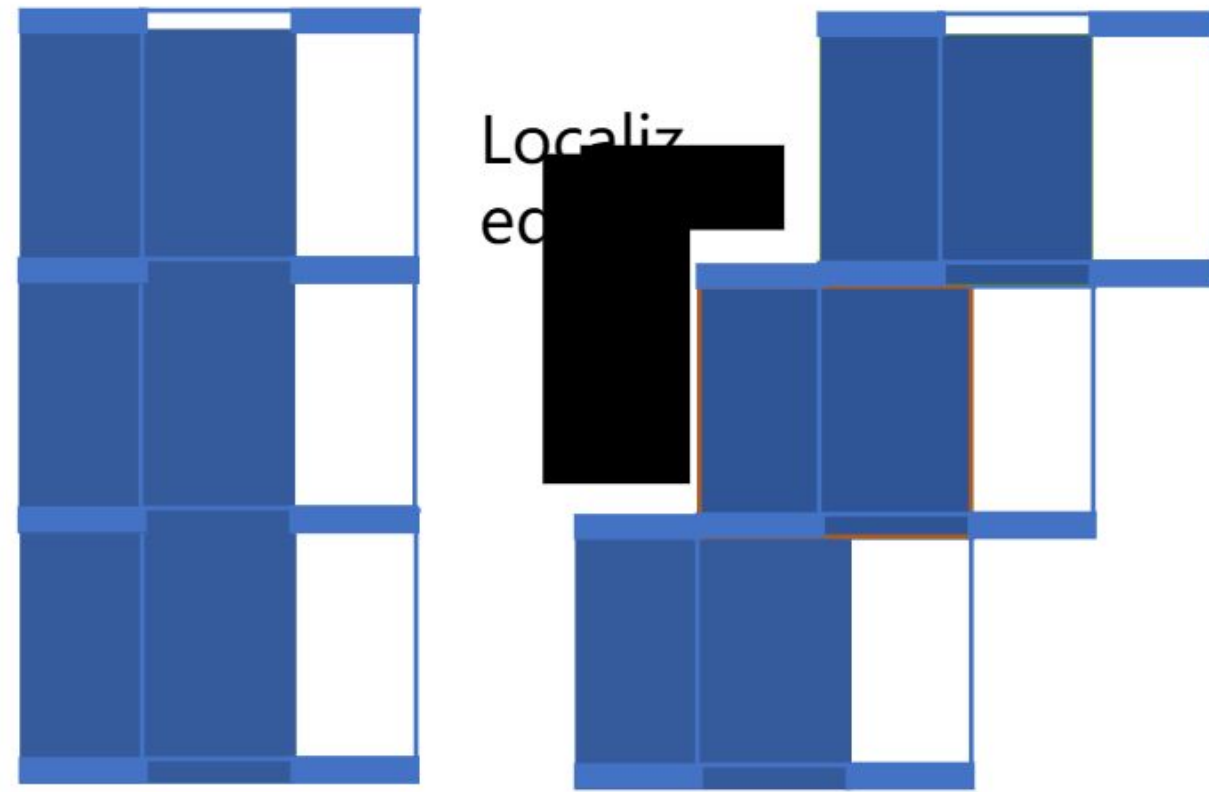
Ruby, Fused Alumin a

Mechanism: Cleavage

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



Mechanism: Slip

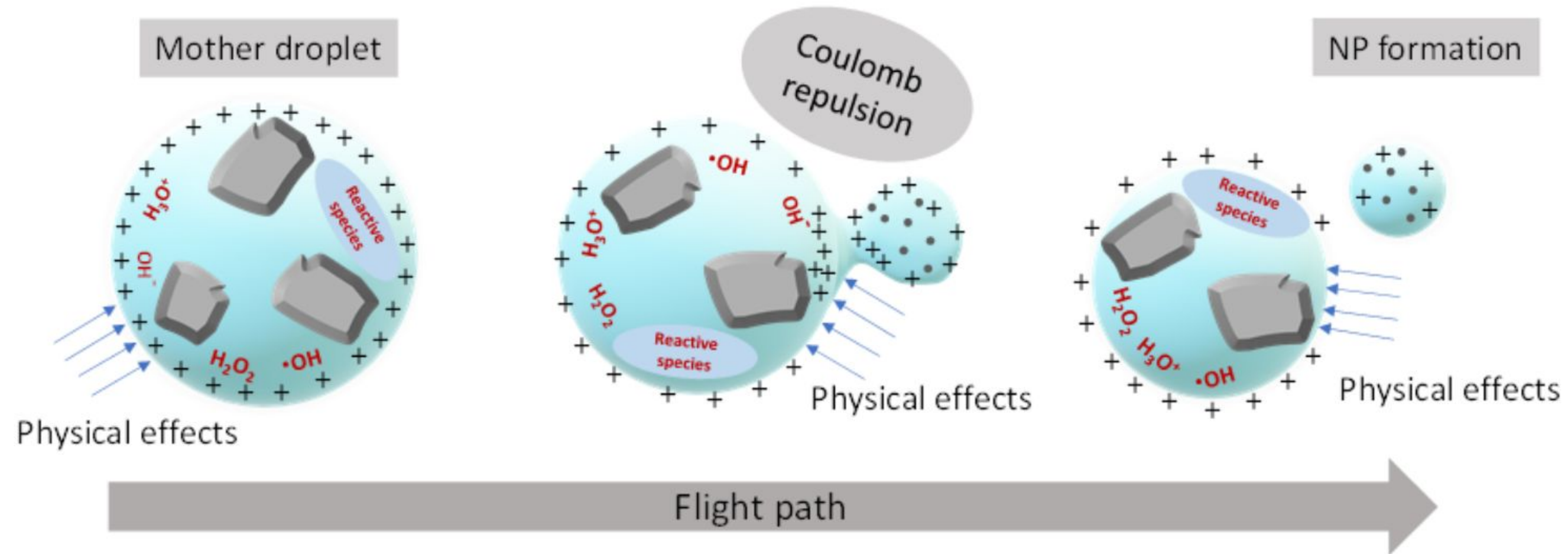


This instability leads to the formation of a stacking fault on the (010) plane, achieved with slip localized at (010) plane

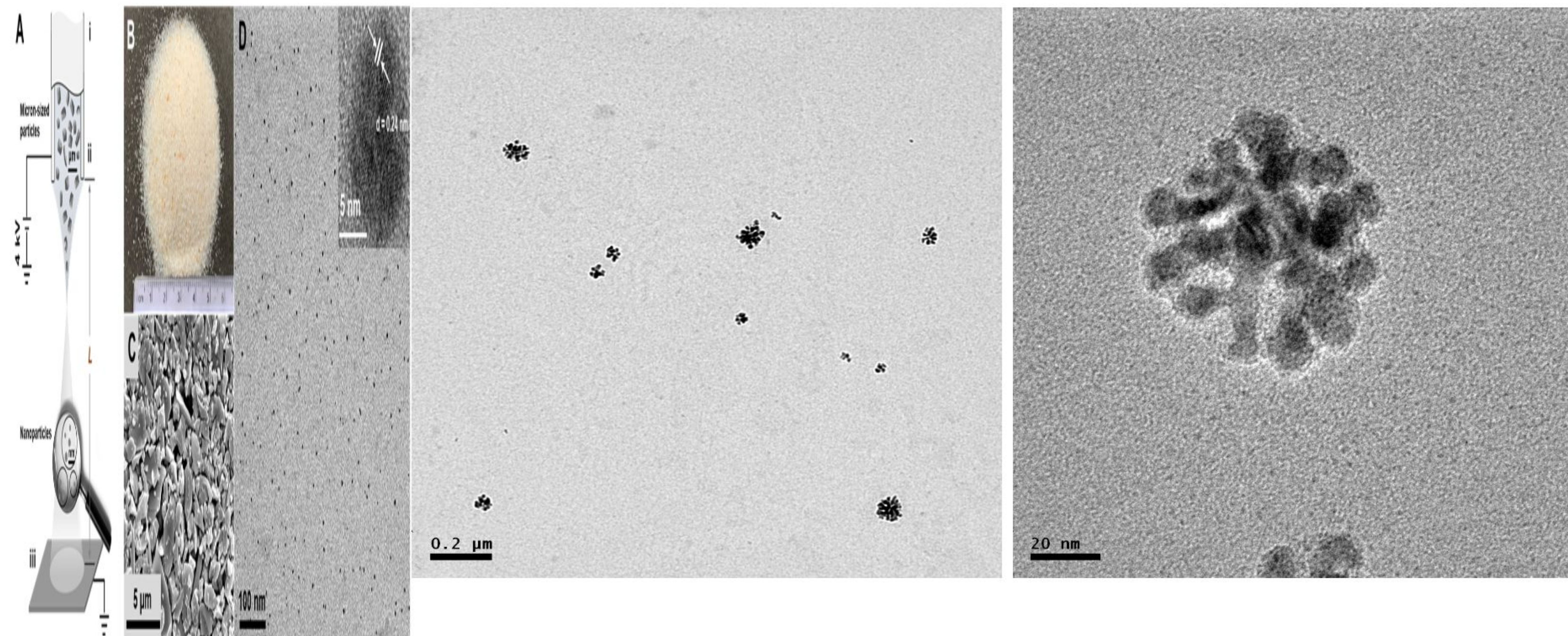
Stacking fault
 $\vec{b} \rightarrow \vec{b}_0 + (x, 0, z)$

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

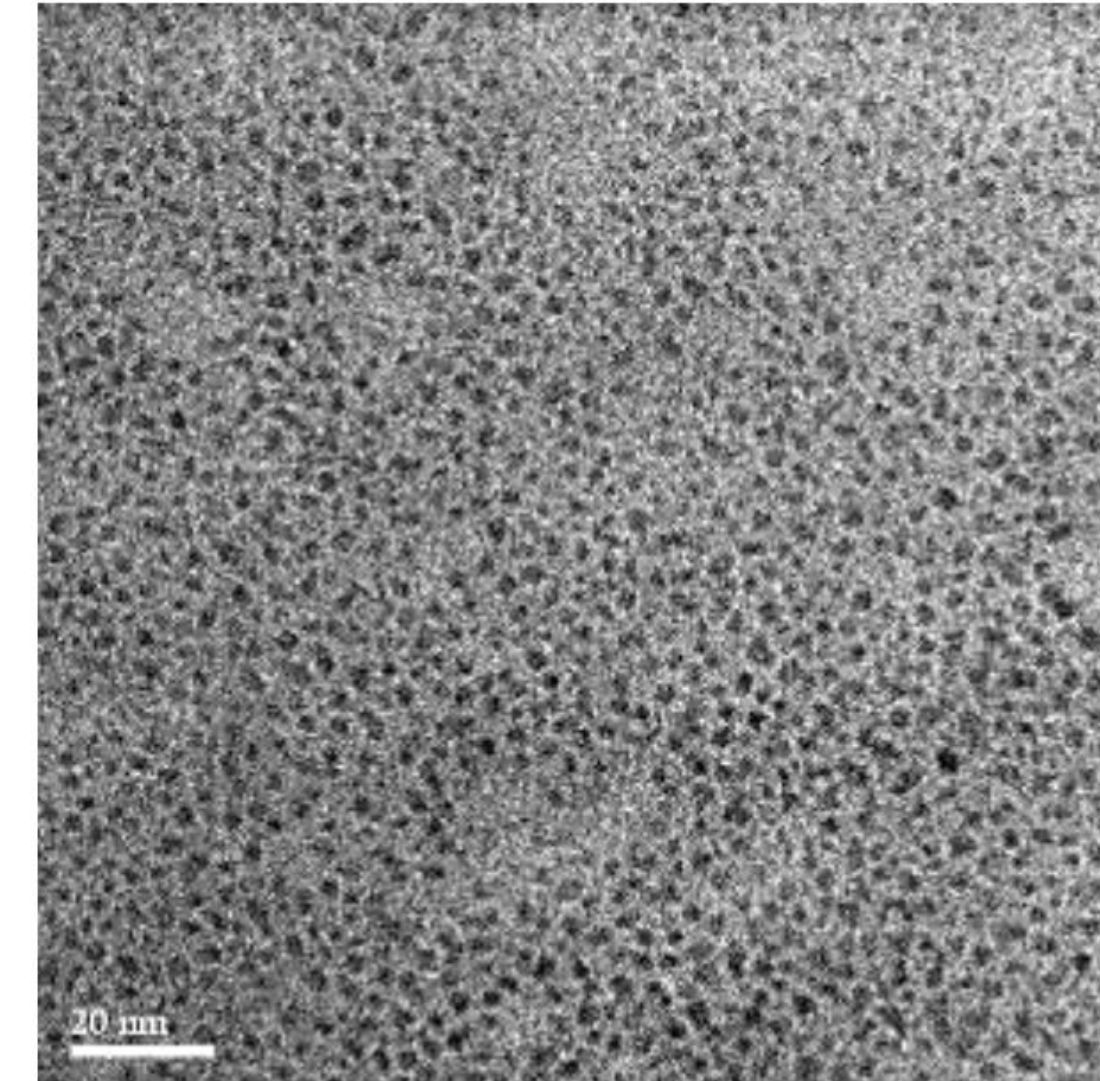
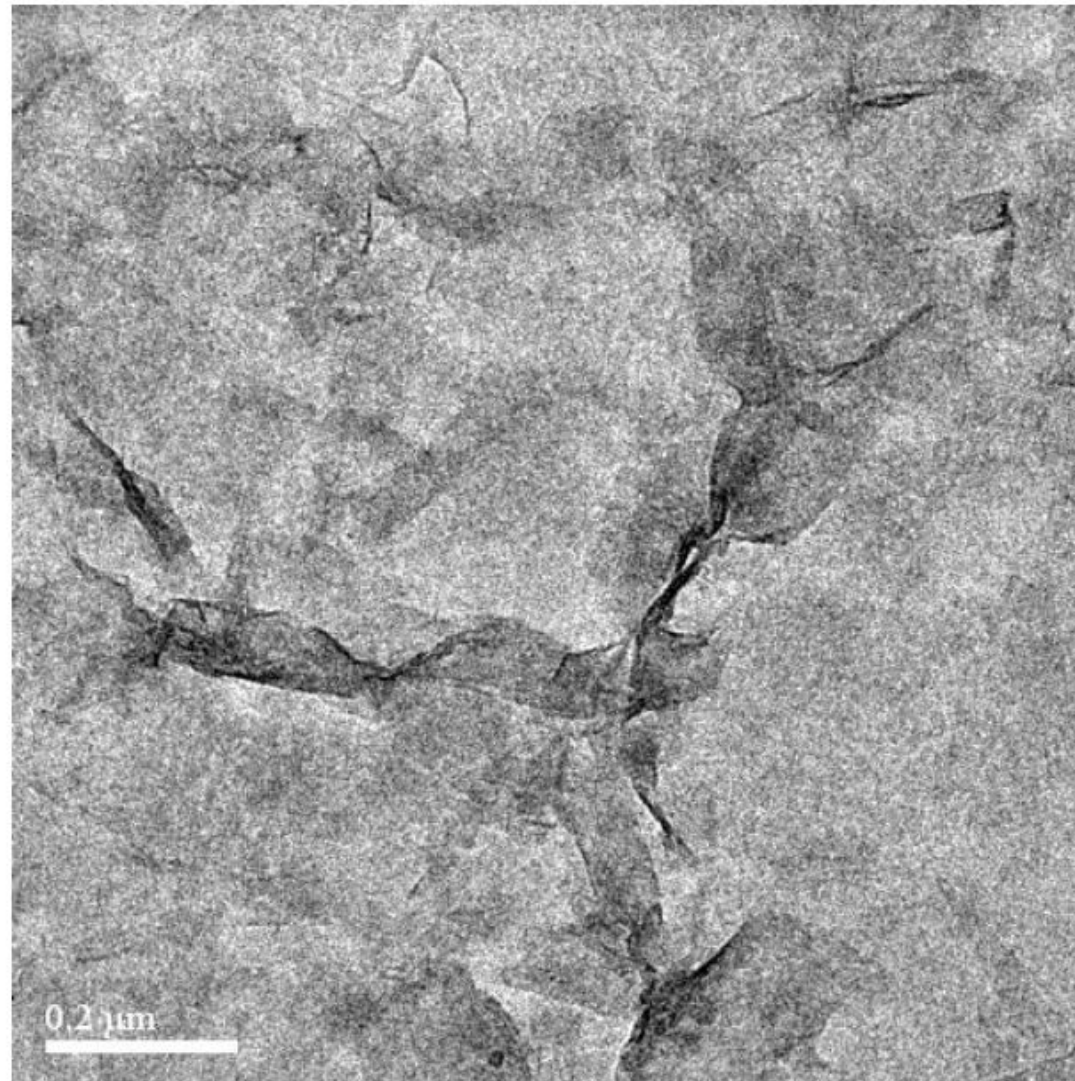
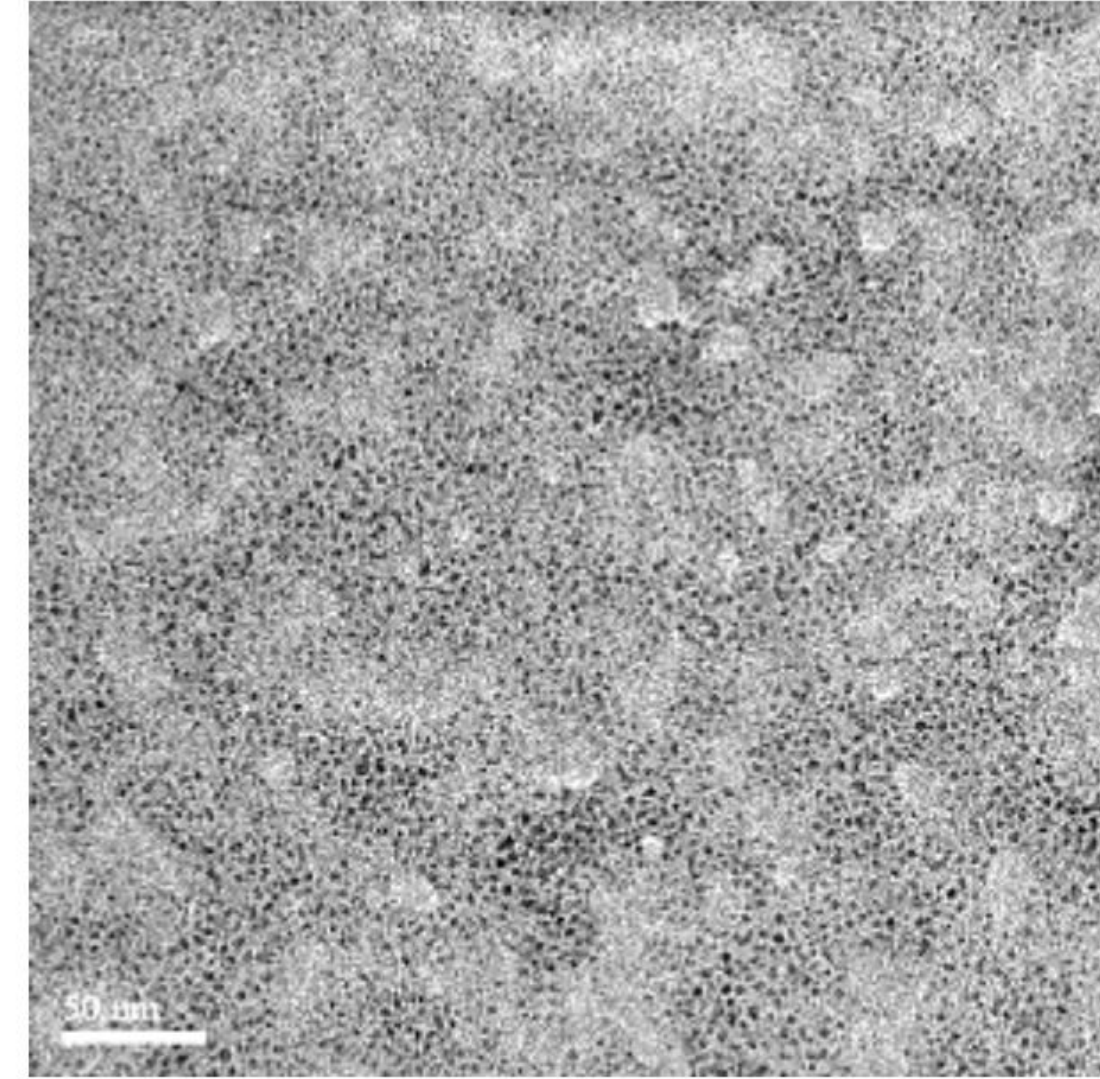
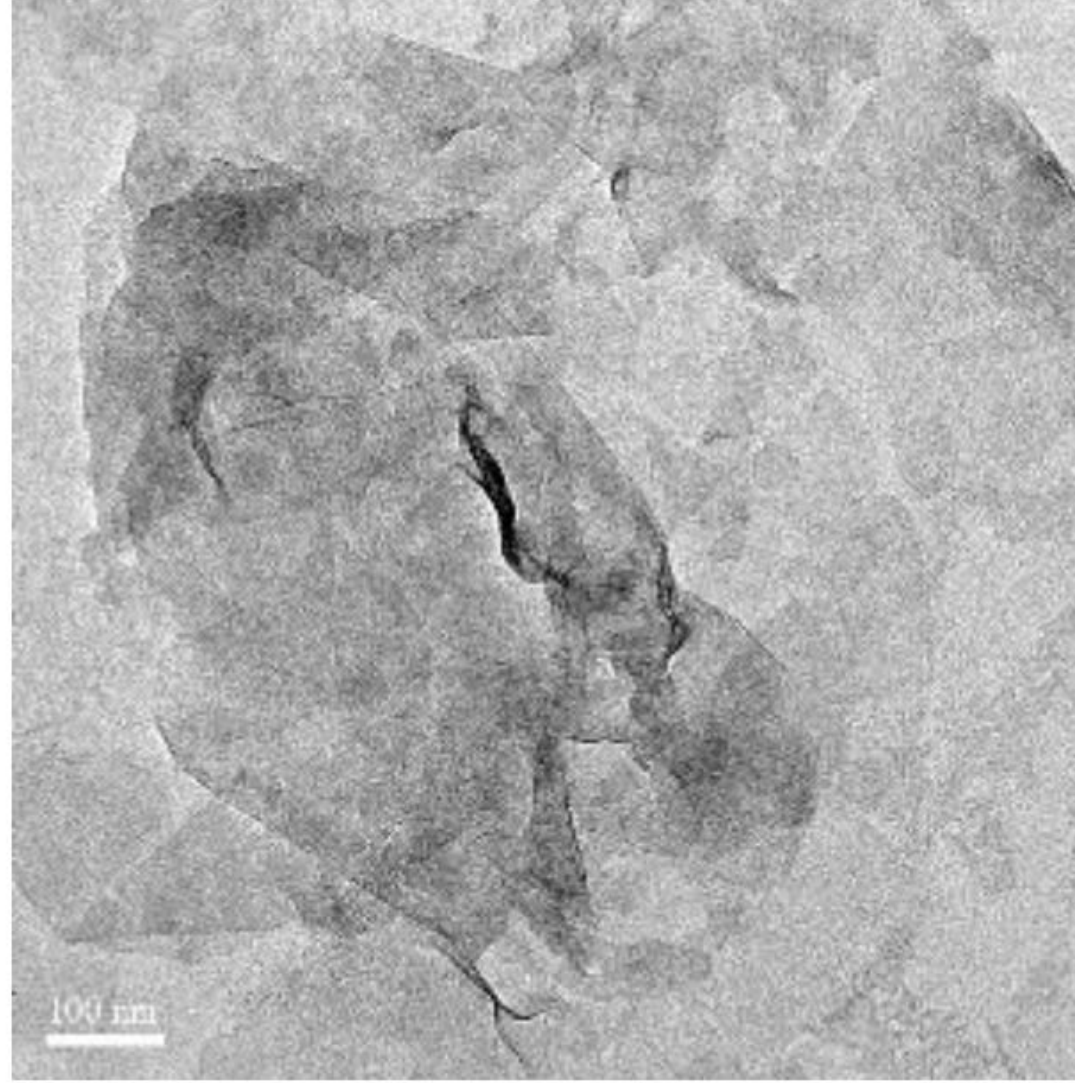
Mechanism of nanoparticle formation



How do they form?



MoS₂ Nanosheets



MoS₂ Nanosheet

MoS₂ Nanoparticles

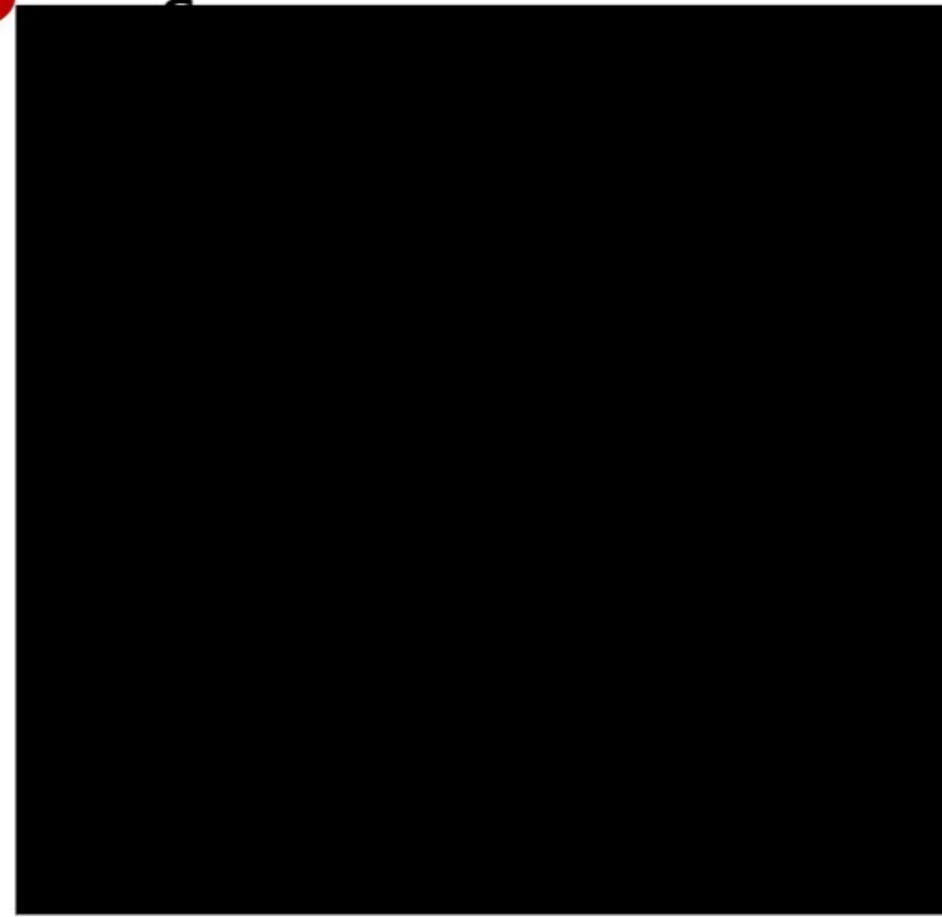
Grand unification of synthesis

s

Radicals, ion

Transient specie

S



s

Electric field

E

Field
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Pressure fluctuatio
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M

MV cm
-1

MP
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Thanks to ChatGP
T

Vision

Make soil using processed wastewater and make deserts bloom.



Thanks to ChatGP
T



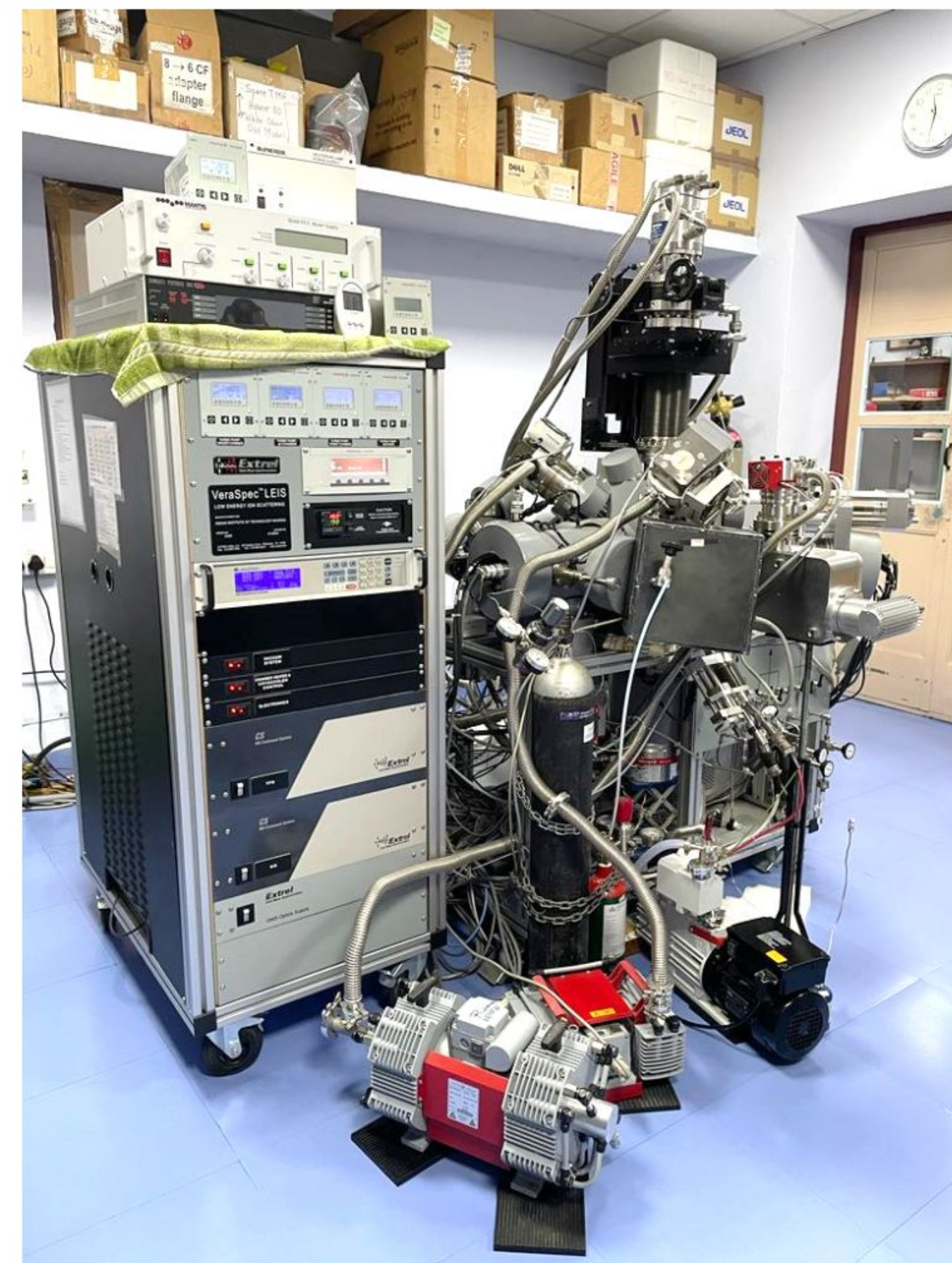
International Centre for Clean Water

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

Can Clathrate Hydrates Exist in Space?

Exploring astrobiology

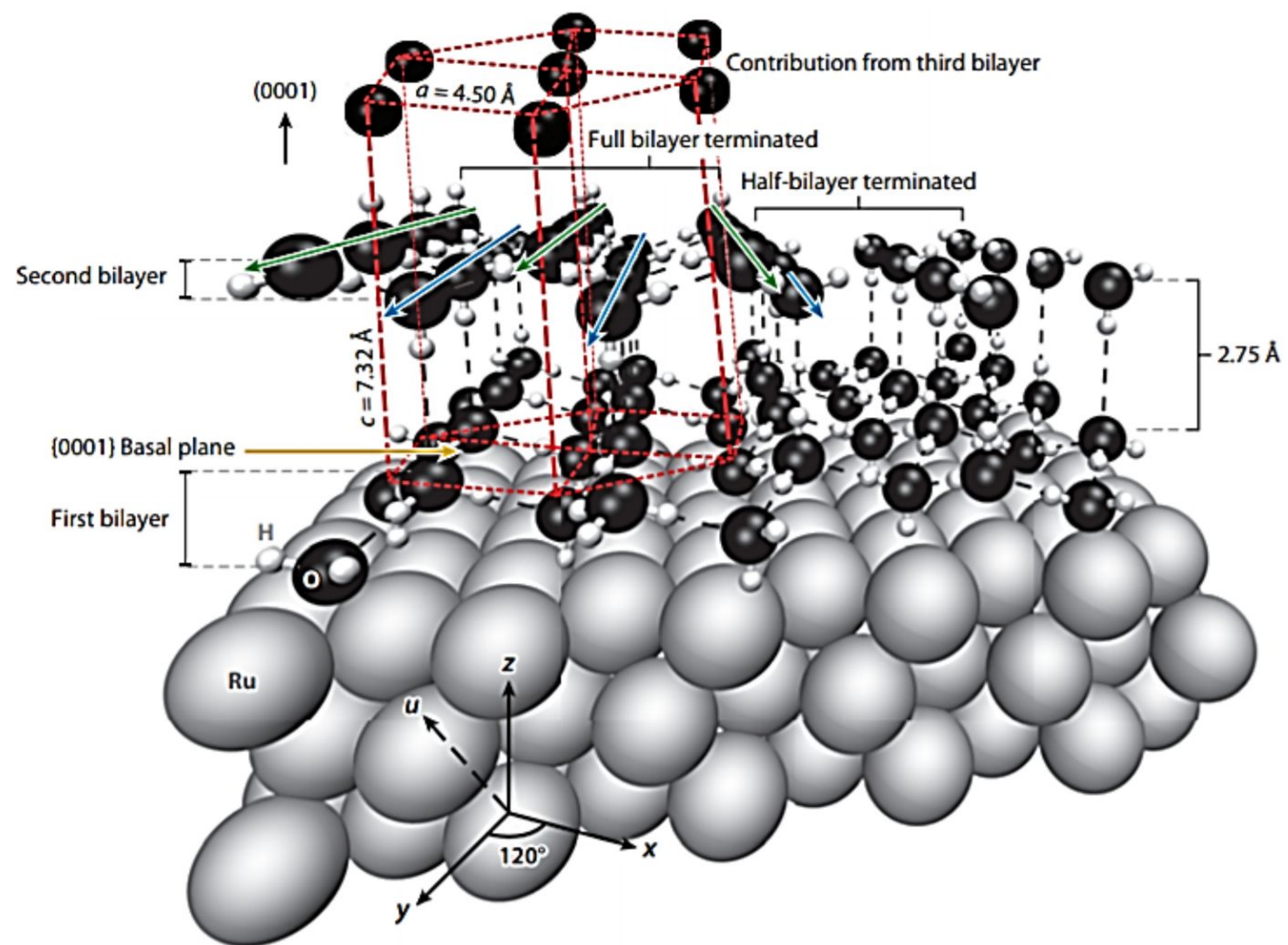
Instrumentation



115-400 nm

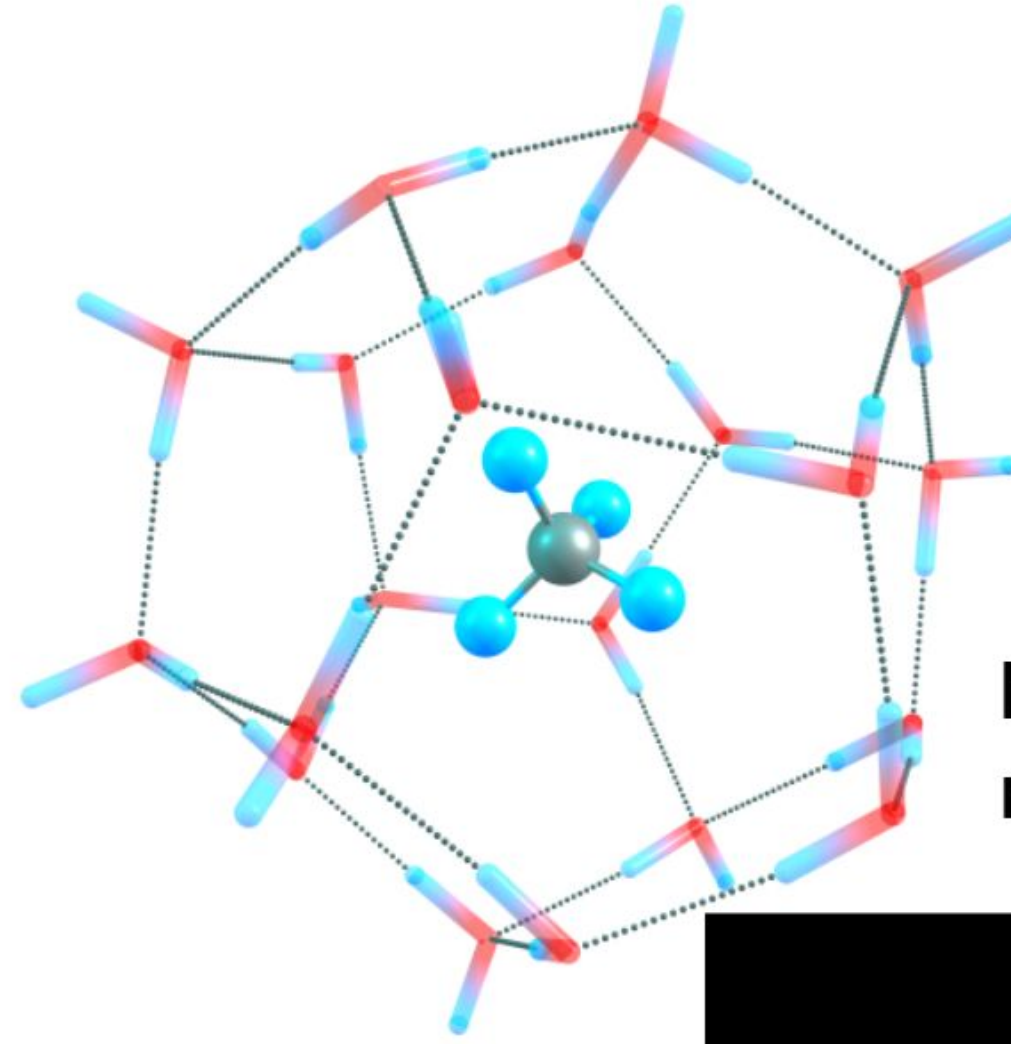
Bag, S. *et al.*, *Rev. Sci. Instrum.* **2014**, 85, 014103/1-014103/7

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

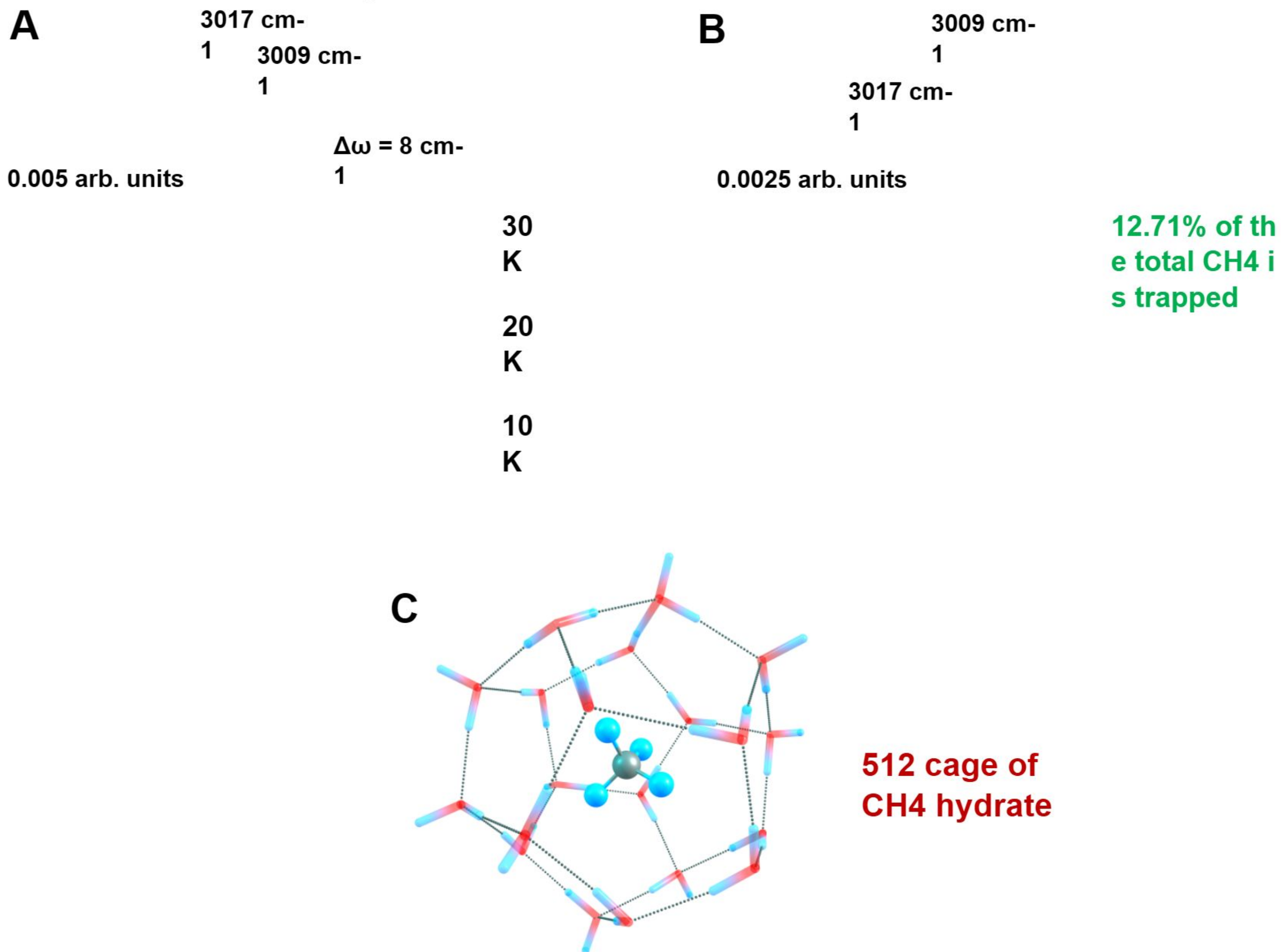
Annealing

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>



Read Online

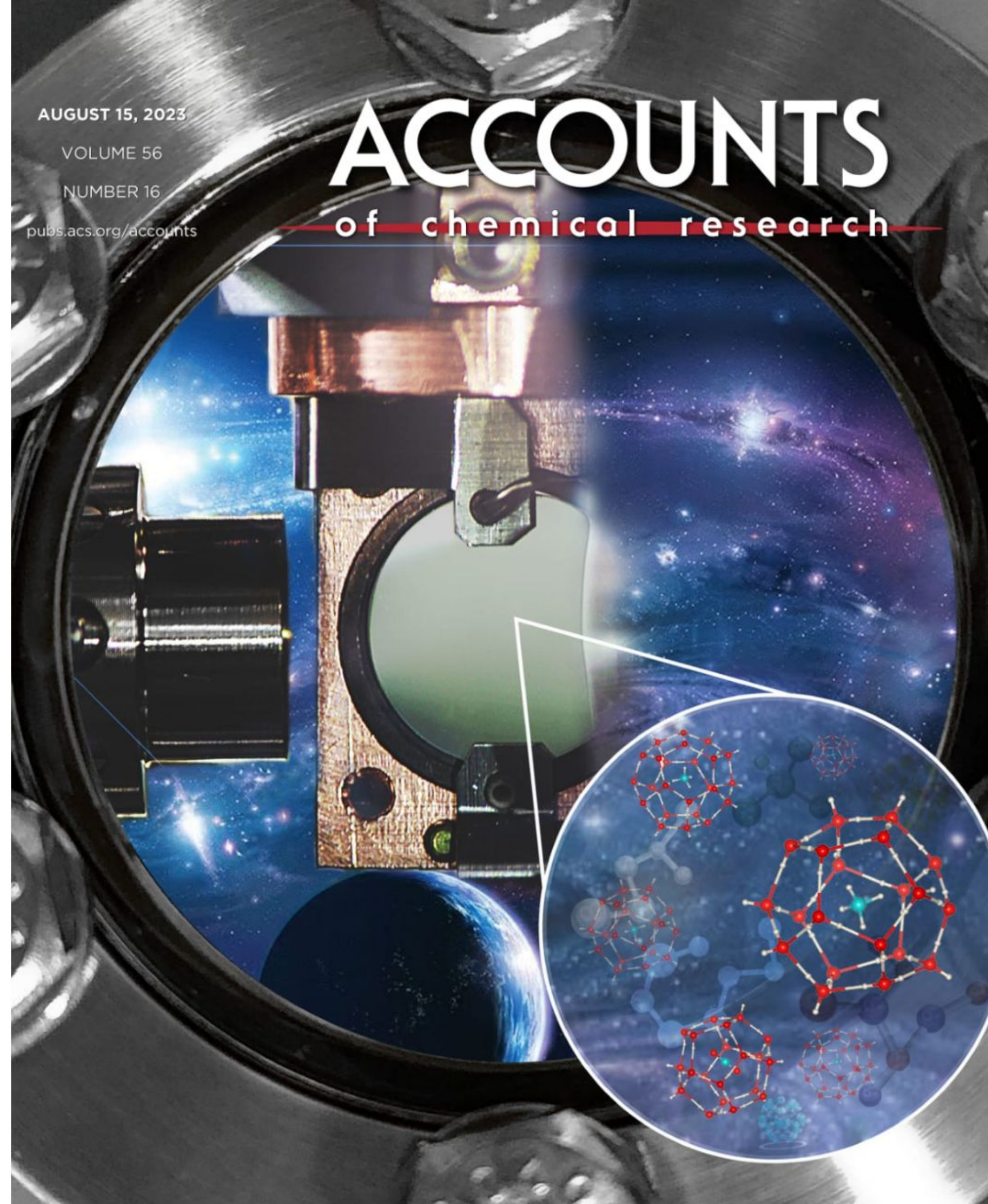
AUGUST 15, 2023

VOLUME 56

NUMBER 16

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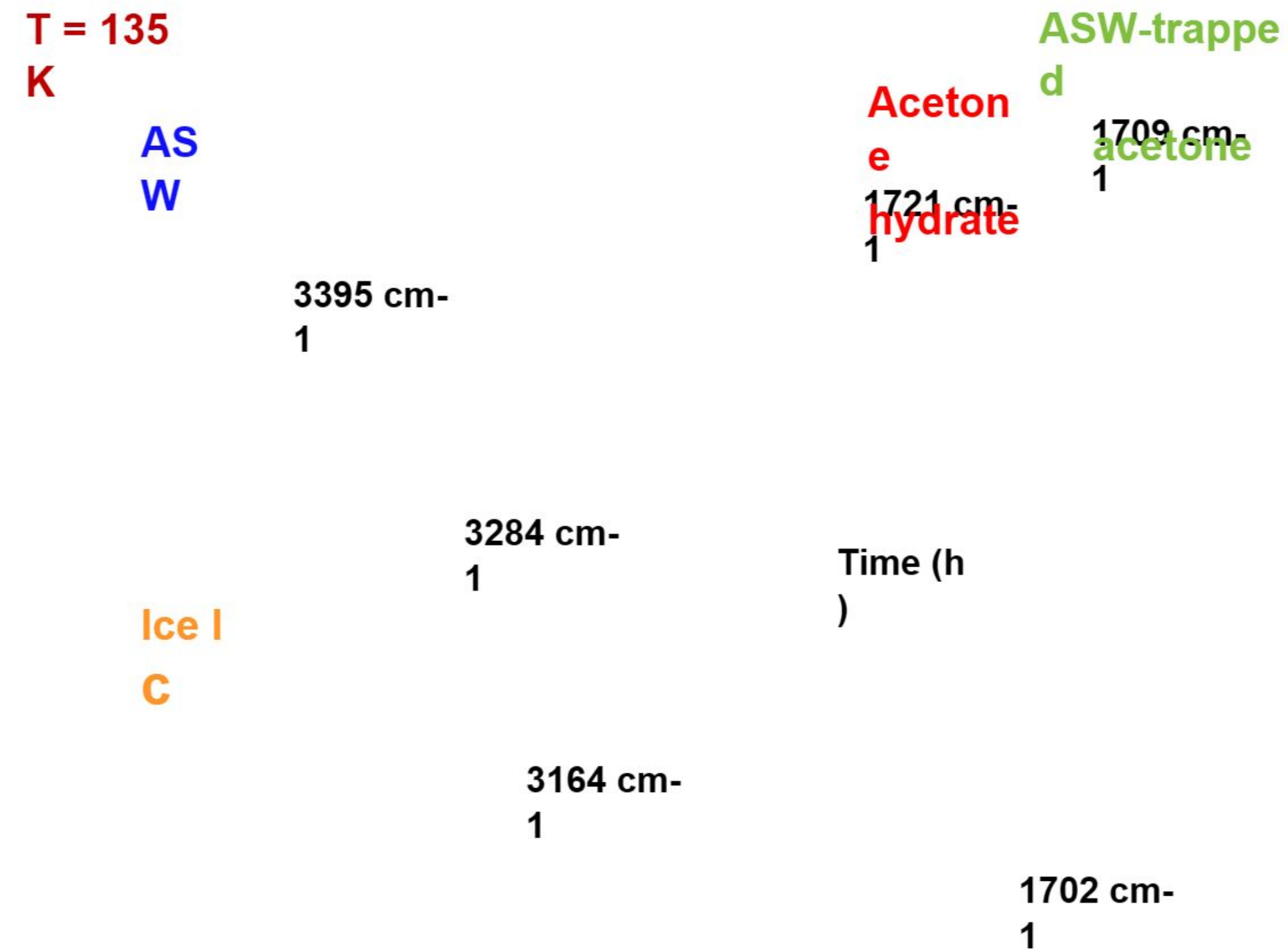
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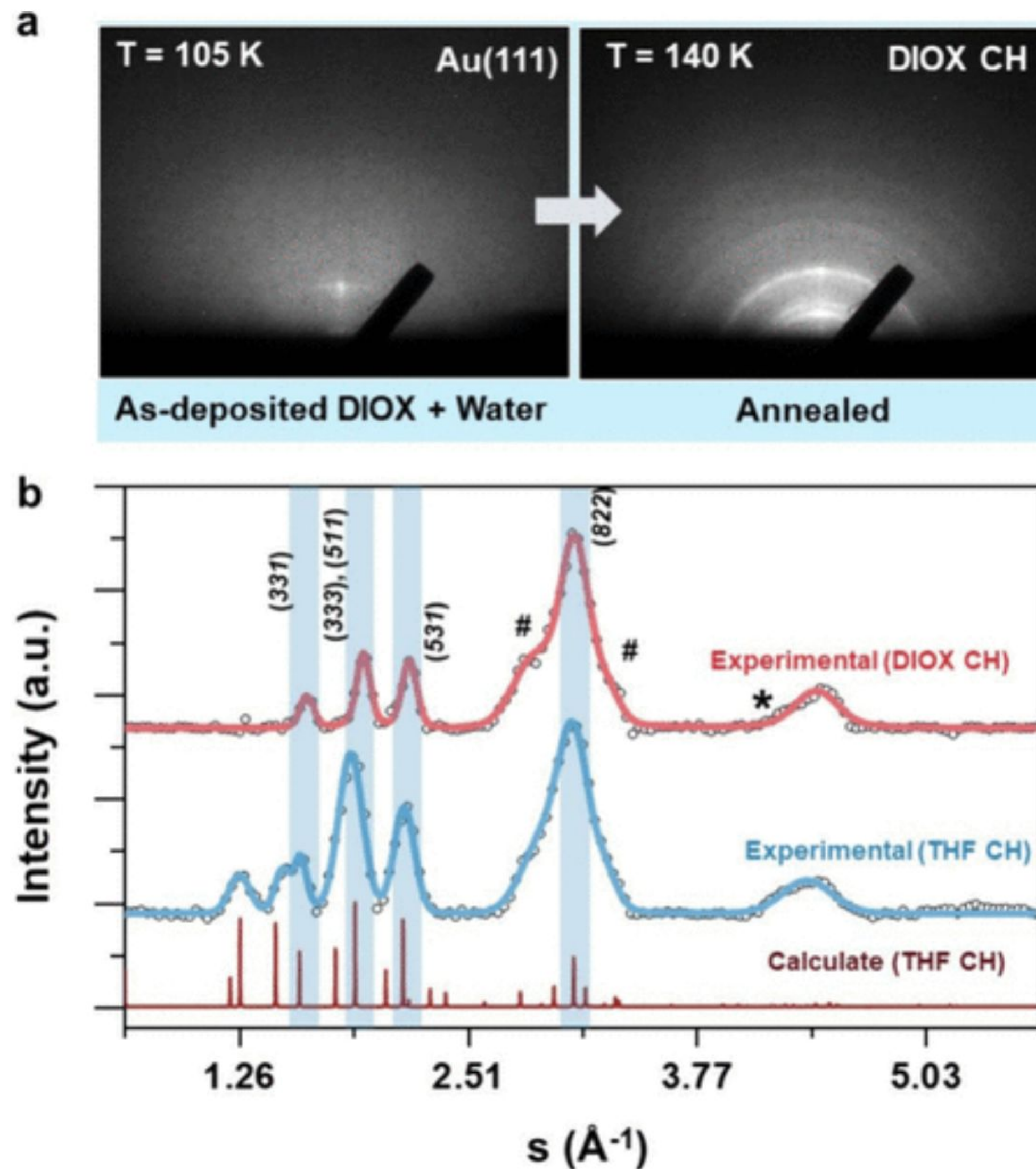
Cubic ice via clathrate hydrate



Cubic ice via clathrate hydrate

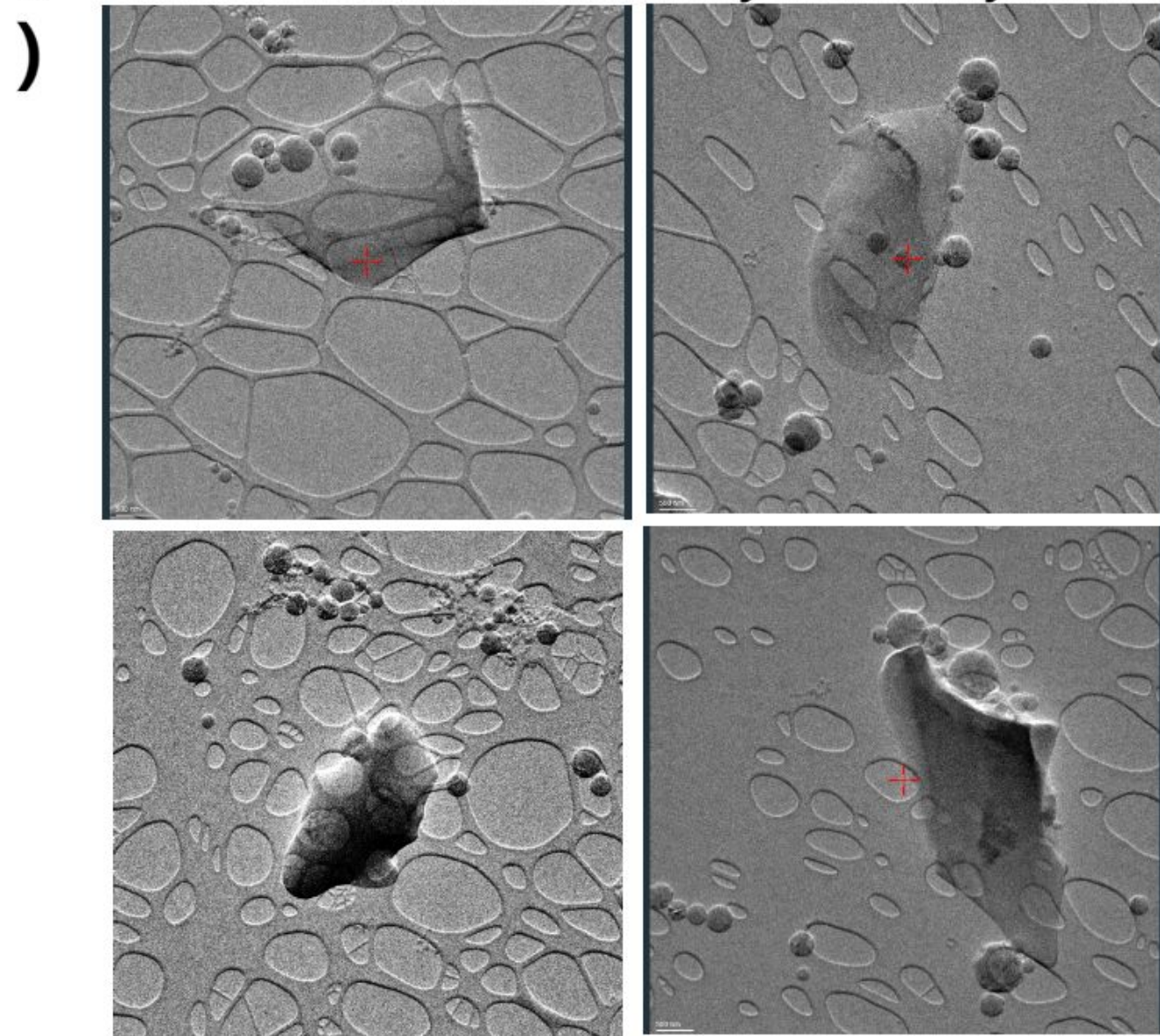
Dr. Ryutaro Soda,
NIMS, Tsukuba,
Japan

Hydrate structures by RHEED



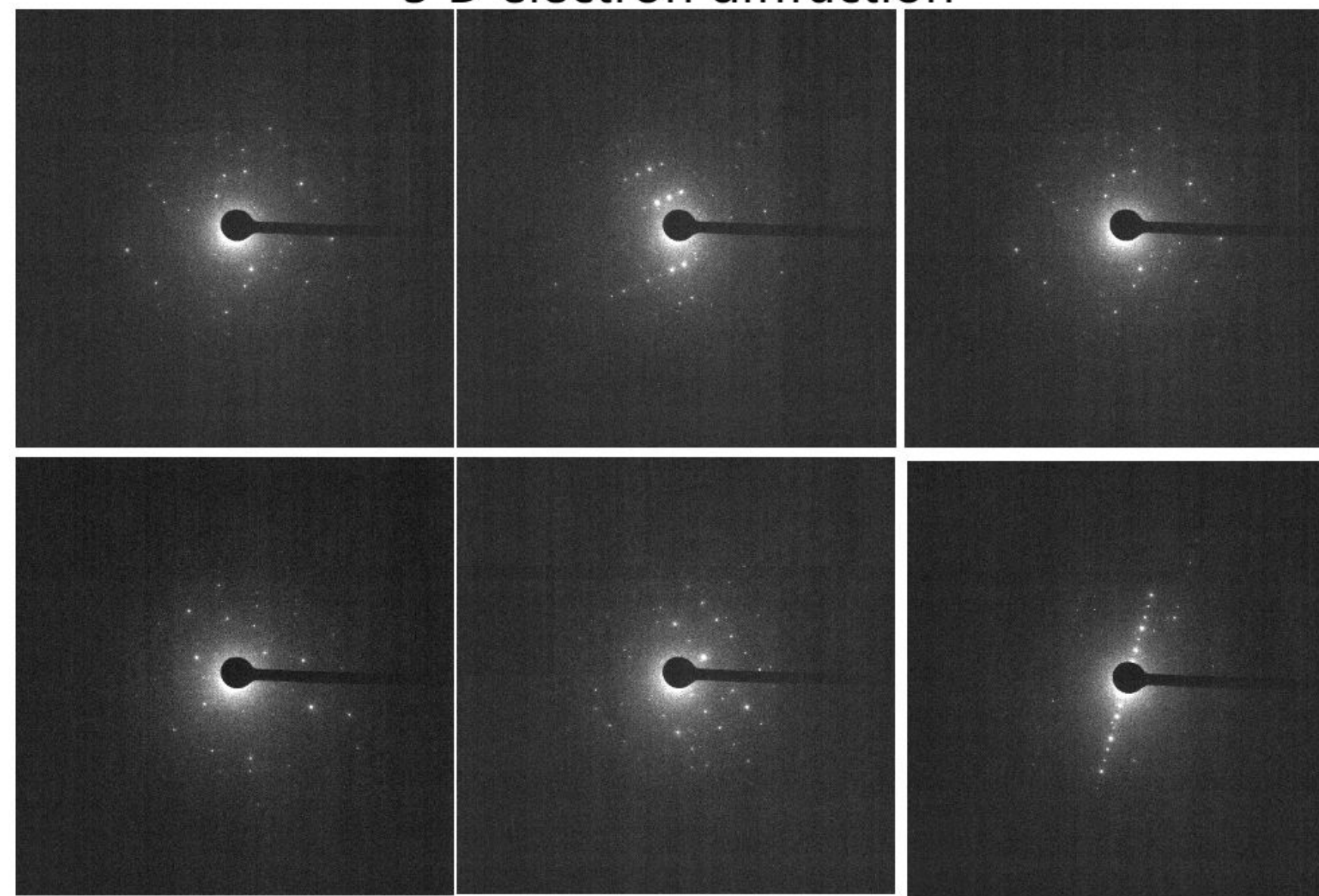
Micro-ED of nanometer-scale crystals of clathrate hydrates

(a) THF-CH₄ Clathrate hydrate crystal

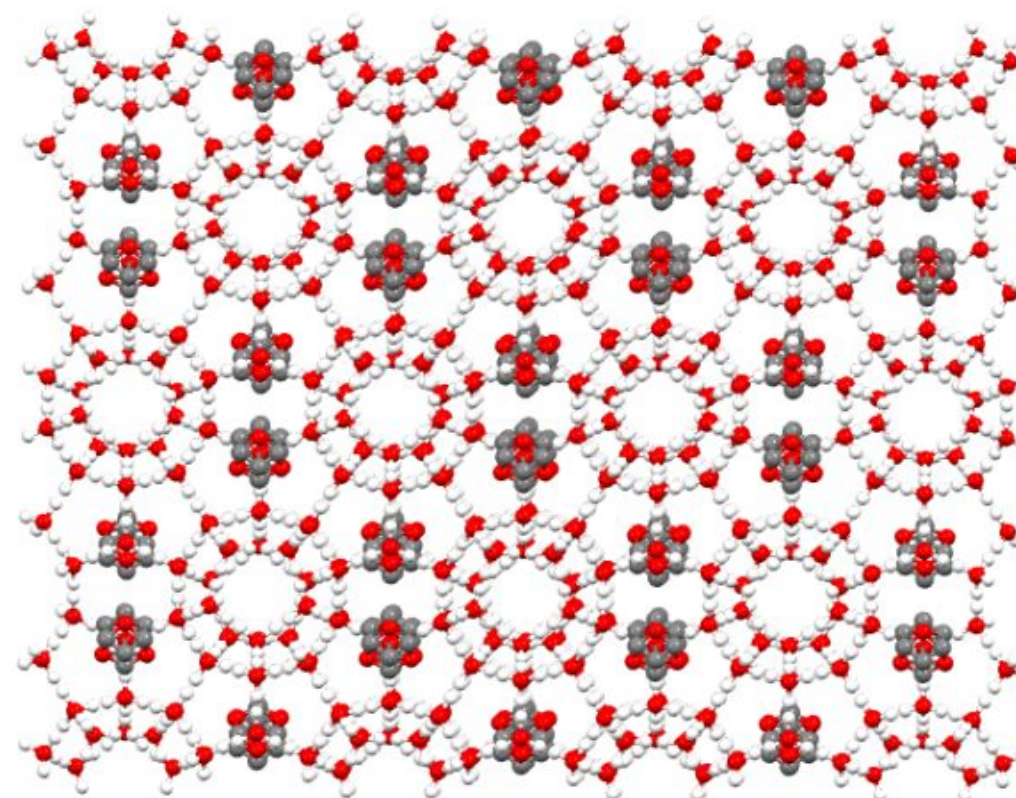
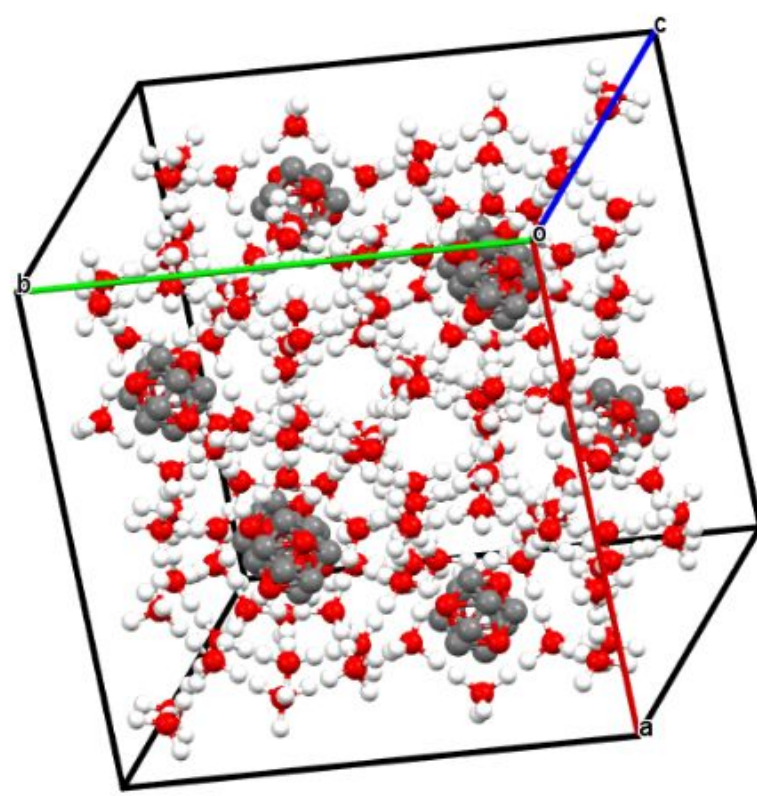


(b)

3 D electron diffraction

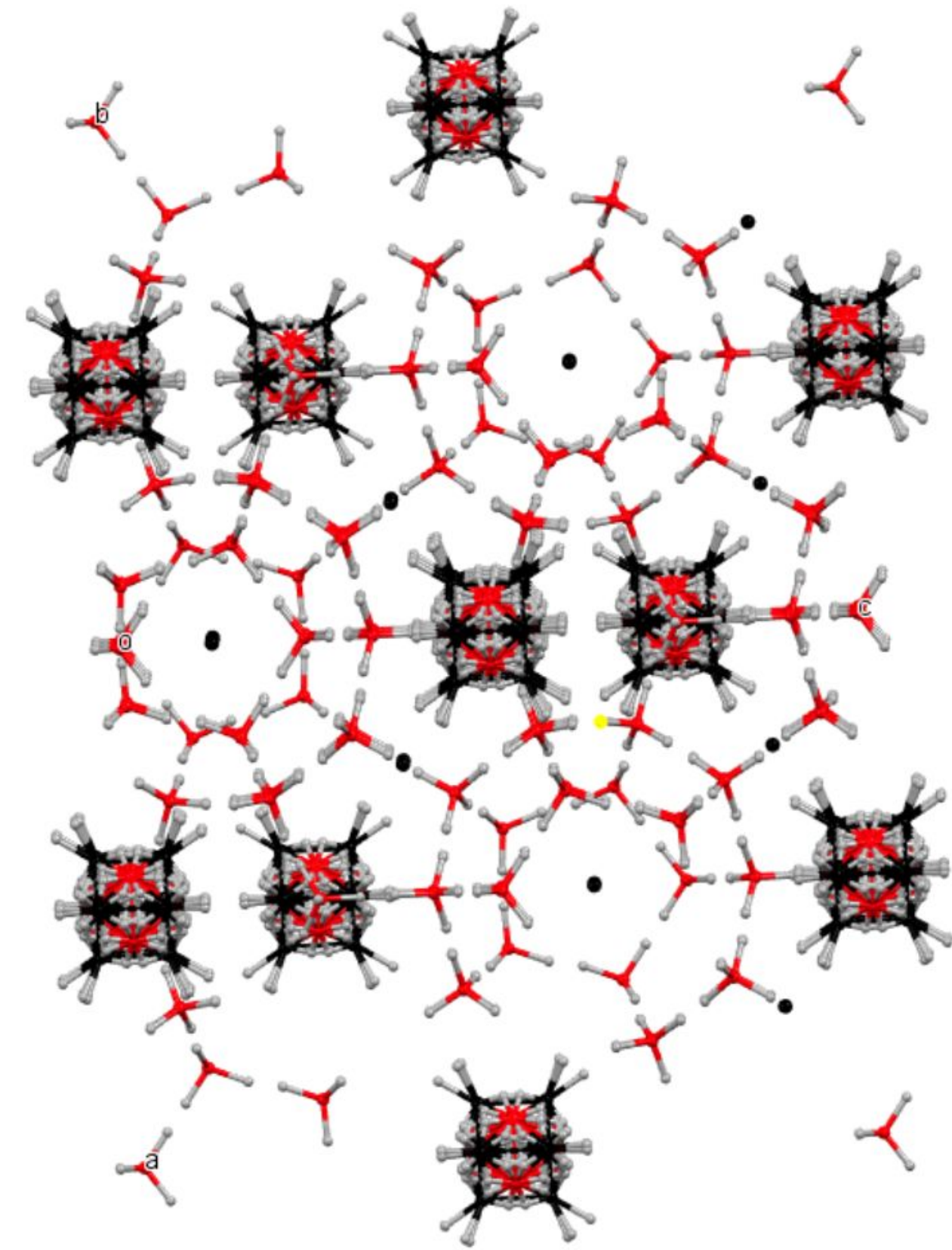
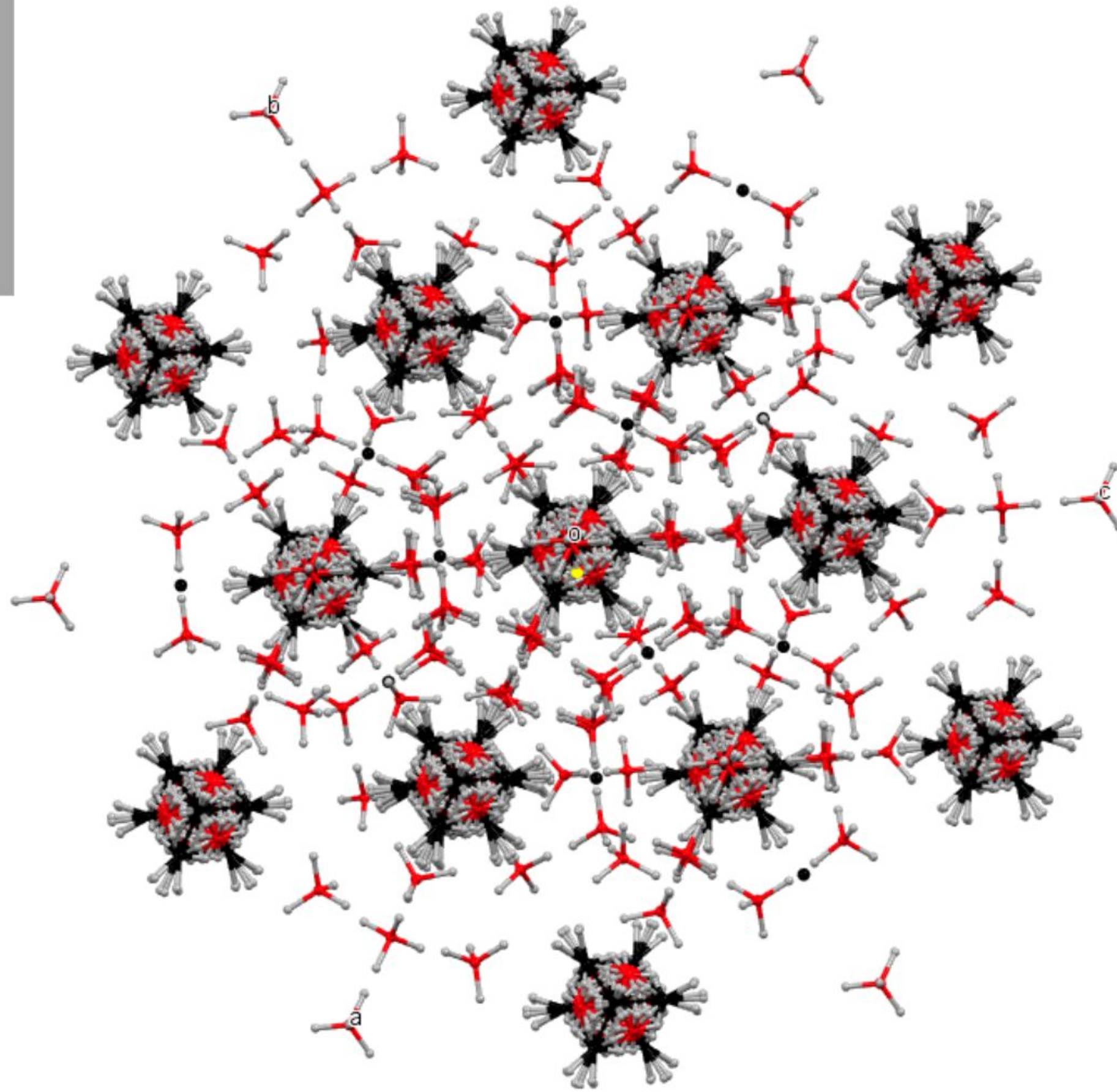
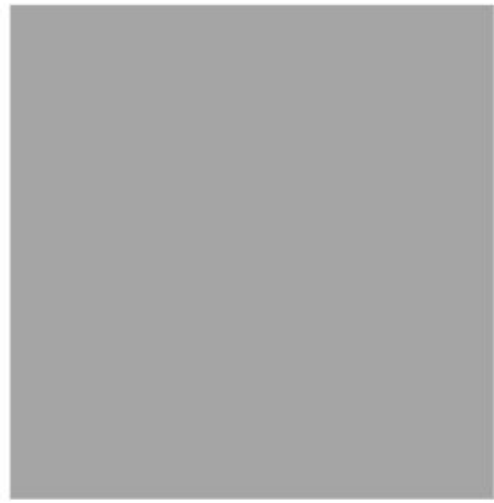


(c)



Crystal structure

MicroED – THF CH₄ clathrate hydrate



An ocean of opportunities

Water presents unique opportunities to find a purpose in life.

Conclusions

Atomically precise clusters and new molecular materials.

Affordable clean water with advanced materials is possible at scale.

Natural minerals break spontaneously in charged water microdroplets.

Clathrate hydrates exist in ultrahigh vacuum.

Implications of all these are profound for sustainability.

New research is needed in these areas.

Affordable, inclusive, sustainable and contextual 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

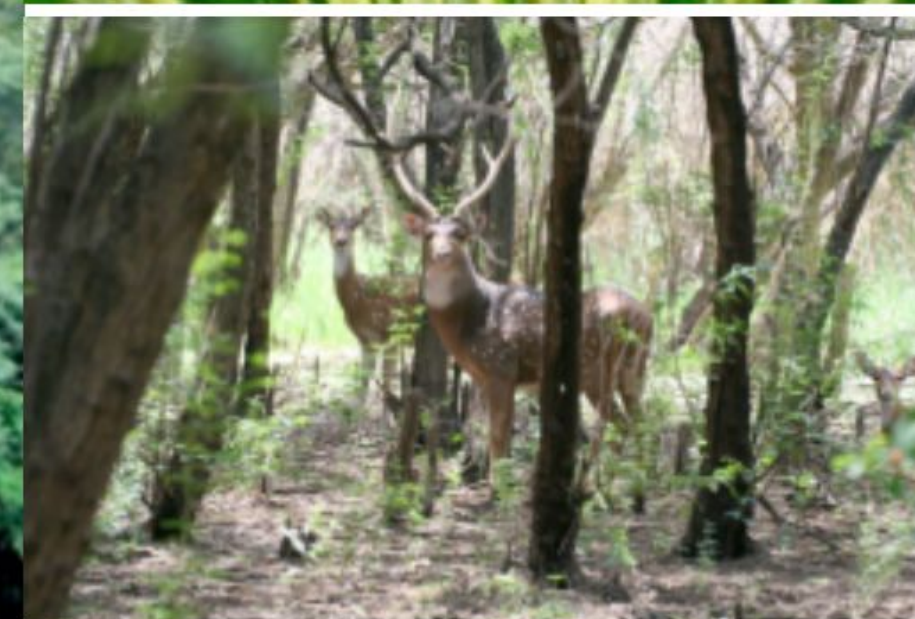
MS Theses: Ananthu Mahendranath, Ramesh Kumar Soni

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





Indian Institute of Technology Madras



Associate Editor
ACS
Sustainable
Resource Management

ramurthi/V. Kamakoti



**Single particle
s**

Structural Transitions and Micro- ED

Atomic precision does not end

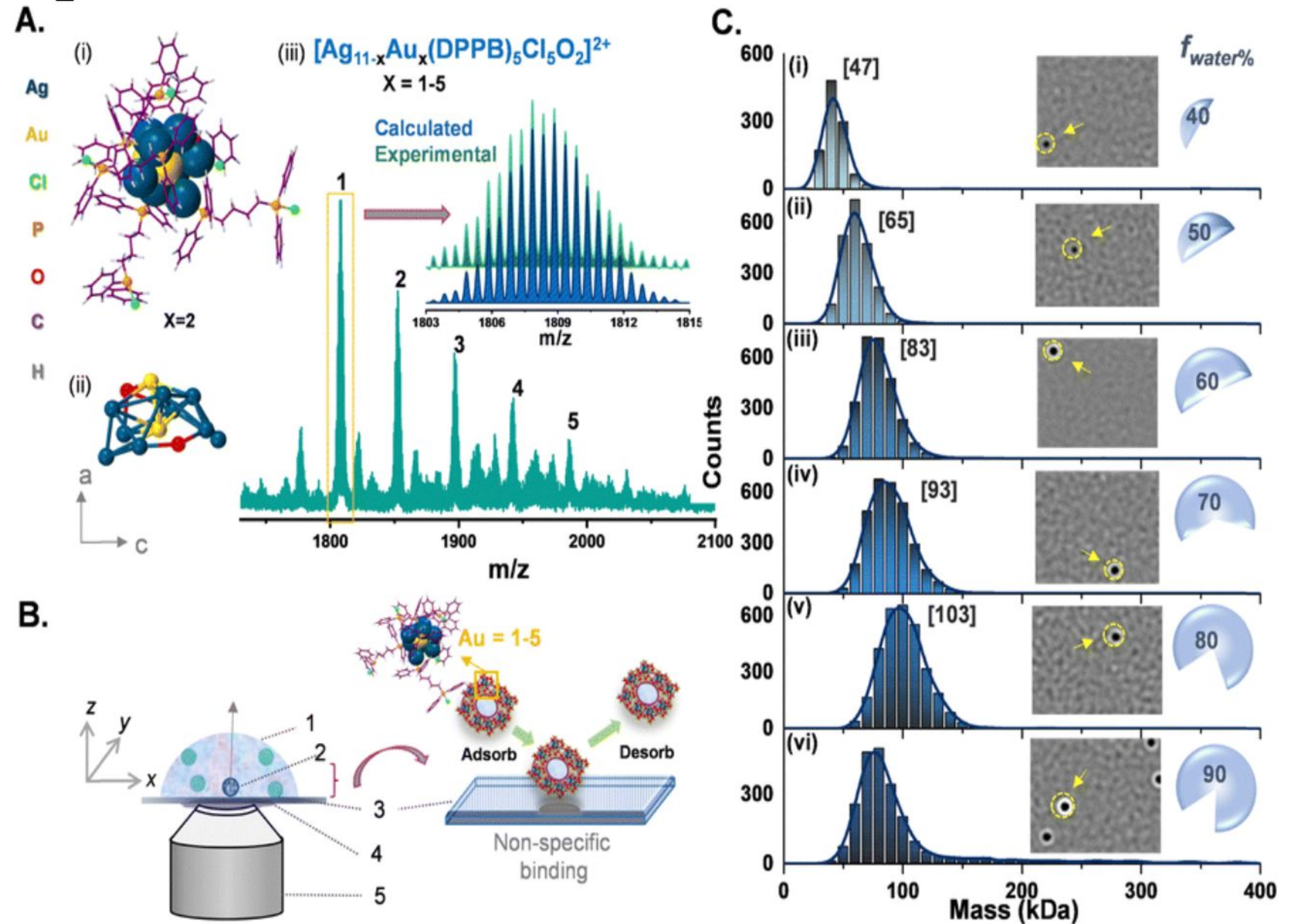
Mass Photometry



Key features :

Mass Range: 30 kDa to 5 MD

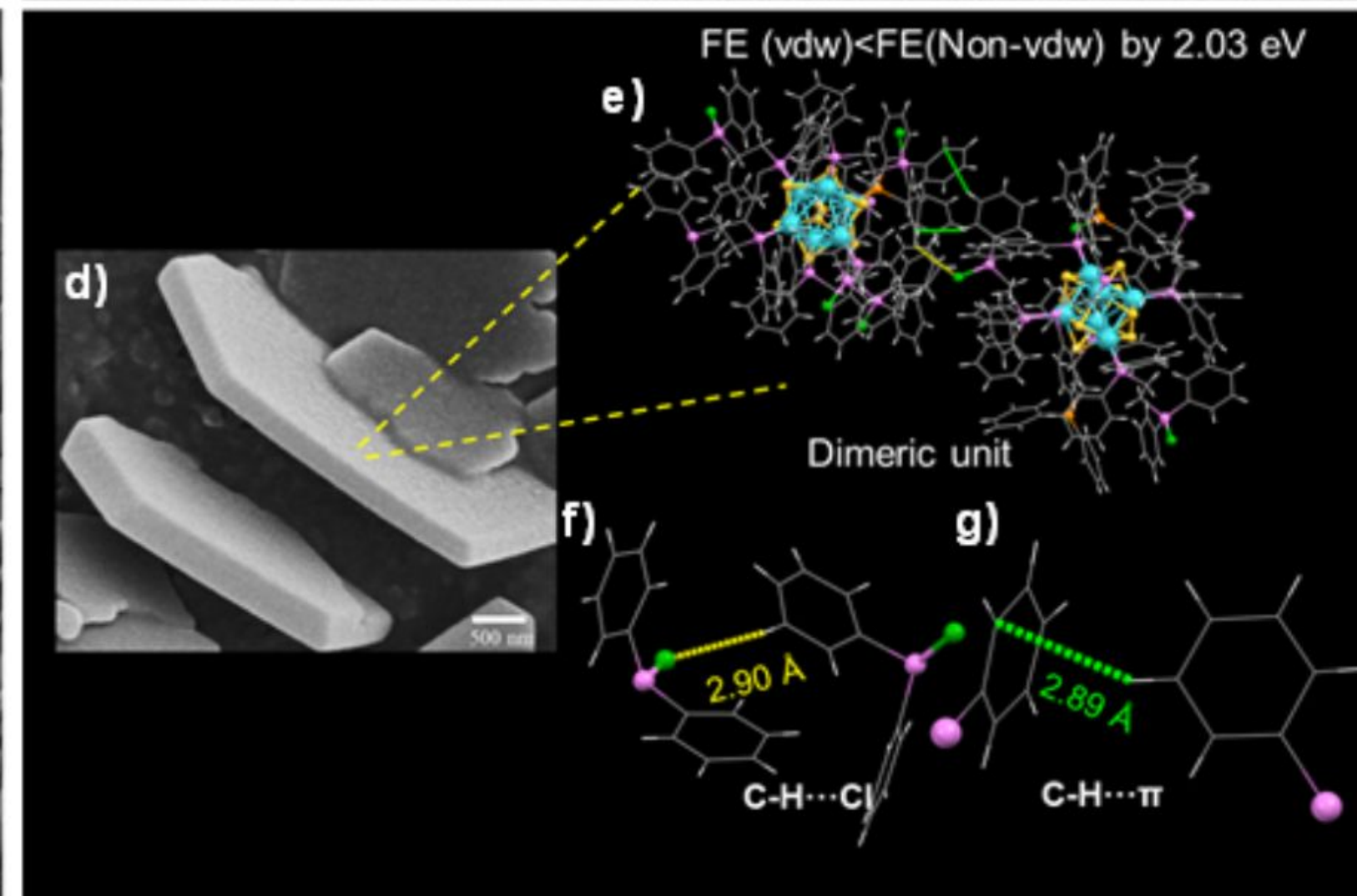
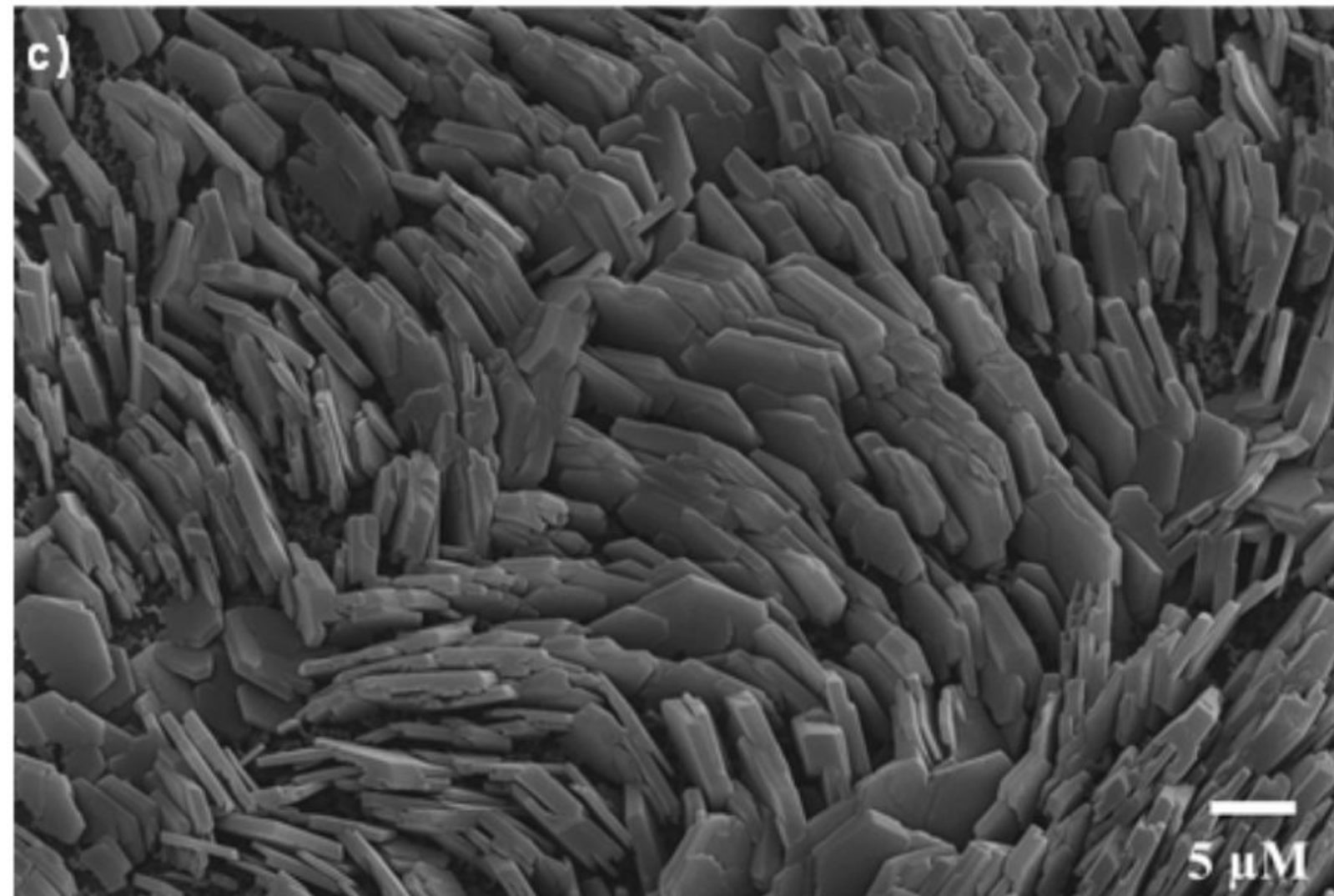
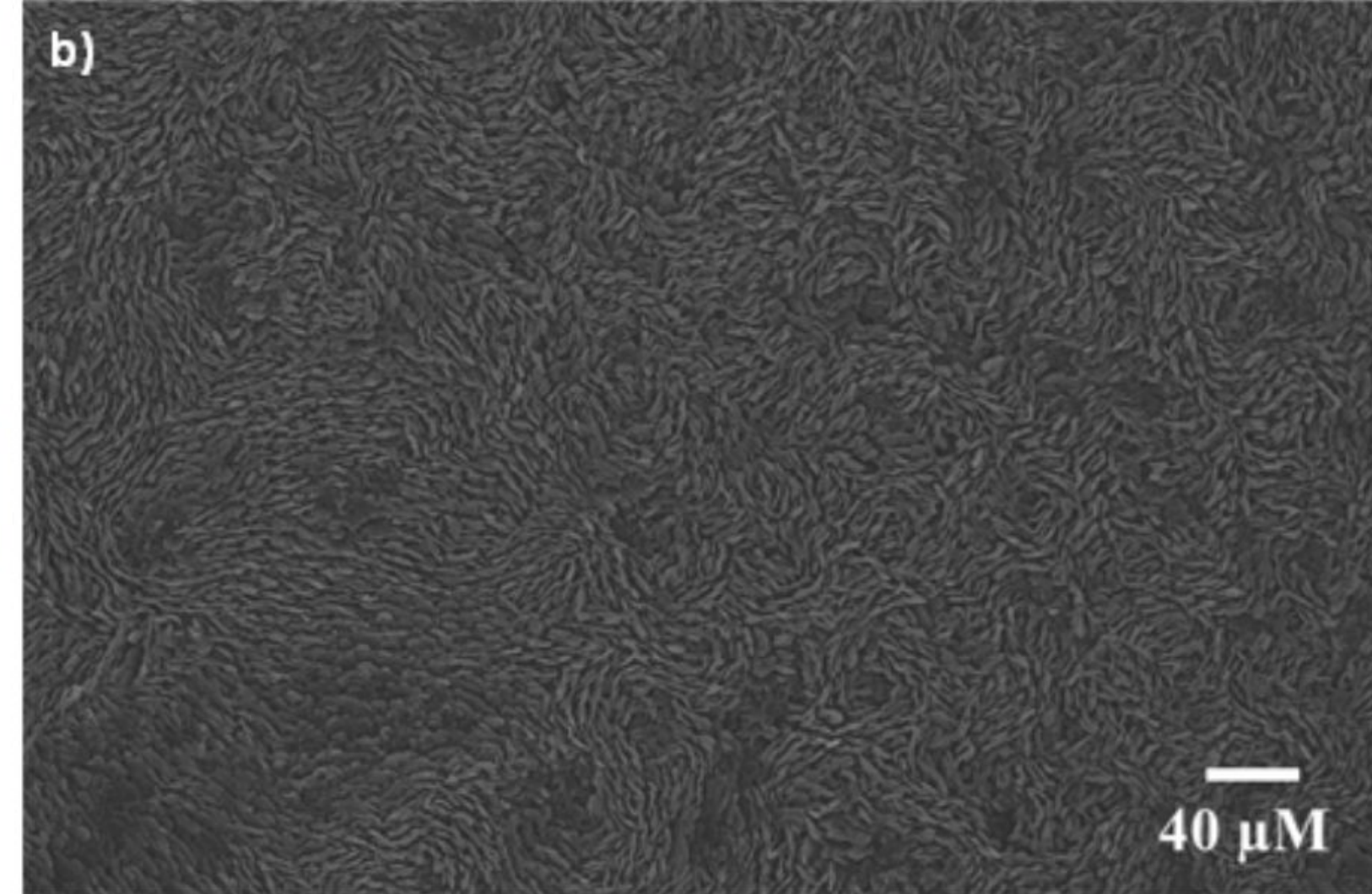
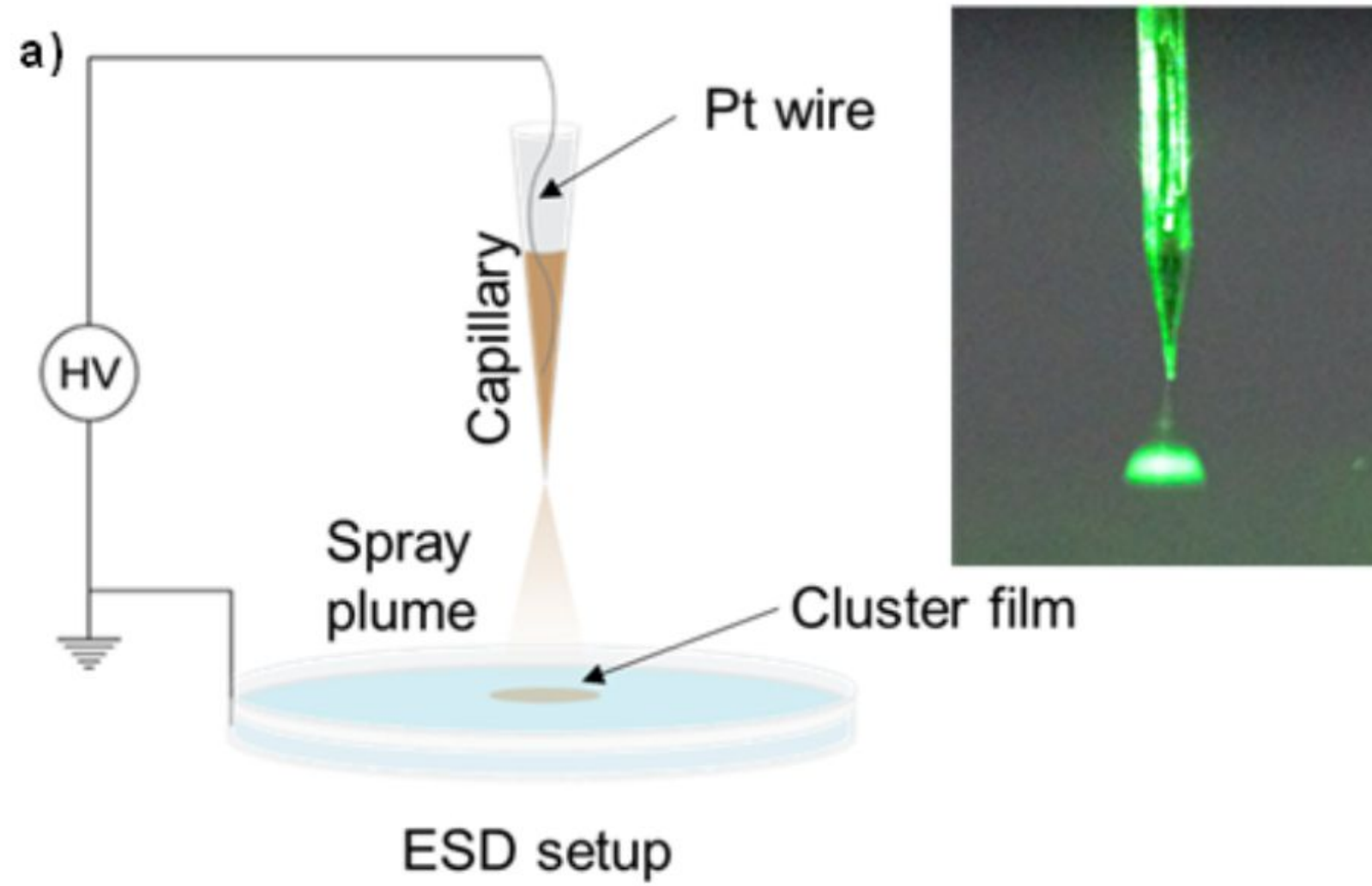
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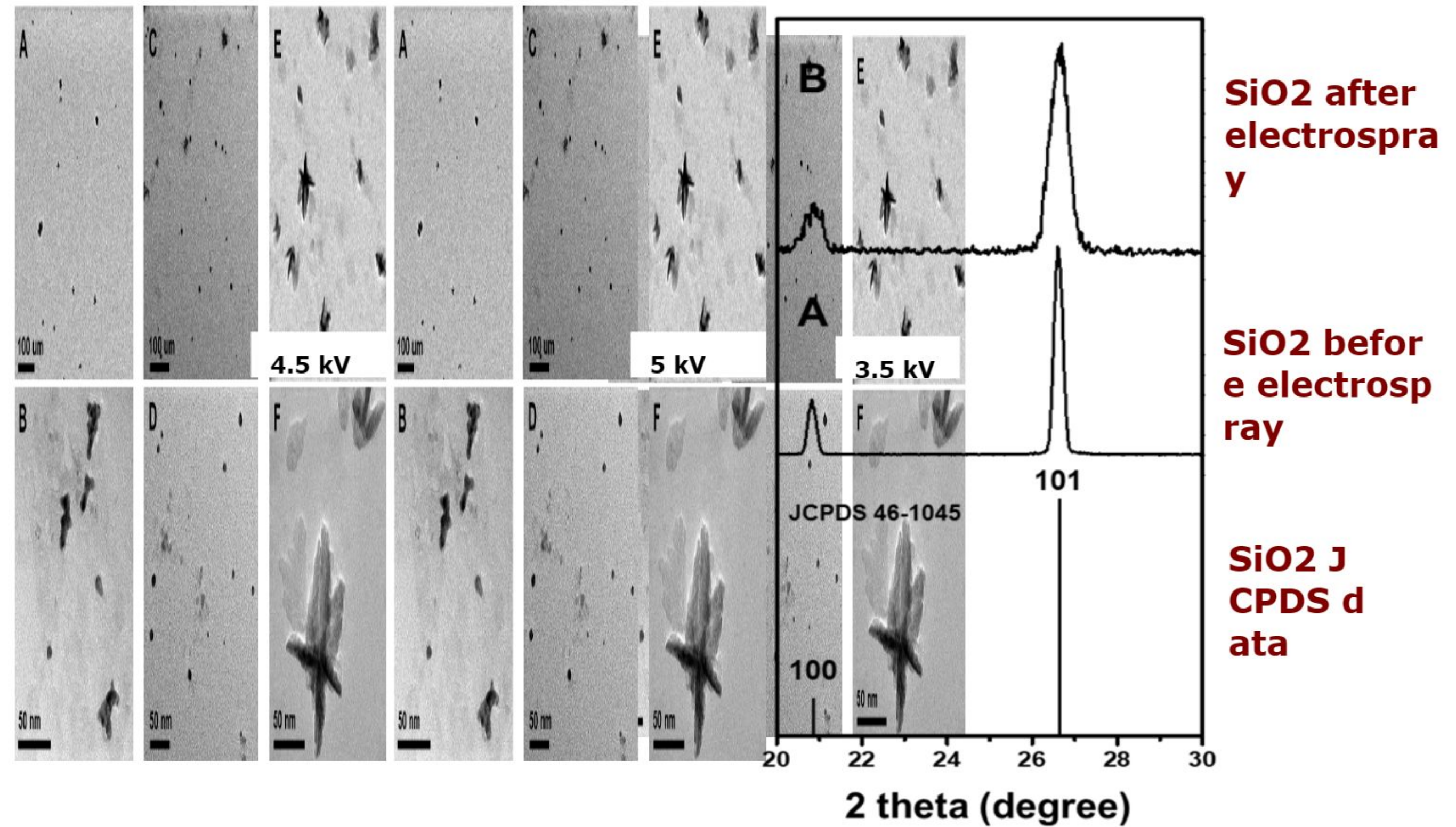
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Electrospray deposition

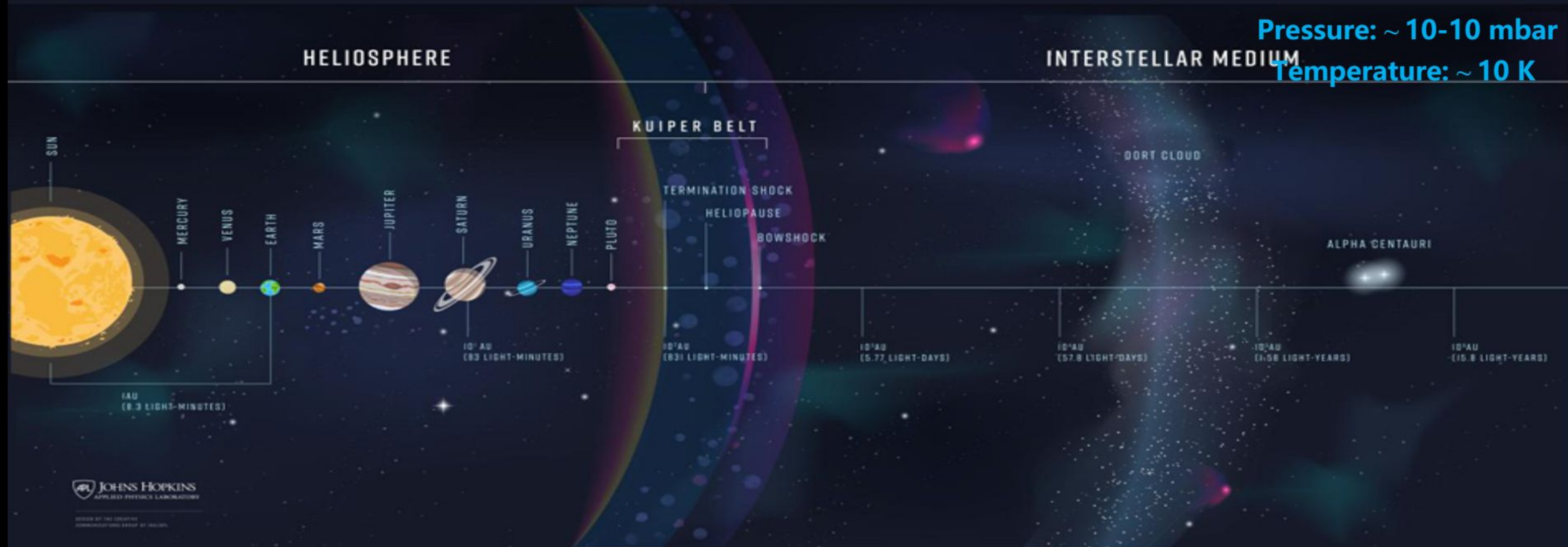


Functional Nanomaterials

Fragmentation of Silica – Varying Conditions



Interstellar medium



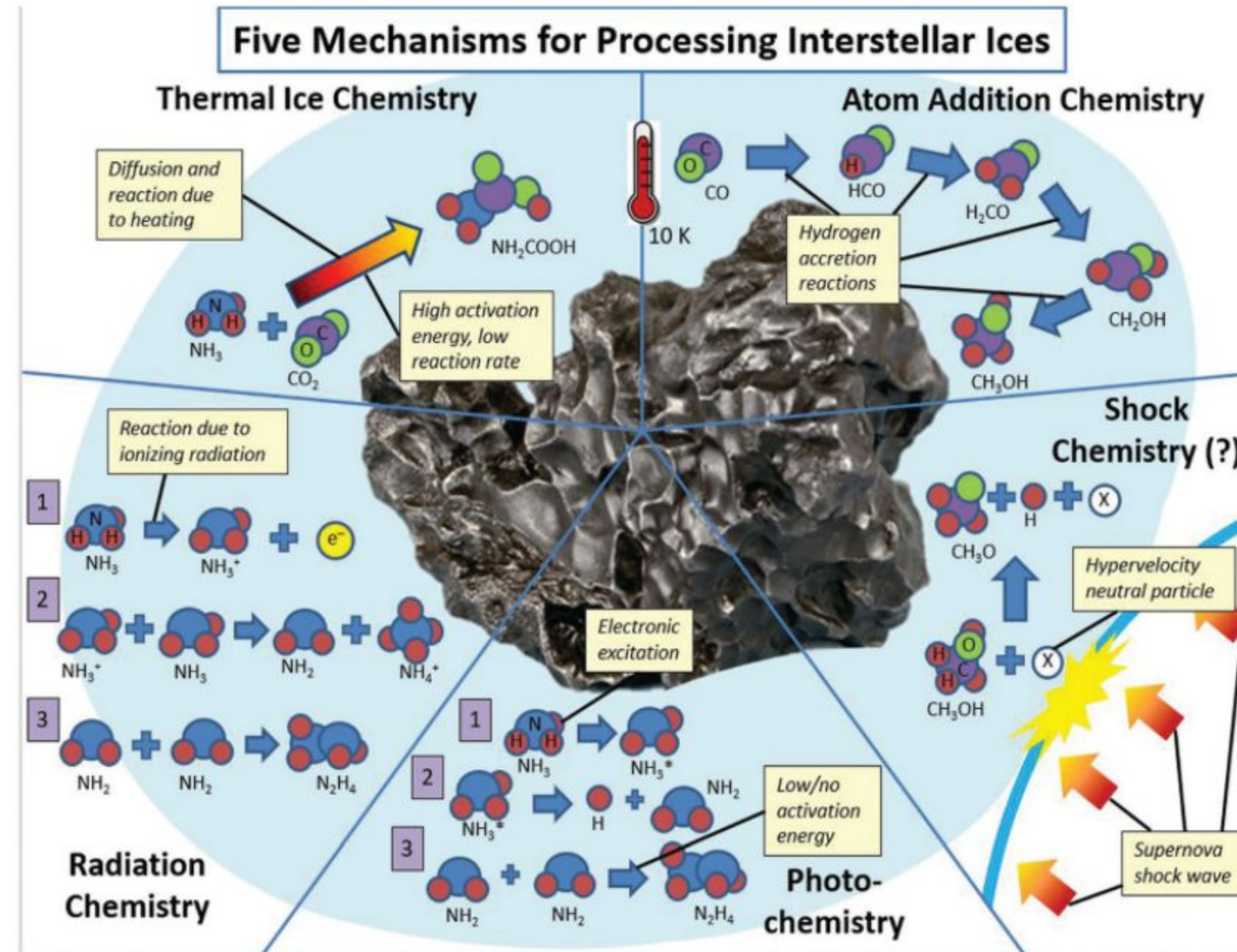
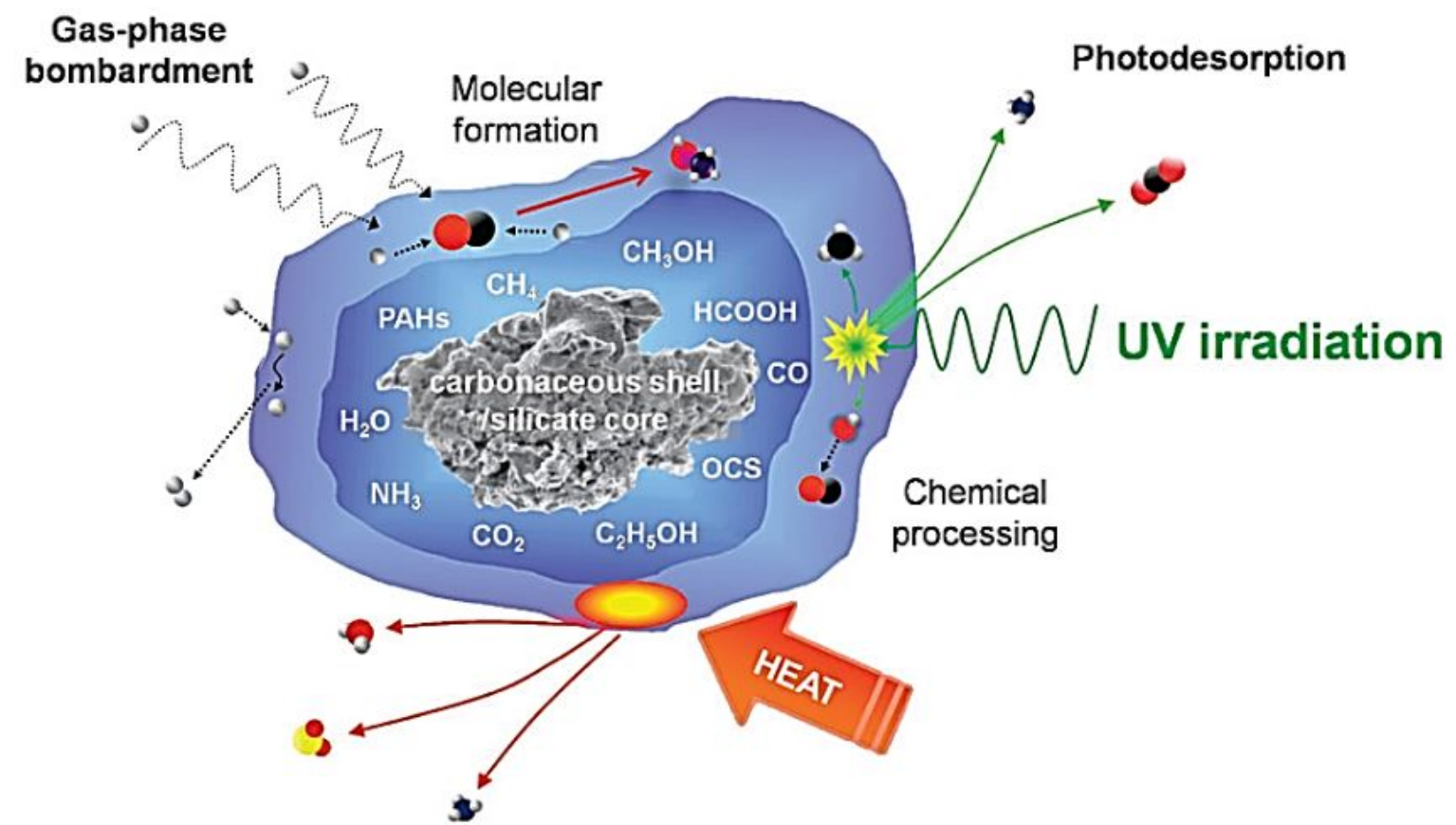
Diffuse clouds: $T \sim 100$ K, $n \sim 100$ molecules per cm^3

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

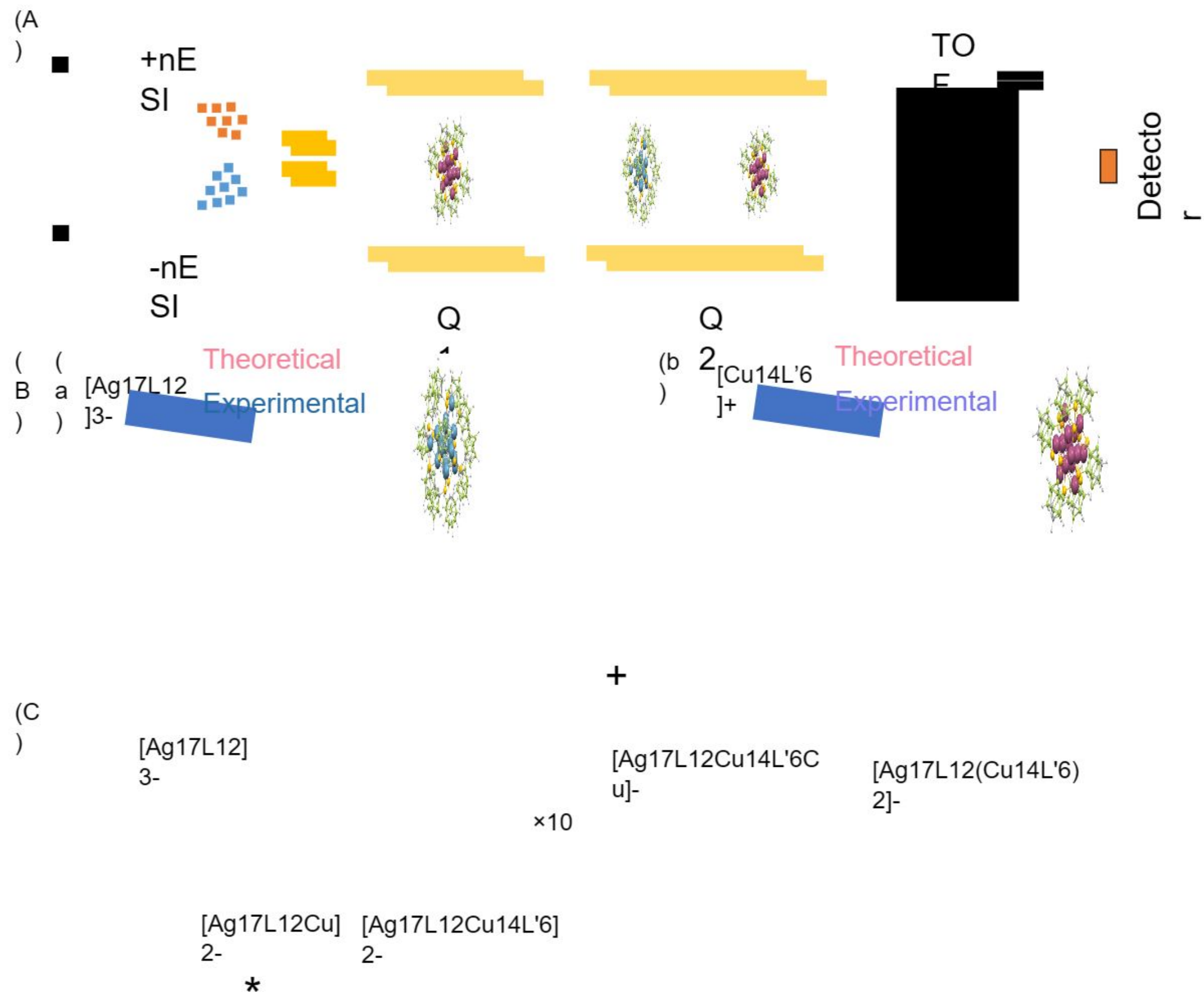


Silicates and carbonaceous material – 0.01-0.5 μm



Coulombic adduct

S



(A) Schematic representation of gas phase ion-ion reaction of atomically precise nanoclusters in an MS trap cell. Atomically precise nanoclusters (B) (a) [Ag₁₇(o1-CBT)₁₂]³⁻ and (b) [Cu₁₄(o9,12-CBDT)₆]²⁺ forming (C) Coulombic adducts.

With Scott McLuckey and De-en Jiang