



Now in the 65th year

My research and need for computations

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Co-founder

InnoNano Research Pvt. Ltd.

InnoDI Water Technologies Pvt. Ltd.

VayuJAL Technologies Pvt. Ltd.

Aqueasy Innovations Pvt. Ltd.

Hydromaterials Pvt. Ltd.

EyeNetAqua Solutions Pvt. Ltd.

DeepSpectrum Innovations Pvt. Ltd.

Professor-in-charge



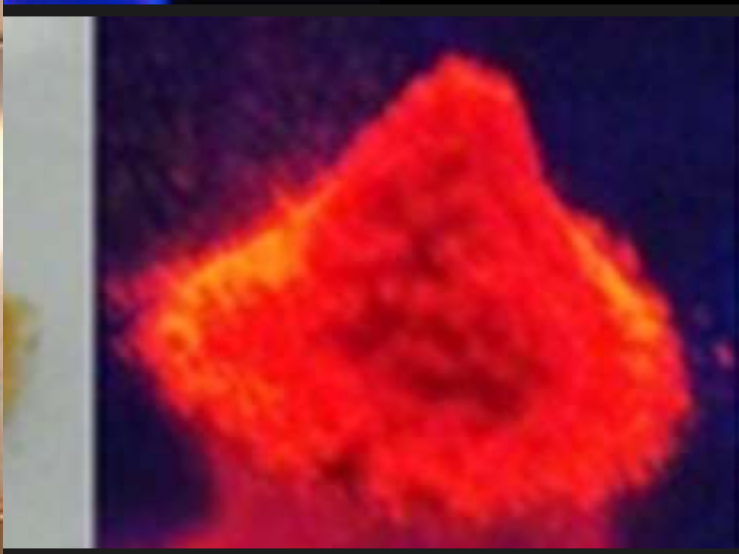
International Centre for Clean Water



Associate Editor

ACS
Sustainable
Resource Management



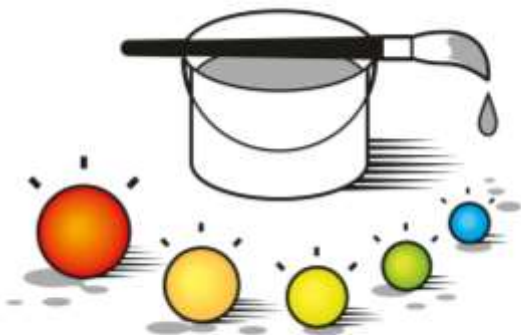


Quantum Dots – Seeds of Nanoscience



THE NOBEL PRIZE IN CHEMISTRY 2023

The Royal Swedish Academy of Sciences has decided to award the Nobel Prize in Chemistry 2023 to



©Johan Jarnestad/The Royal Swedish Academy of Sciences

Moungi G. Bawendi

Massachusetts Institute of Technology (MIT),
Cambridge, MA, USA



Louis E. Brus

Columbia University, New York, NY, USA



Alexei I. Ekimov

Nanocrystals Technology Inc., New York,
NY, USA



‘for the discovery and synthesis of quantum dots’

C₆₀: Buckminsterfullerene

**H. W. Kroto*, J. R. Heath, S. C. O'Brien, R. F. Curl
& R. E. Smalley**

Rice Quantum Institute and Departments of Chemistry and Electrical Engineering, Rice University, Houston, Texas 77251, USA

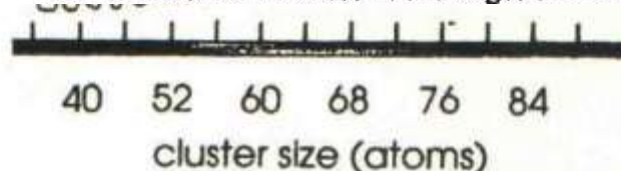
During experiments aimed at understanding the mechanisms by which long-chain carbon molecules are formed in interstellar space and circumstellar shells¹, graphite has been vaporized by laser irradiation, producing a remarkably stable cluster consisting of 60 carbon atoms. Concerning the question of what kind of 60-carbon atom structure might give rise to a superstable species, we suggest a truncated icosahedron, a polygon with 60 vertices and 32 faces, 12 of which are pentagonal and 20 hexagonal. This object is commonly encountered as the football shown in Fig. 1. The C₆₀ molecule which results when a carbon atom is placed at each vertex of this structure has all valences satisfied by two single bonds and one double bond, has many resonance structures, and appears to be aromatic.

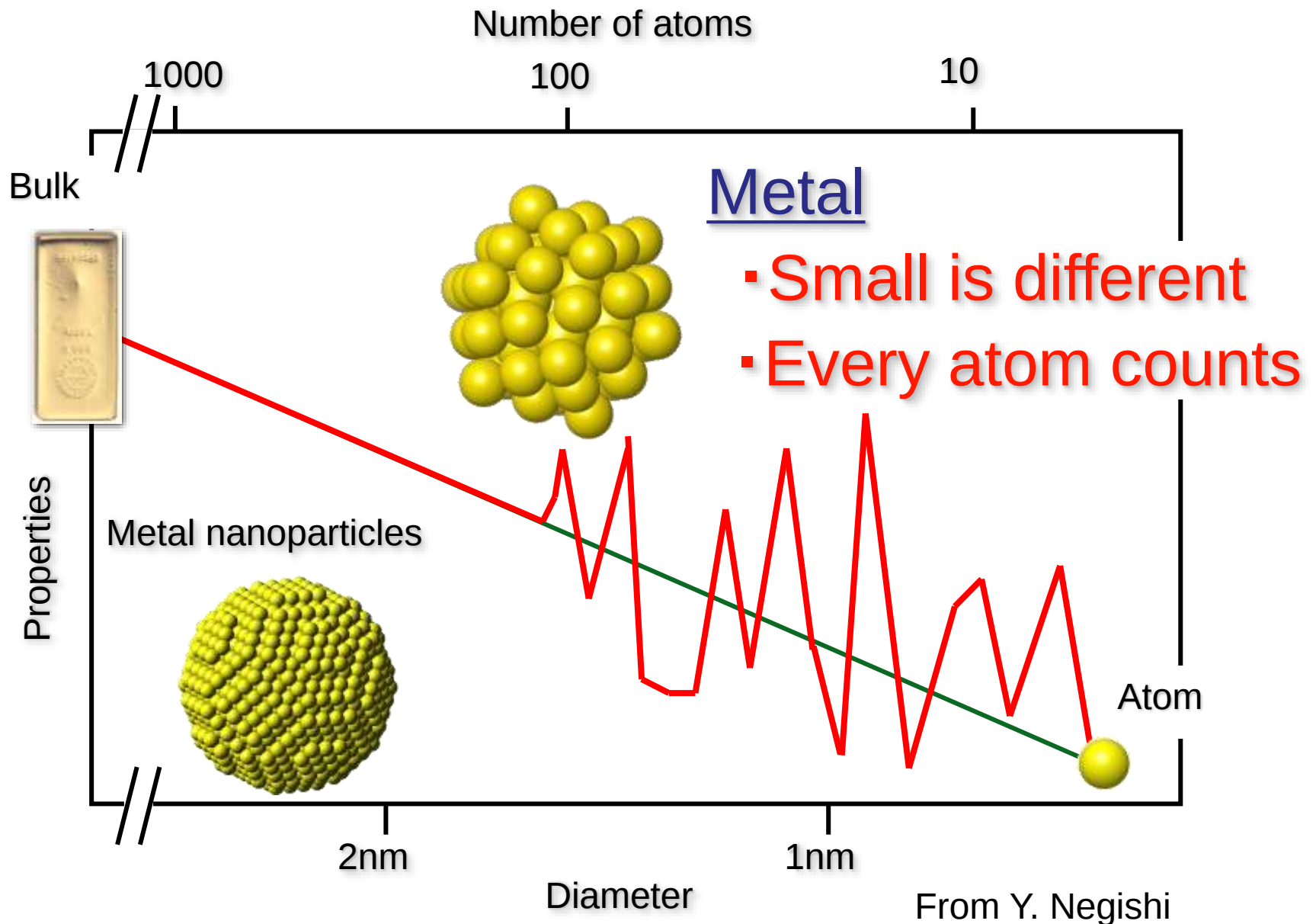
Fig. 1 A football (in the United States, a soccerball) on Texas grass. The C₆₀ molecule featured in this letter is suggested to have the truncated icosahedral structure formed by replacing each vertex on the seams of such a ball by a carbon atom.



graphite fused six-membered ring structure. We believe that the distribution in Fig. 3c is fairly representative of the nascent distribution of larger ring fragments. When these hot ring clusters are left in contact with high-density helium, the clusters equilibrate by two- and three-body collisions towards the most stable species, which appears to be a unique cluster containing 60 atoms.

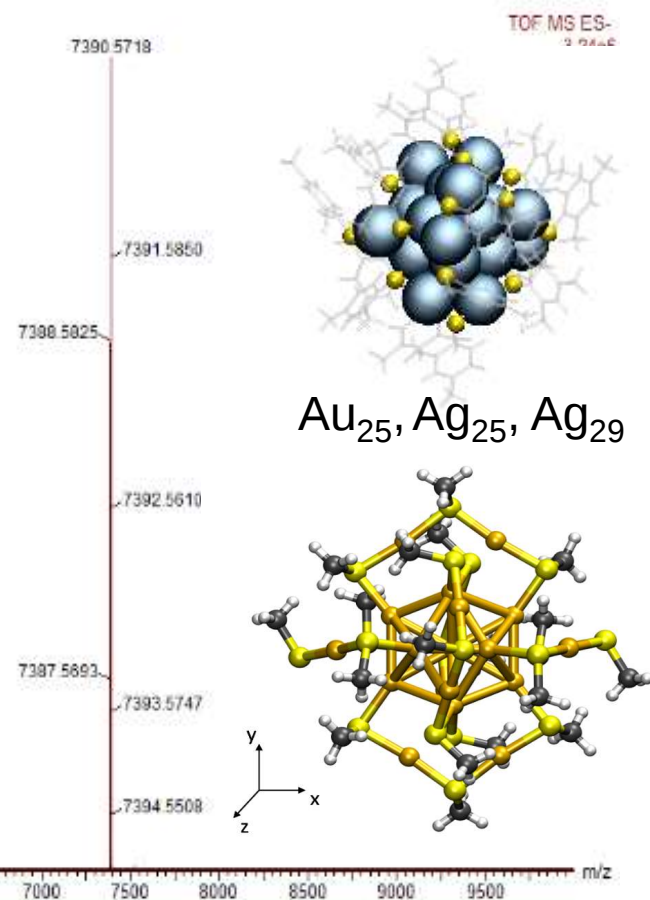
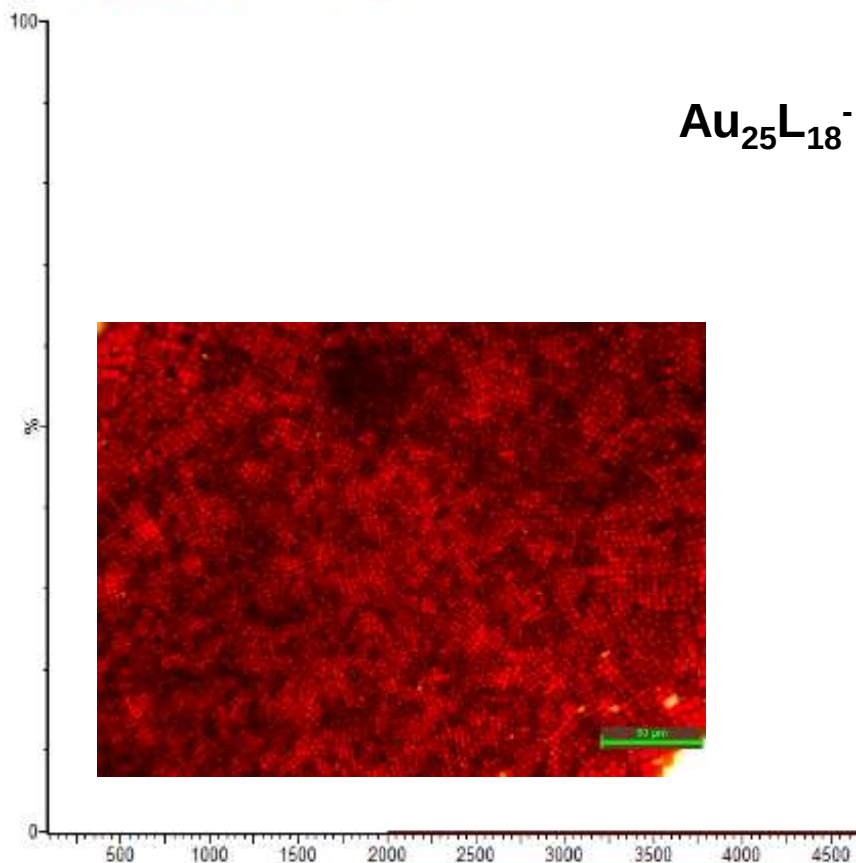
When one thinks in terms of the many fused-ring isomers with unsatisfied valences at the edges that would naturally arise





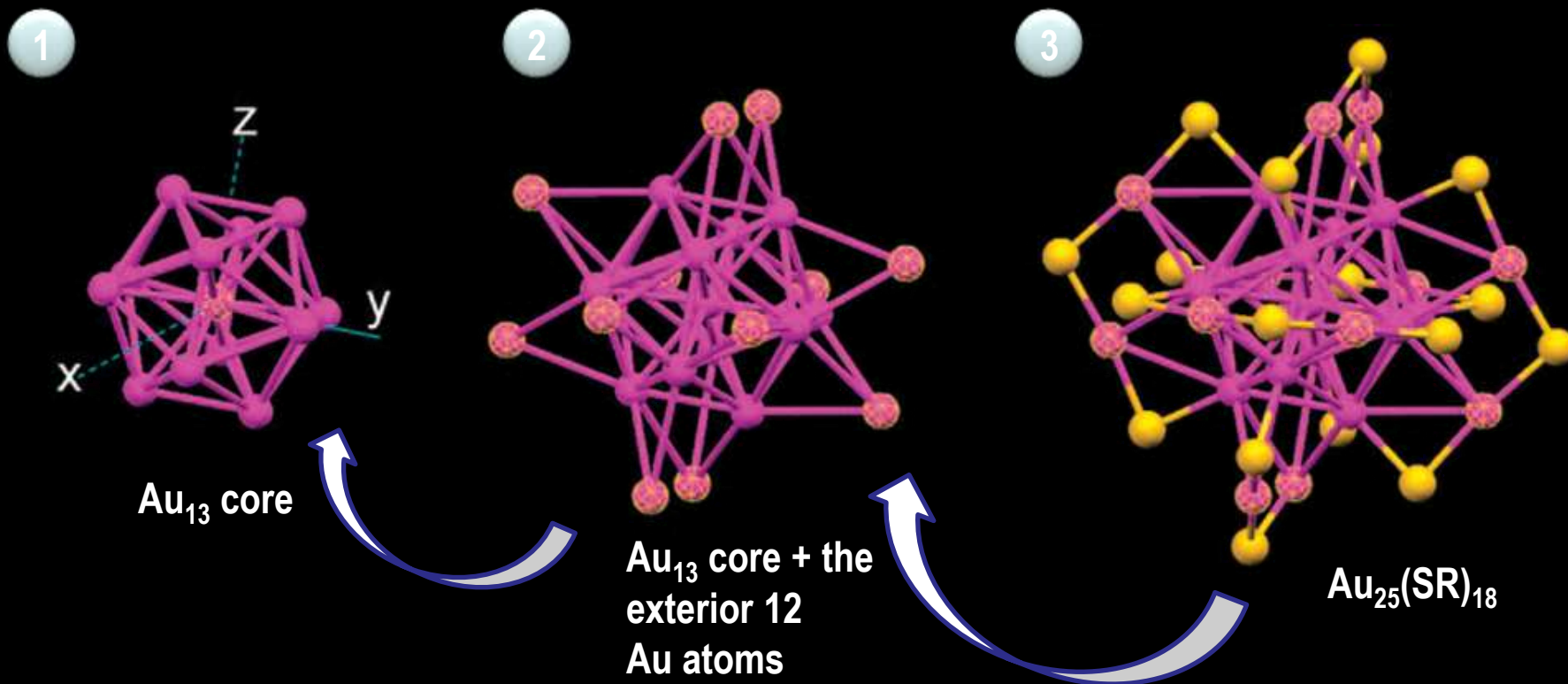
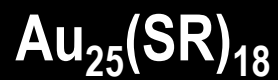
Atomically precise metal clusters as materials

AU25PET16_RES_NEG_MS_3 32 (0.658) Cm (5:00)

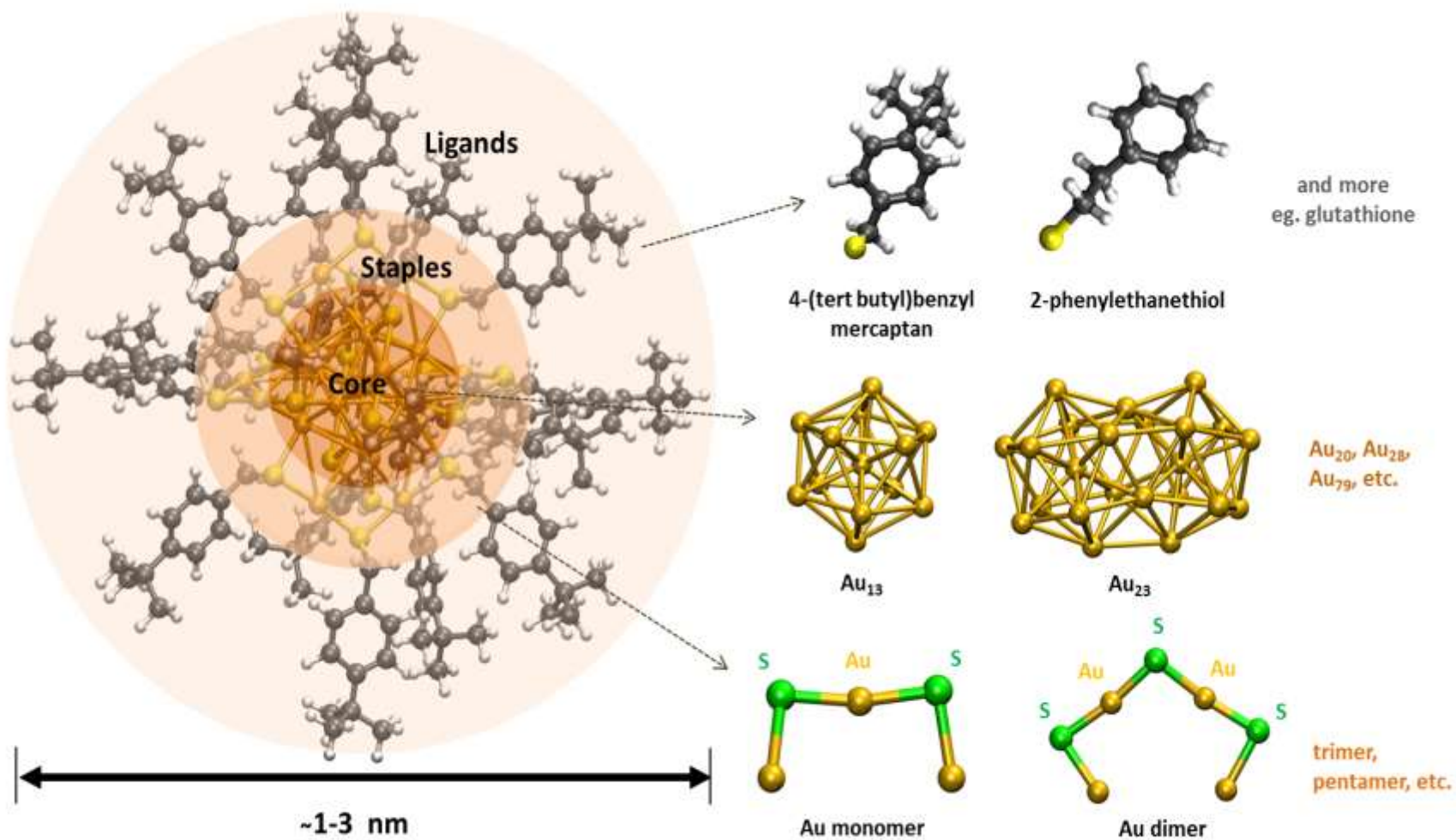


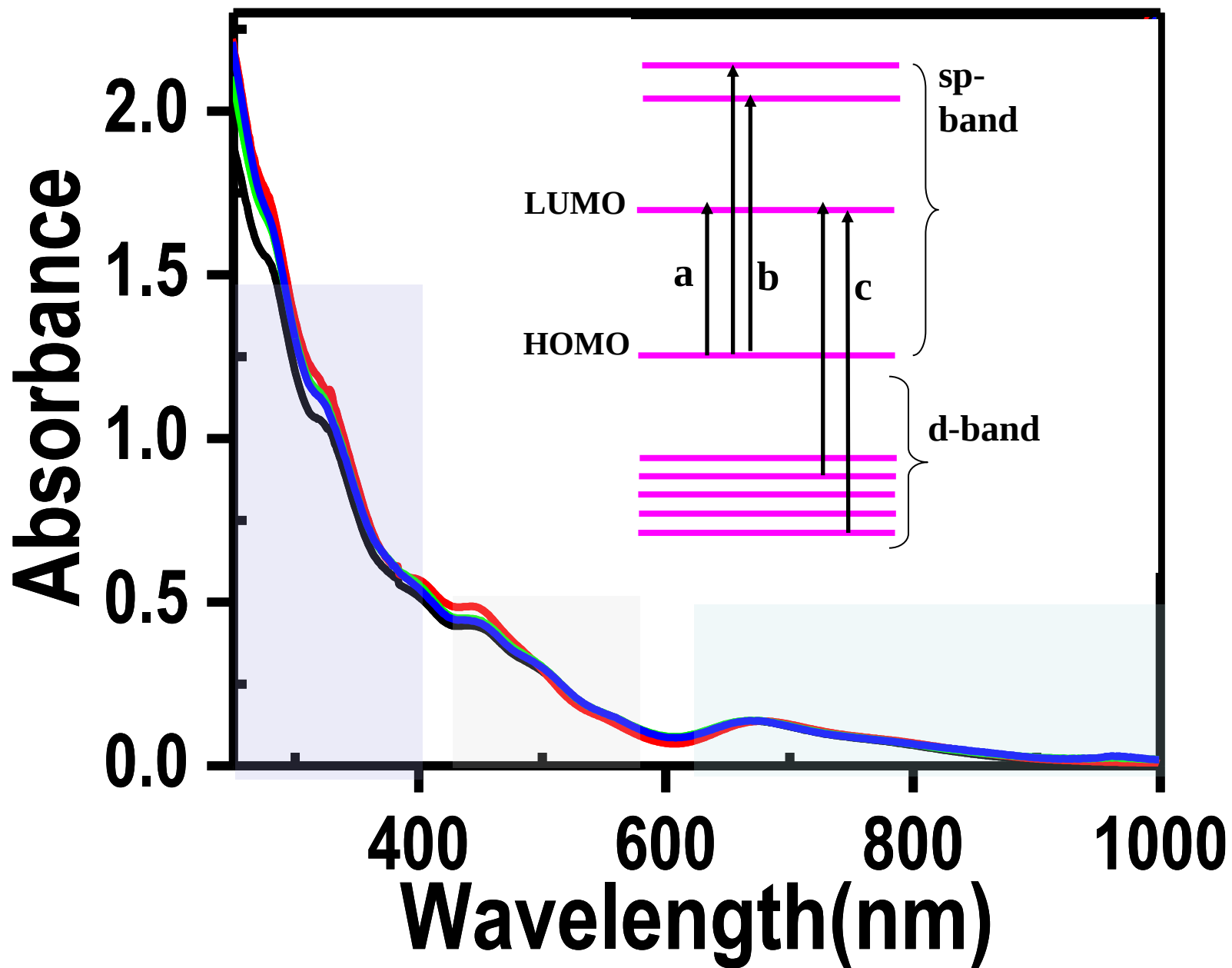
T. Pradeep et. al. *Acc. Chem. Res.* 2018; 2019.

Structures



>150 such clusters





Atomically Precise Clusters of Noble Metals: Emerging Link between Atoms and Nanoparticles

Indranath Chakraborty[†] and Thalappil Pradeep^{*}

DST Unit of Nanoscience (DST UNS) and Thematic Unit of Excellence, Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, India

 Supporting Information

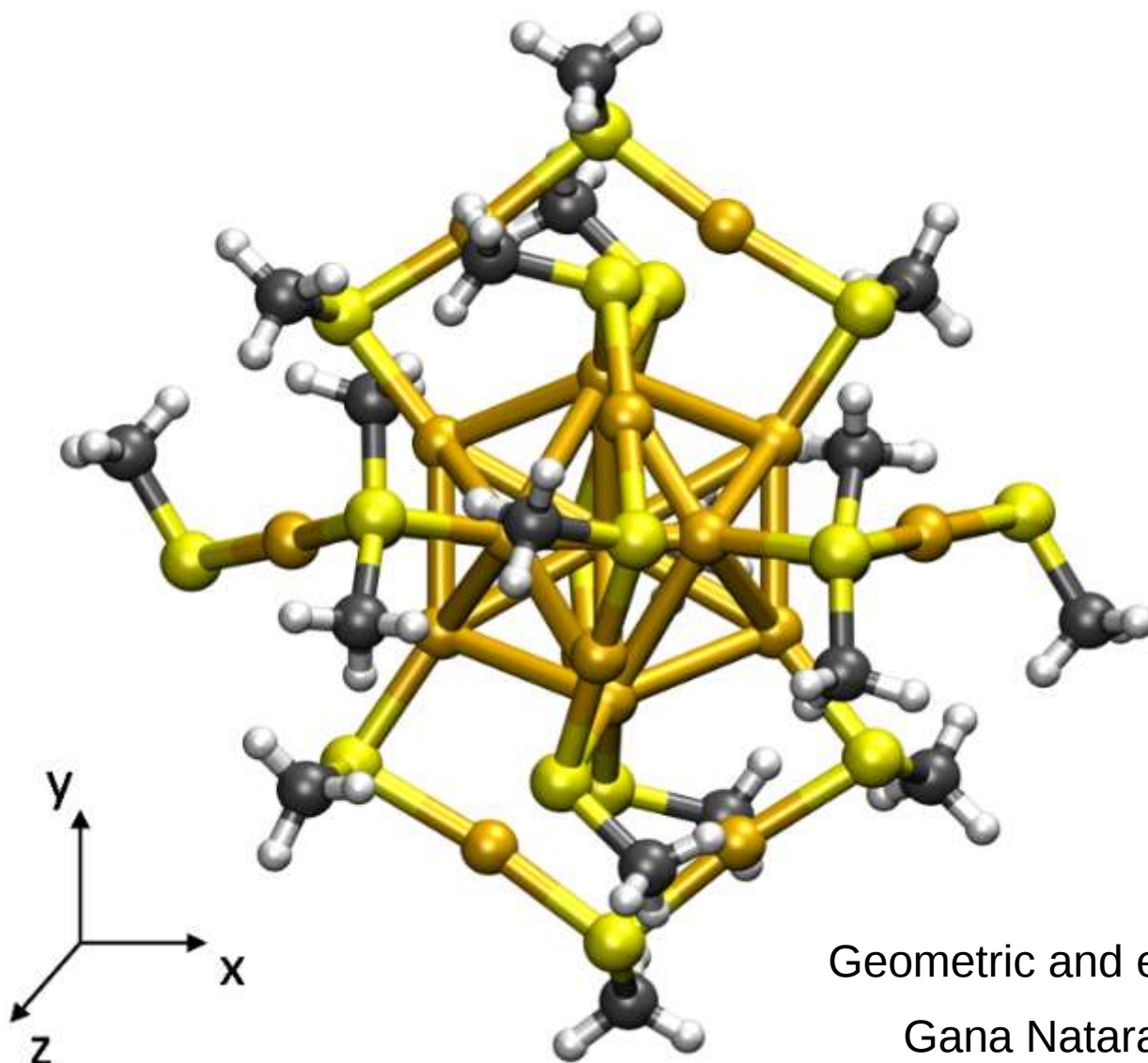
Citations: >2000

ABSTRACT: Atomically precise pieces of matter of nanometer dimensions composed of noble metals are new categories of materials with many unusual properties. Over 100 molecules of this kind with formulas such as $\text{Au}_{25}(\text{SR})_{18}$, $\text{Au}_{38}(\text{SR})_{24}$, and $\text{Au}_{102}(\text{SR})_{44}$ as well as $\text{Ag}_{25}(\text{SR})_{18}$, $\text{Ag}_{29}(\text{S}_2\text{R})_{12}$, and $\text{Ag}_{44}(\text{SR})_{30}$ (often with a few counterions to compensate charges) are known now. They can be made reproducibly with robust synthetic protocols, resulting in colored solutions, yielding powders or diffractable crystals. They are distinctly different from nanoparticles in their spectroscopic properties such as optical absorption and emission, showing well-defined features, just like molecules. They show isotopically resolved molecular ion peaks in mass spectra and provide diverse information when examined through multiple instrumental methods. Most important of these properties is luminescence, often in the visible–near-infrared window, useful in biological applications. Luminescence in the visible region, especially by clusters protected with proteins, with a large Stokes shift, has been used for various sensing applications, down to a few tens of molecules/ions, in air and water. Catalytic properties of clusters, especially oxidation of organic substrates, have been examined. Materials science of these systems presents numerous possibilities and is fast evolving. Computational insights have given reasons for their stability and unusual properties. The molecular nature of these materials is unequivocally manifested in a few recent studies such as intercluster reactions forming precise clusters. These systems manifest properties of the core, of the ligand shell, as well as that of the integrated system. They are better described as protected molecules or *aspicules*, where *aspis* means shield and *cules* refers to molecules, implying that they are “shielded molecules”. In order to understand their diverse properties, a nomenclature has been introduced with which it is possible to draw their structures with positional labels on paper, with some training. Research in this area is captured here, based on the publications available up to December 2016.



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

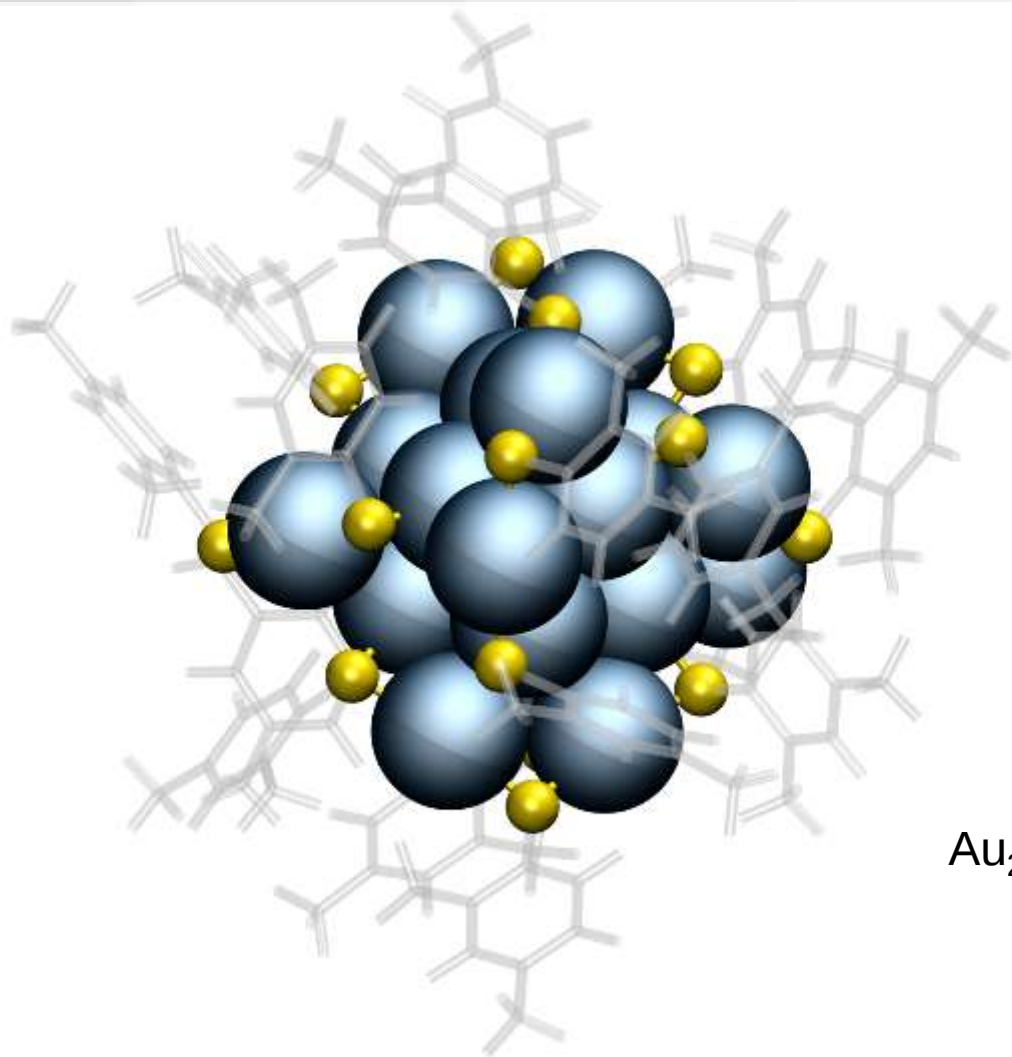
Molecular structure



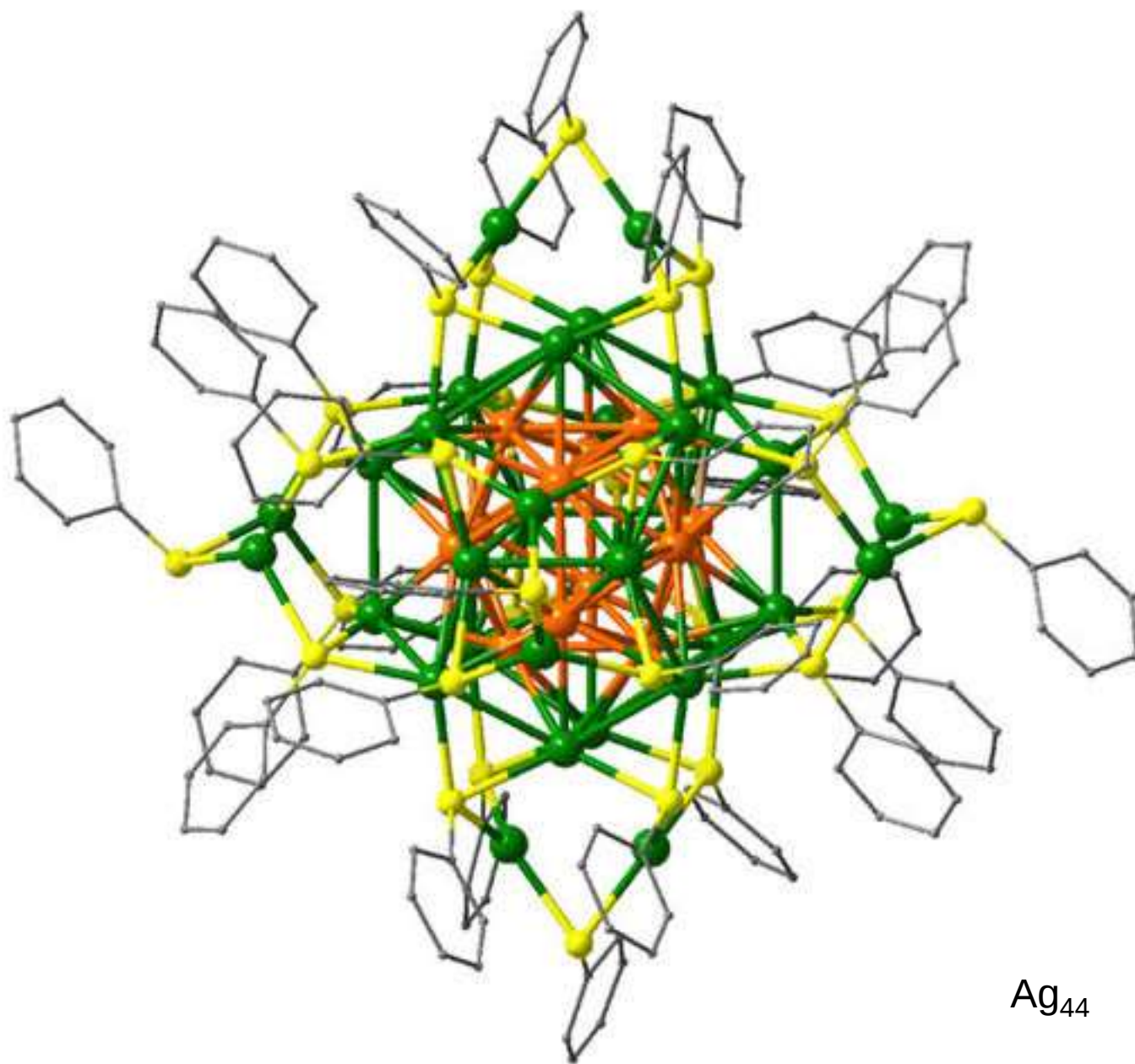
Geometric and electronic shells

Gana Natarajan

New molecules

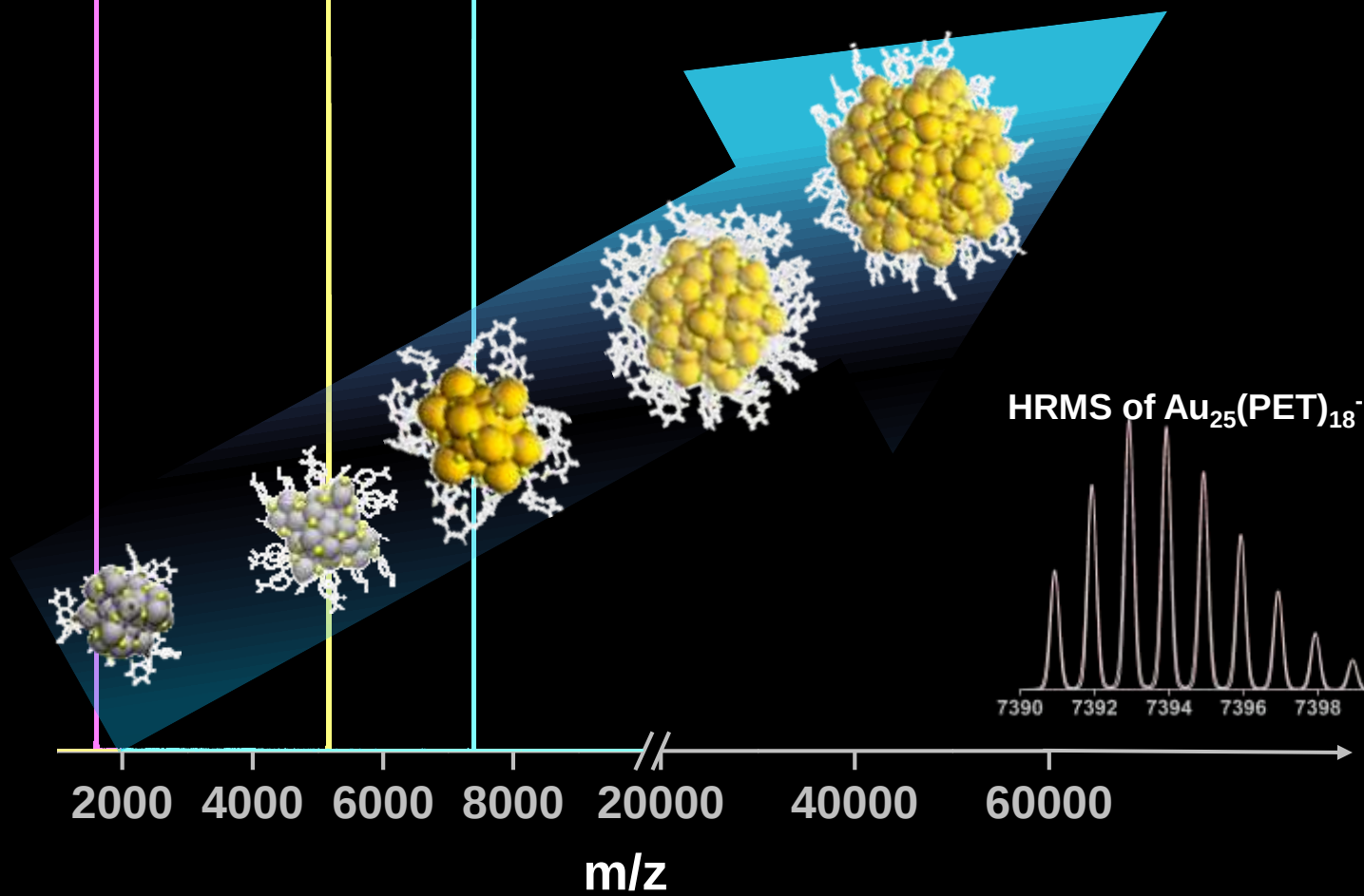


$\text{Au}_{25}, \text{Ag}_{25}, \text{Ag}_{29}$



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

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



Molecules and their properties

Chemical formula	H ₂ O
Molecular weight	18.0148
Critical temperature	373.91°C
Critical pressure	22.05 MPa
Critical density	315.0 kg/m ³
Triple point temperature	0.01°C
Triple point pressure	615.066 Pa
Normal boiling point	100.0°C
Normal freezing point	0.0°C
Density of ice at normal melting point	918.0 kg/m ³
Maximum density, 3.98°C	999.973 kg/m ³
Viscosity, 25°C	0.889 mN s/m ²
Surface tension, 25°C	72 mN/m
Heat Capacity, 25°C	4.1796 kJ/kg.K
Enthalpy of vaporisation, 100°C	2,257.7 kJ/kg
Enthalpy of fusion, 0°C	333.8 kJ/kg
Velocity of sound, 0°C	1.403 km/s
Dielectric constant, 25°C	78.40
Electrical conductivity, 25°C	8 µS/m
Refractive index, 25°C	1.333
Liquid compressibility, 10°C	480. × 10 ⁻¹² m ² /N
Coefficient of thermal expansion, 25°C	256.32 × 10 ⁻⁶ K ⁻¹
Thermal Conductivity, 25°C	0.608 W/m.K

Molecular formula
 Molecular weight
 Molecular structure
 Molecular absorption and emission
 Molecular reactions
 Molecular assembly
 Molecular co-crystals

 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

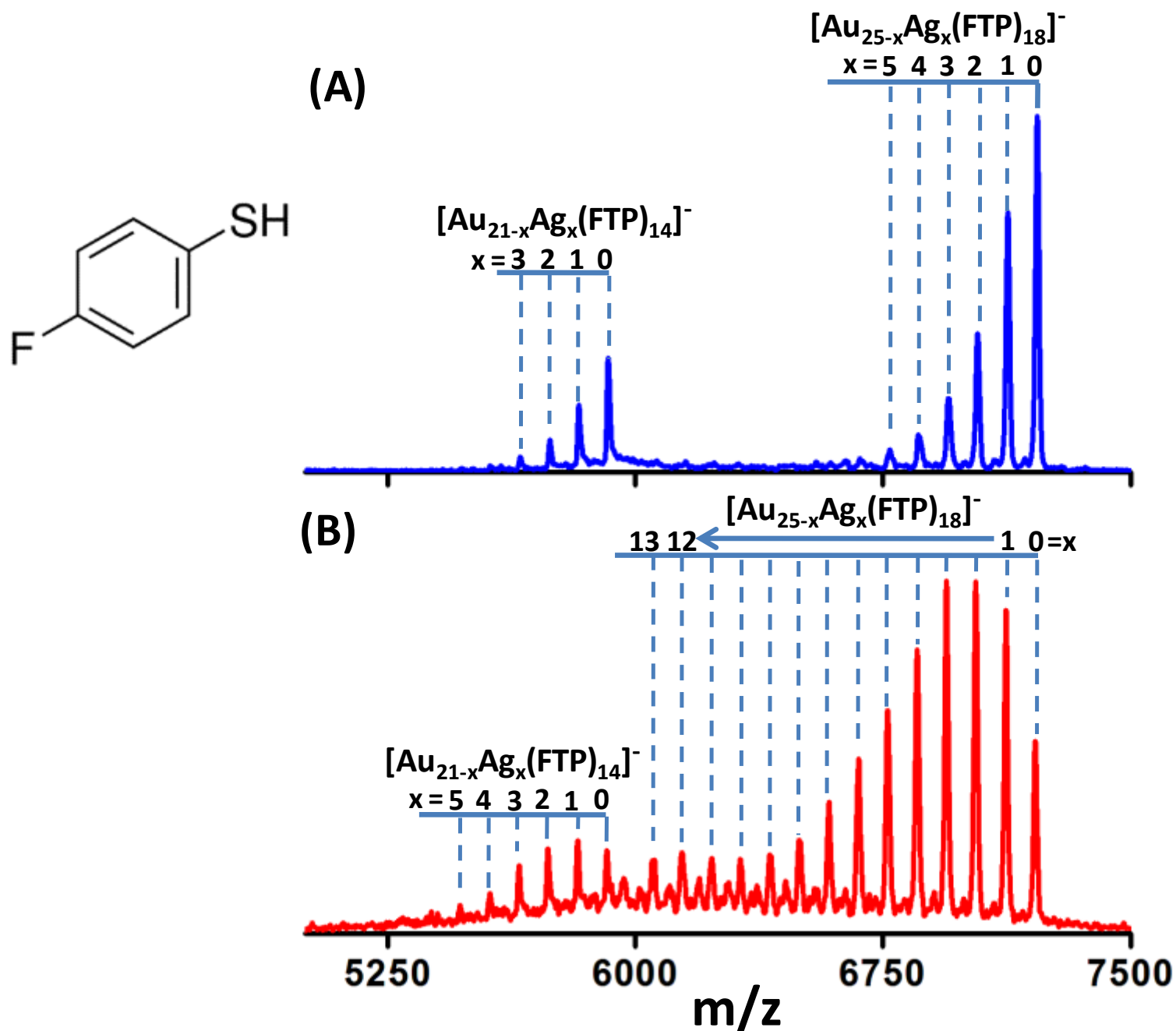
Intercluster Reactions between $\text{Au}_{25}(\text{SR})_{18}$ and $\text{Ag}_{44}(\text{SR})_{30}$

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 $x=1$

(A) Location of Au in $\text{Au}_x\text{Ag}_{44-x}(\text{SR})_{30}$ $\Delta E/\text{eV}$

Icosahedron (I)	-0.72
Dodecahedron: cube vertex (D_{cv})	-0.14
Dodecahedron: cube face (D_{cf})	-0.32
Staples (S)	-0.48

(B) Location of Ag in $\text{Au}_{25-x}\text{Ag}_x(\text{SR})_{18}$ $\Delta E/\text{eV}$

Central atom (C)	+0.71
Icosahedron (I)	+0.23
Staples (S)	+0.44

(C) Locations of Au in $\text{Au}_x\text{Ag}_{44-x}(\text{SR})_{30}$

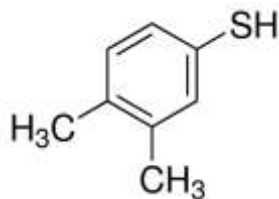
Location of Ag in $\text{Au}_{25-x}\text{Ag}_x(\text{SR})_{18}$	I	D_{cv}	D_{cf}	S
C	-0.015	+0.564	+0.388	+0.226
I	-0.486	+0.093	-0.083	-0.245
S	-0.276	+0.303	+0.127	-0.035

Ag₂₅-Au₂₅ experiments

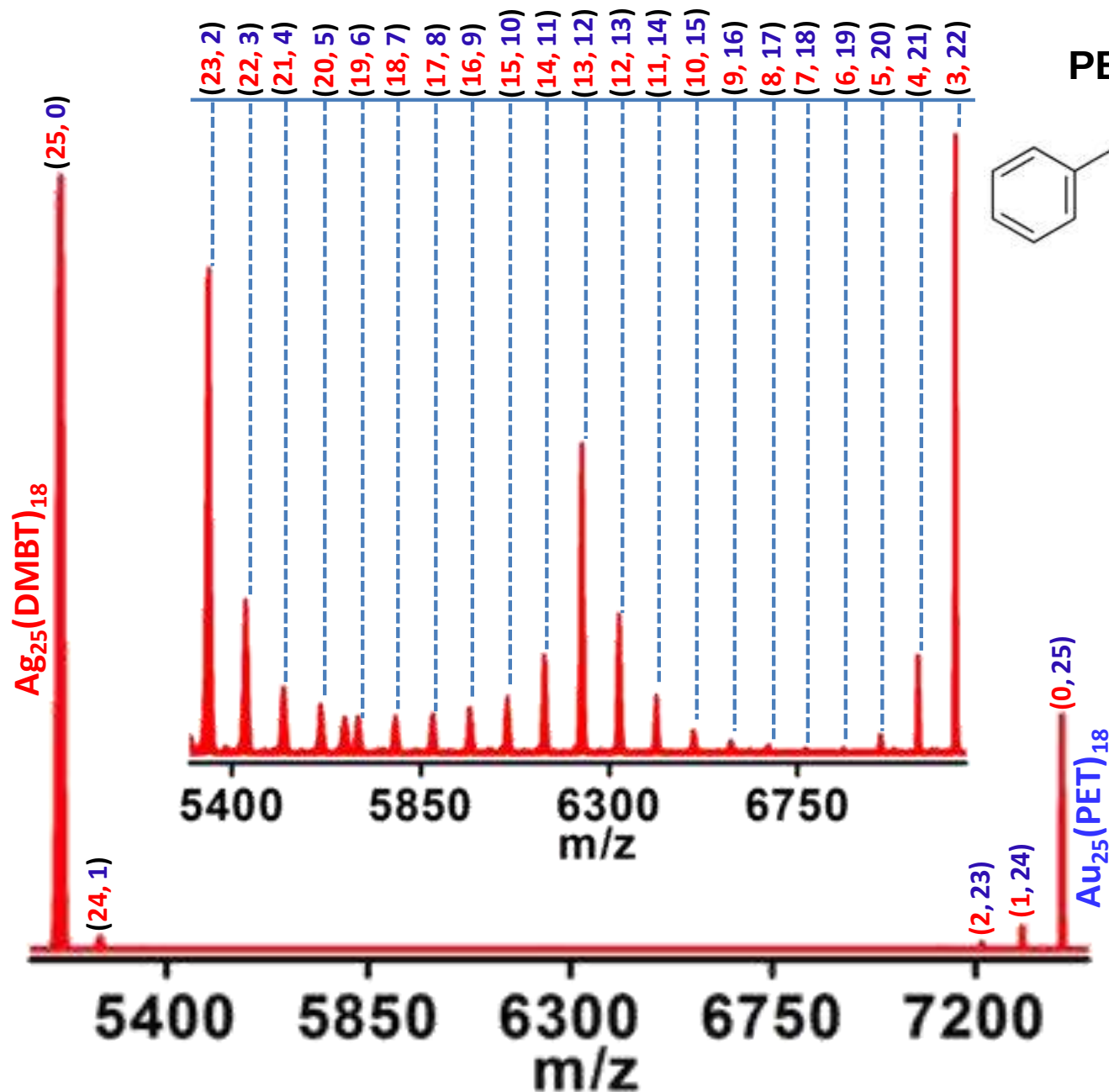
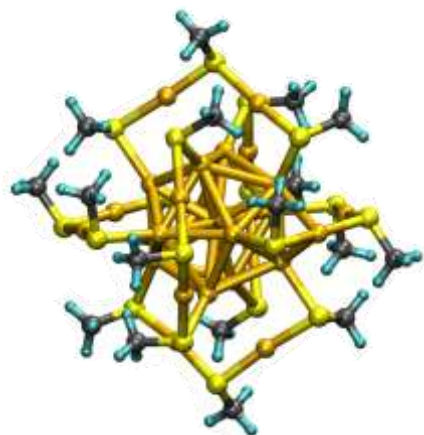
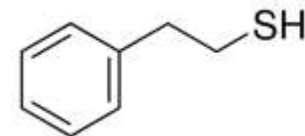
K. R. Krishnadas et al. *Nature Commun.* 2016

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

DMBT

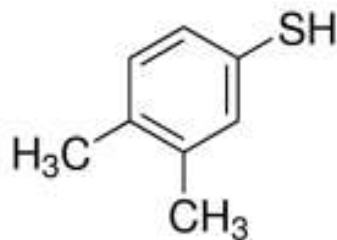


PET

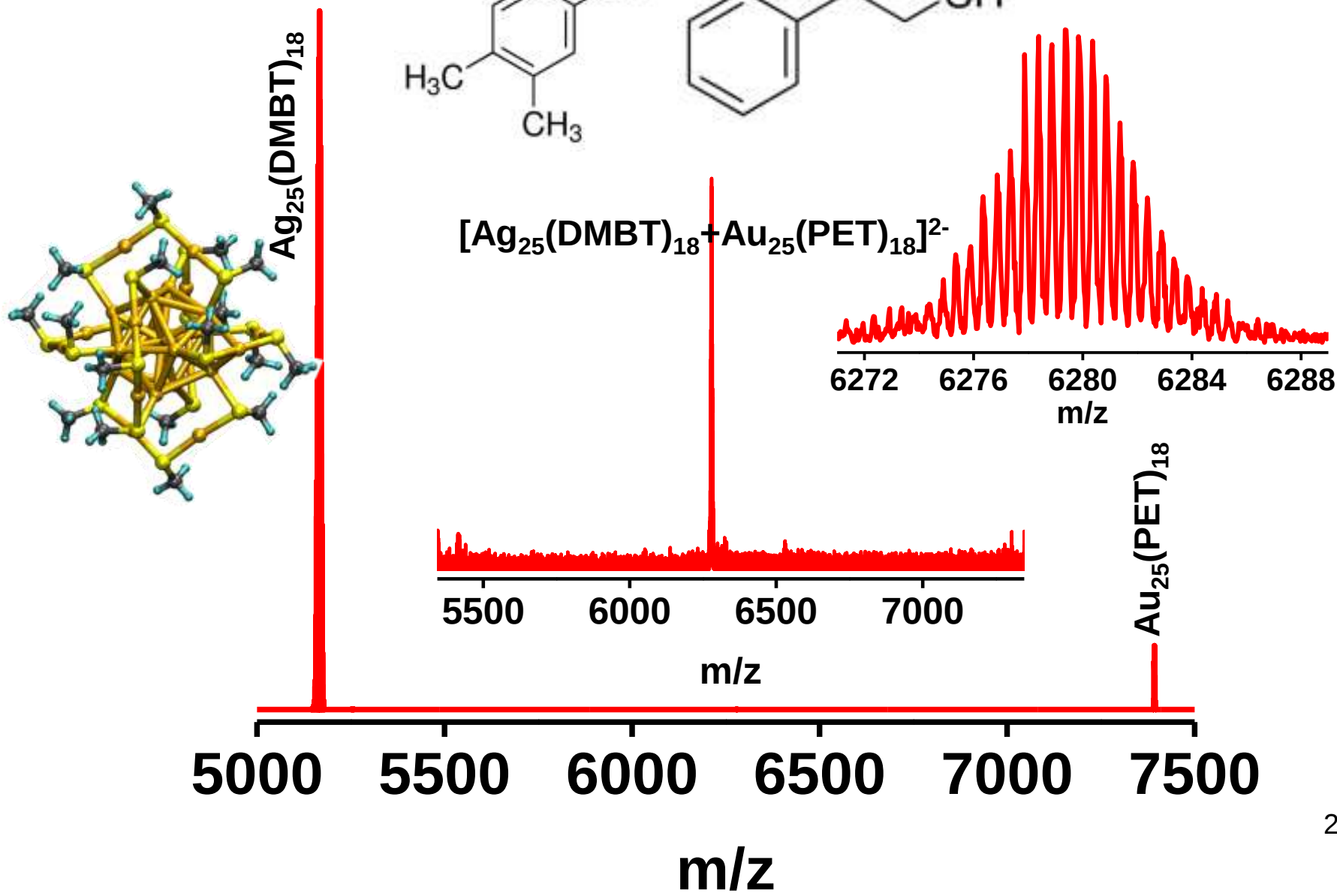
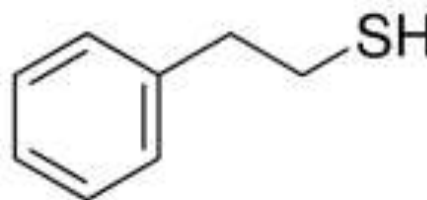




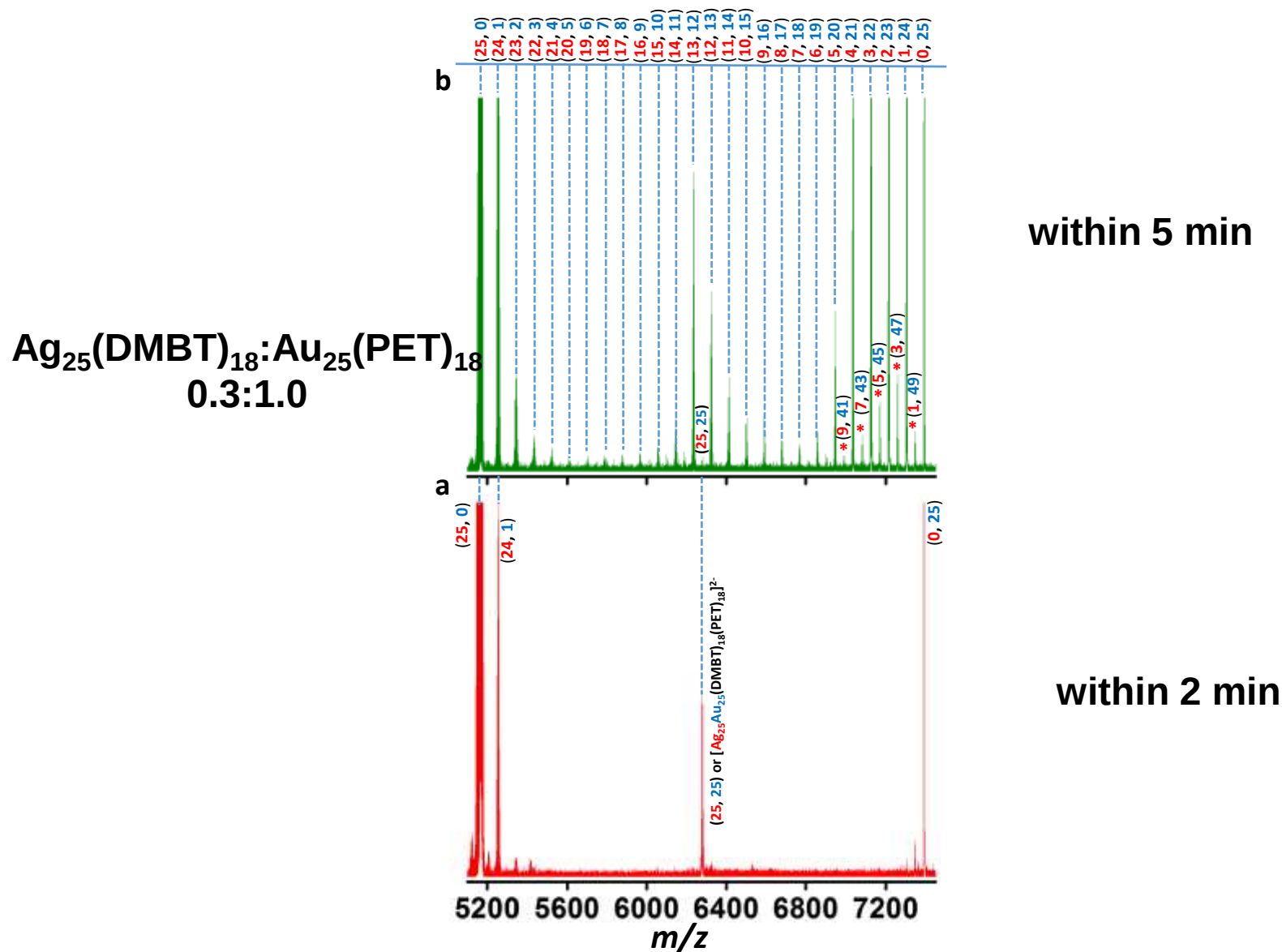
DMBT



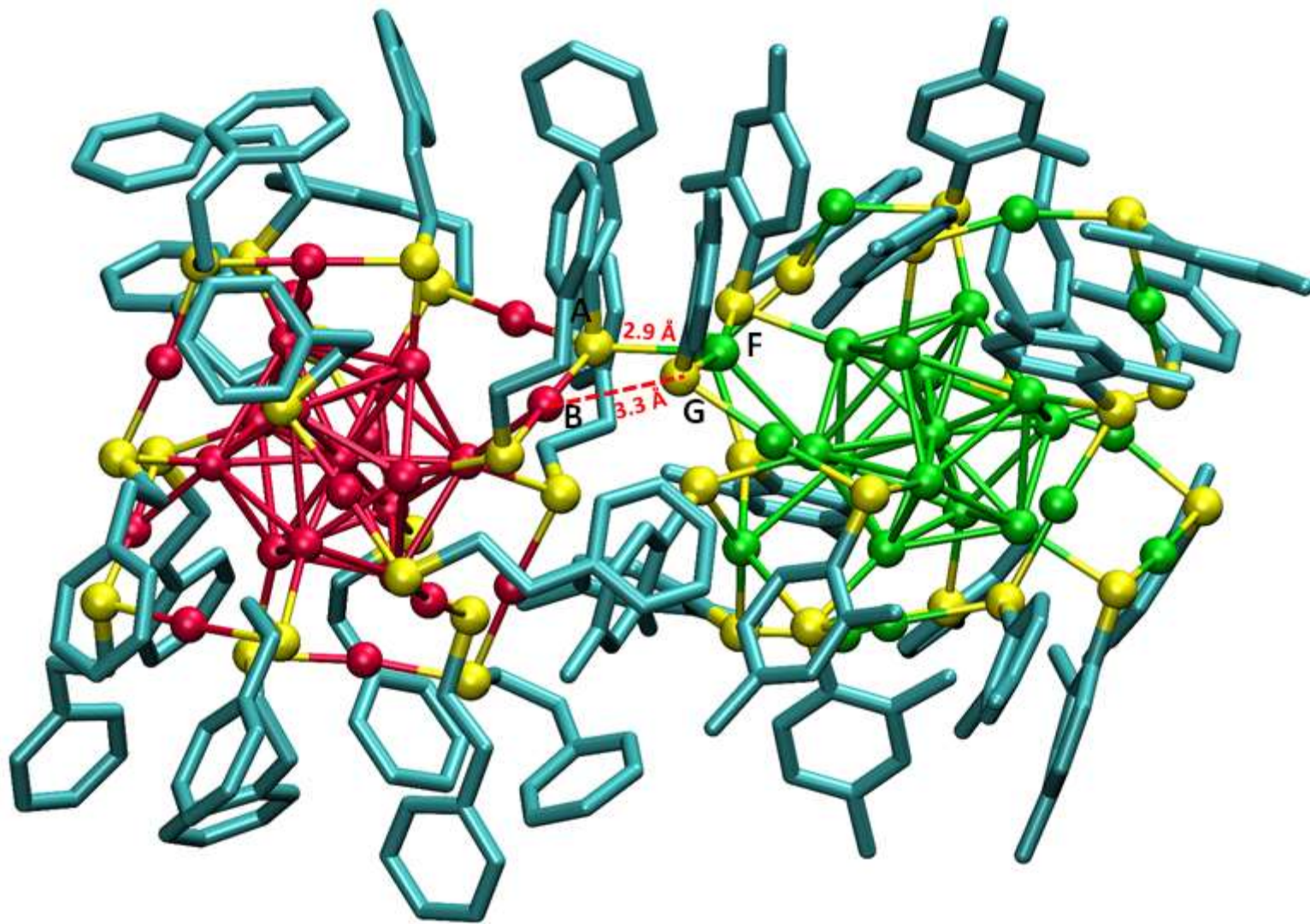
PET

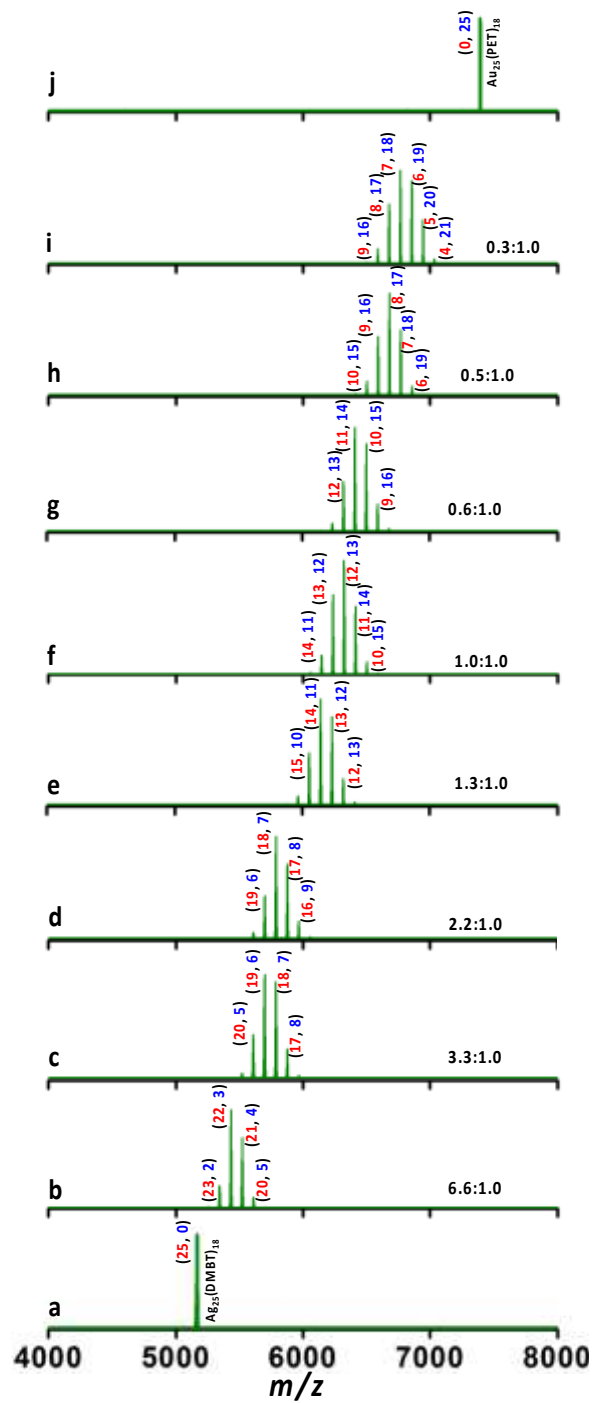


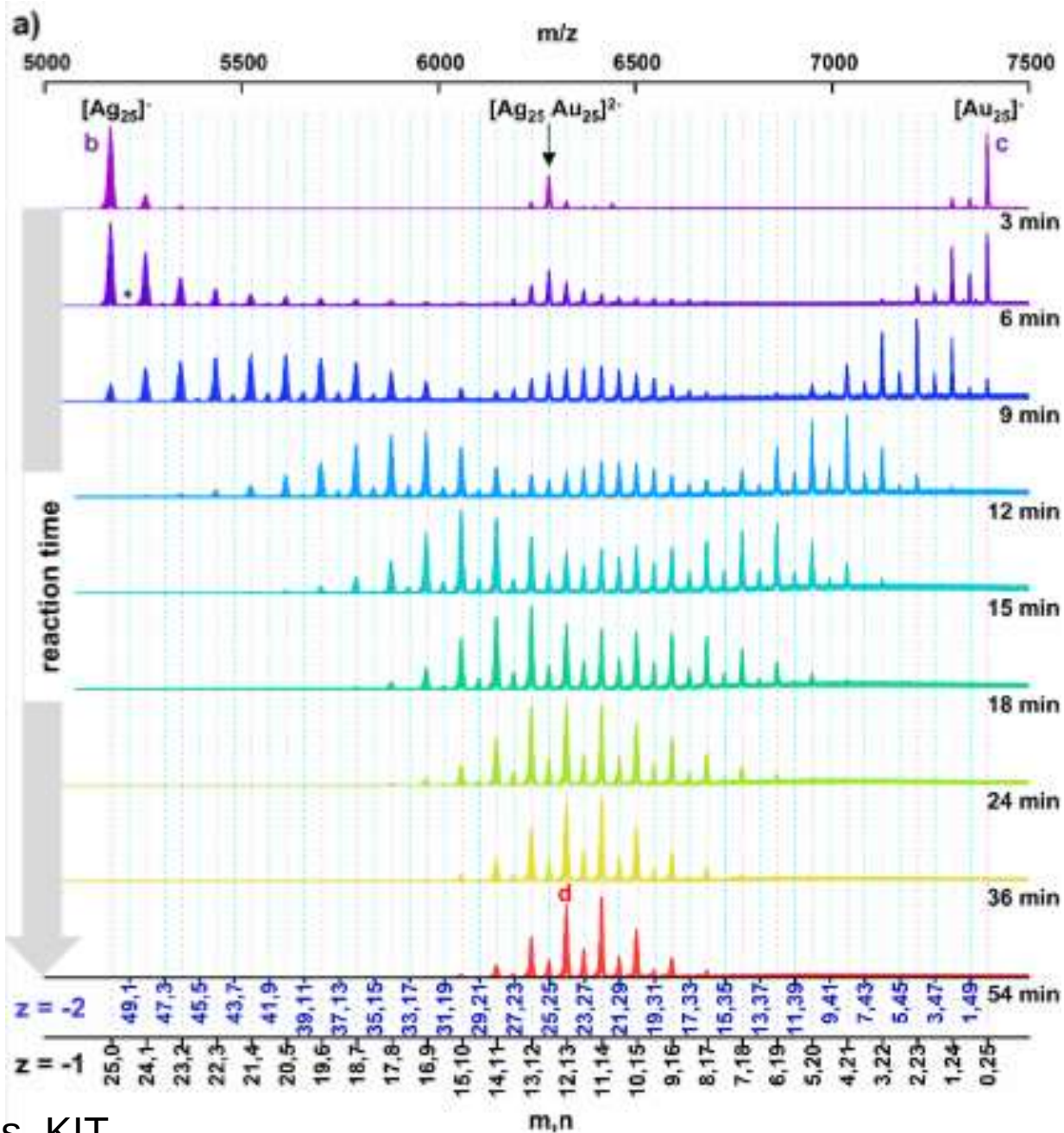
Evolution of alloy clusters from the dianionic adduct, $[\text{Ag}_{25}\text{Au}_{25}(\text{DMBT})_{18}(\text{PET})_{18}]^{2-}$

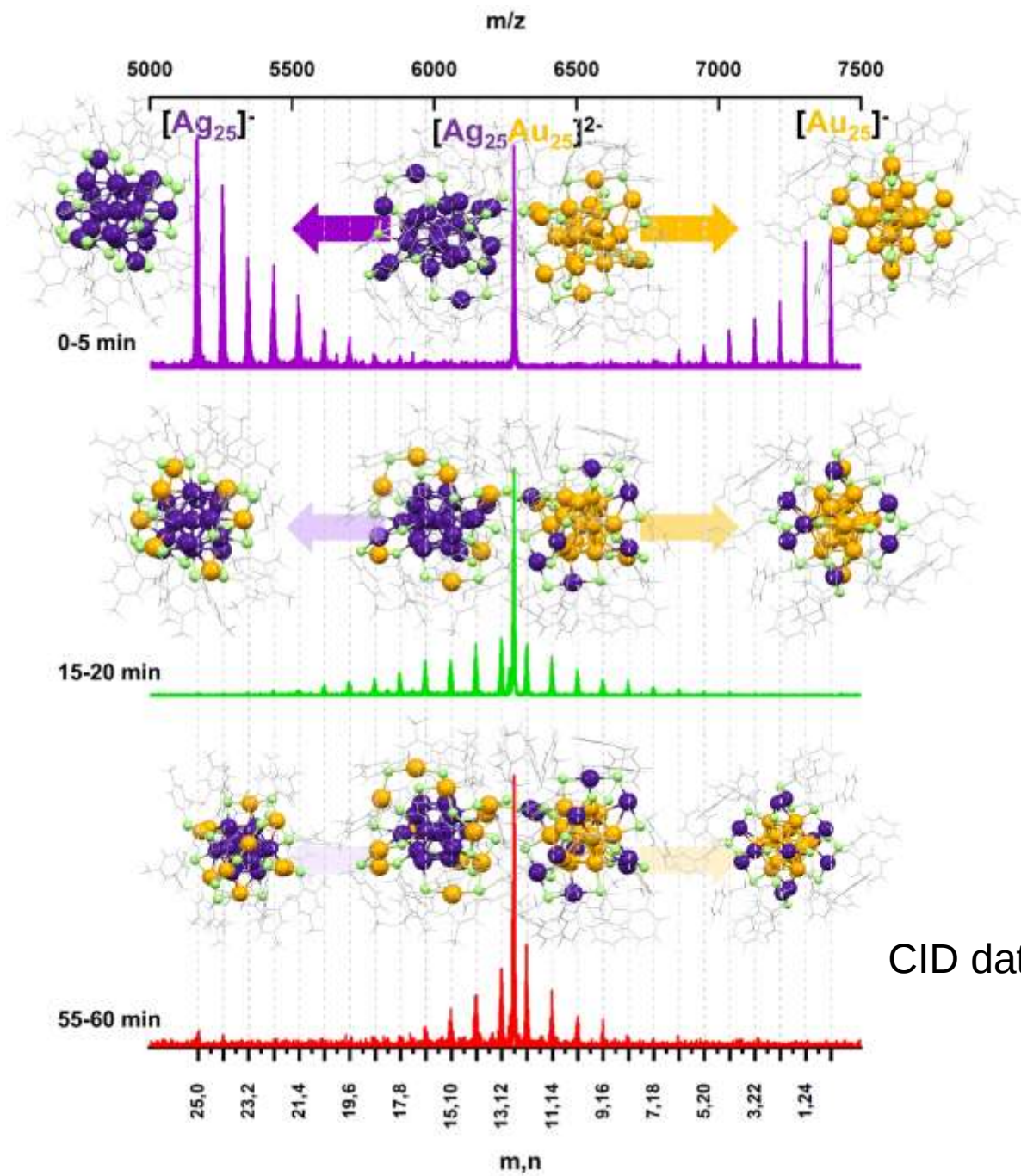


Optimized structure of $[\text{Ag}_{25}\text{Au}_{25}(\text{DMBT})_{18}(\text{PET})_{18}]^{2-}$



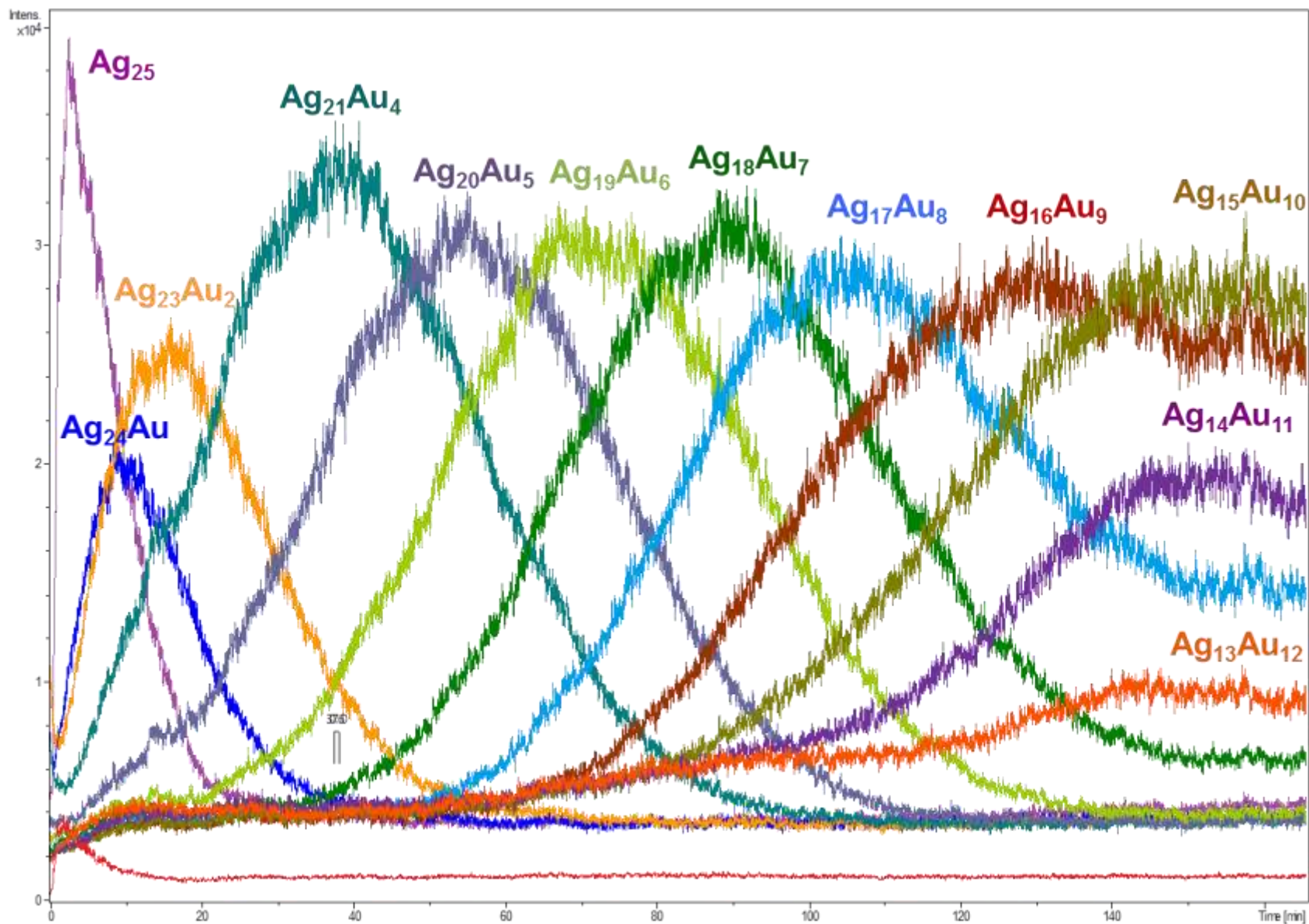






CID data of $[Au_{25}Ag_{25}]^{2-}$

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



CONDENSED MATTER PHYSICS

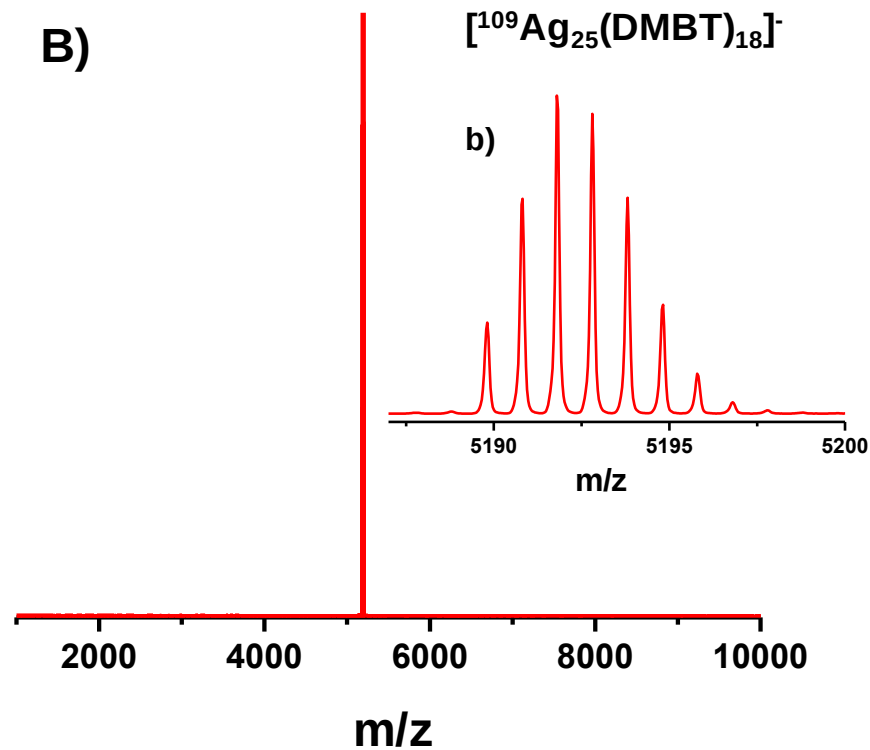
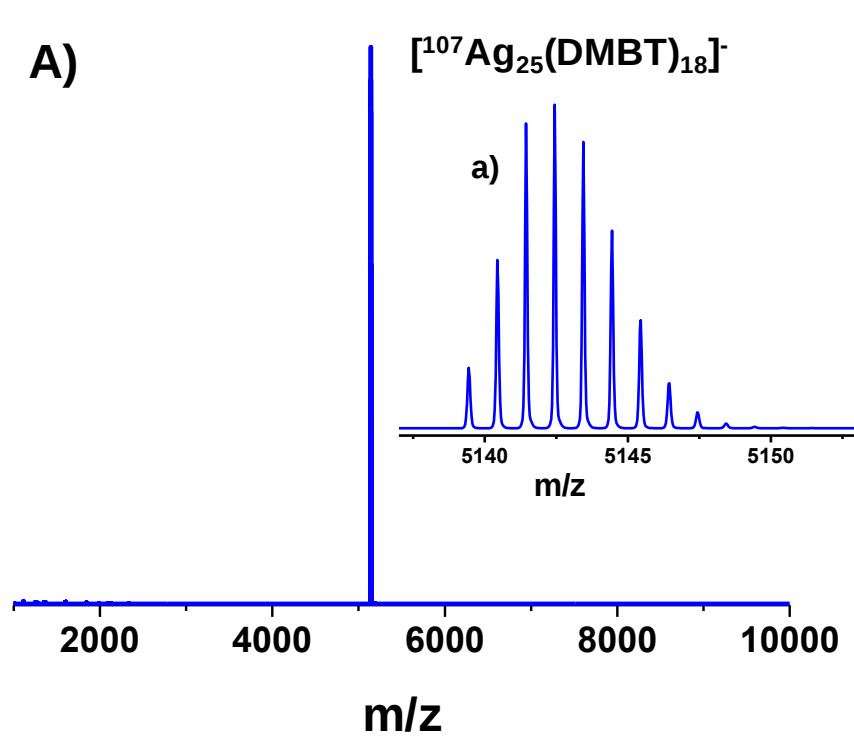
Rapid isotopic exchange in nanoparticles

Papri Chakraborty¹, Abhijit Nag¹, Ganapati Natarajan¹, Nayanika Bandyopadhyay¹, Ganesan Paramasivam¹, Manoj Kumar Panwar¹, Jaydeb Chakrabarti², Thalappil Pradeep^{1*}

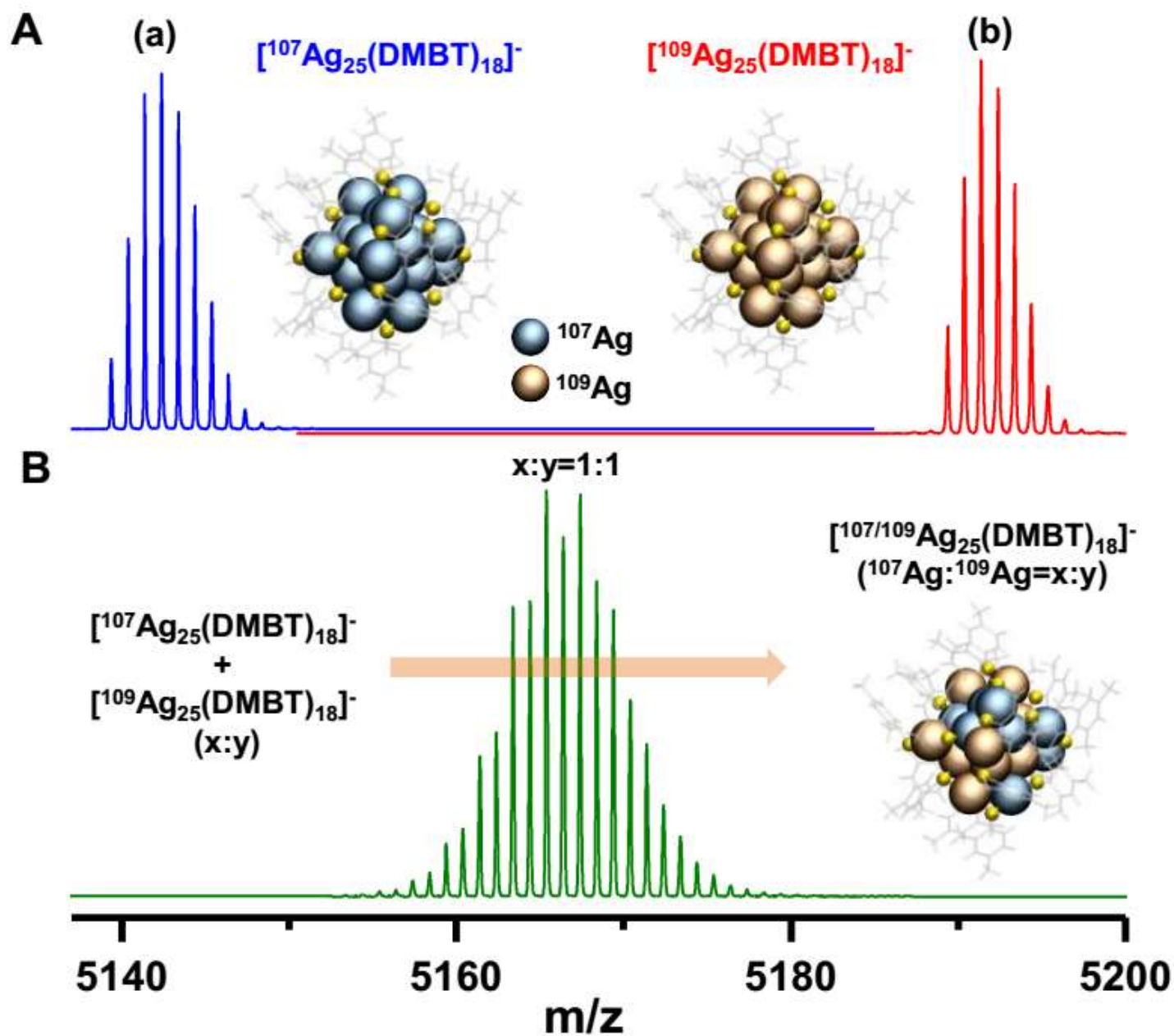
Rapid solution-state exchange dynamics in nanoscale pieces of matter is revealed, taking isotopically pure atomically precise clusters as examples. As two isotopically pure silver clusters made of ^{107}Ag and ^{109}Ag are mixed, an isotopically mixed cluster of the same entity results, similar to the formation of HDO, from H_2O and D_2O . This spontaneous process is driven by the entropy of mixing and involves events at multiple time scales.

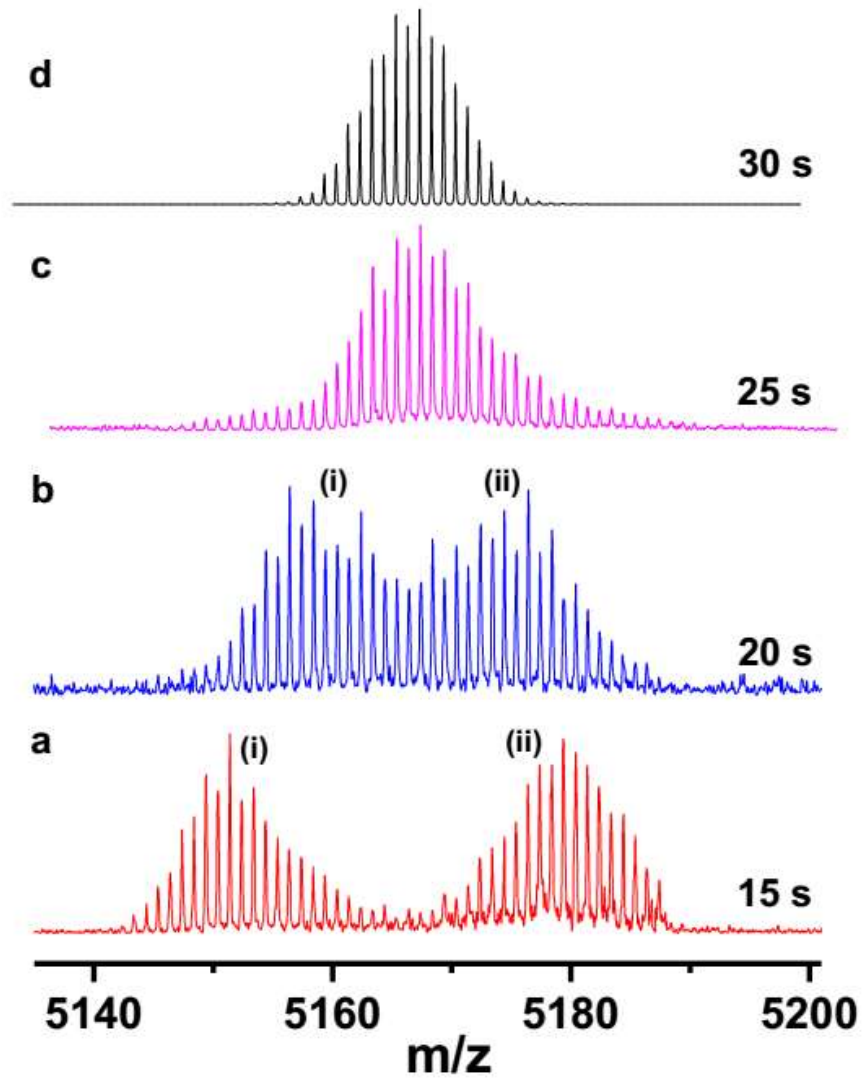


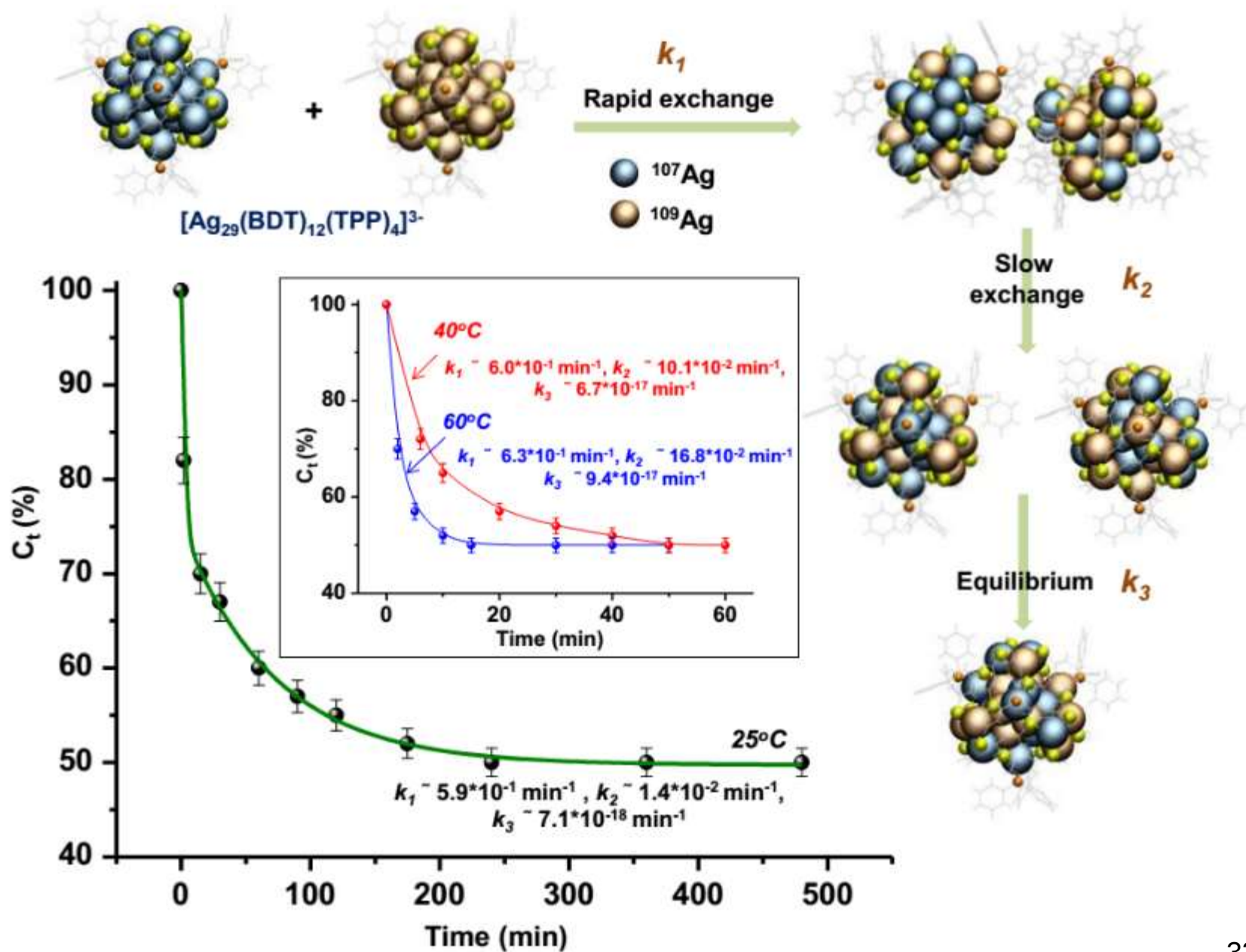
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ESI MS of **A)** $^{107}\text{Ag}_{25}(\text{DMBT})_{18}$ and **B)** $^{109}\text{Ag}_{25}(\text{DMBT})_{18}$. Insets shows the respective isotope patterns.



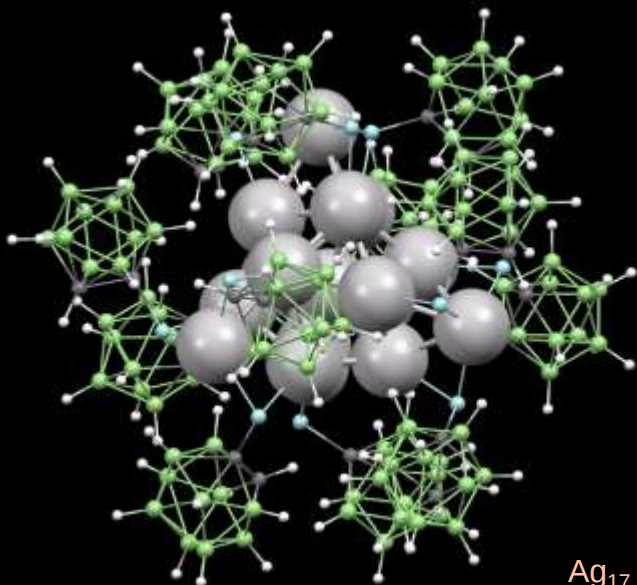




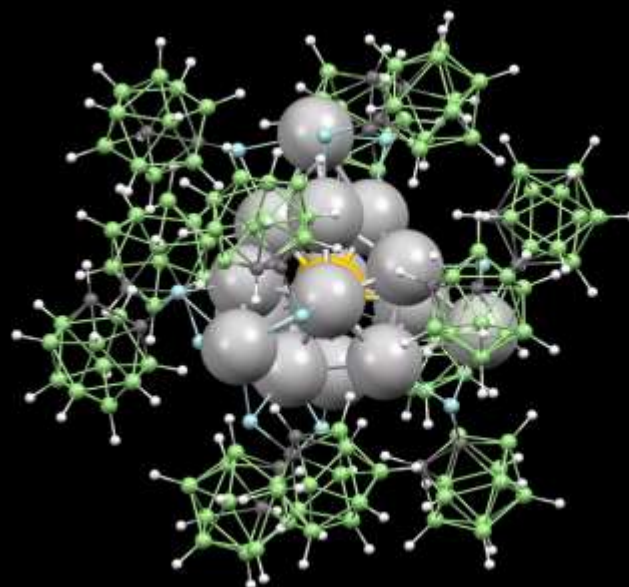


Vivek Yadav, et. al., *Nature Communications*, 2025

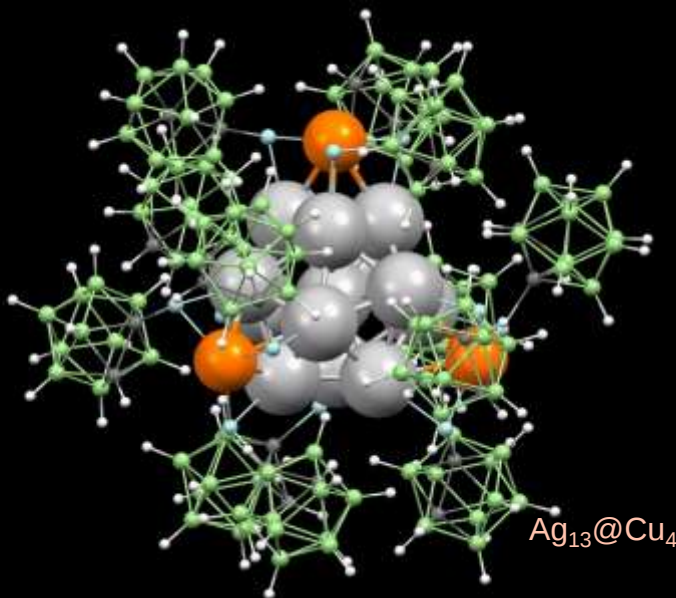
Structure of M_{17} Nanoclusters



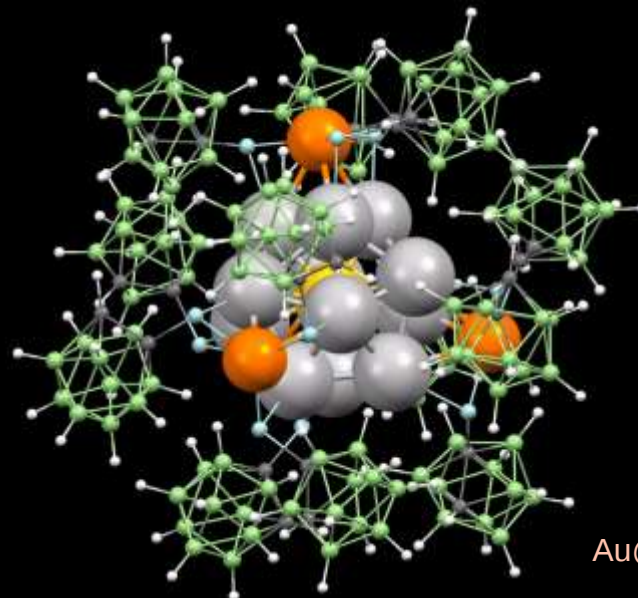
Ag_{17}



$Au@Ag_{16}$

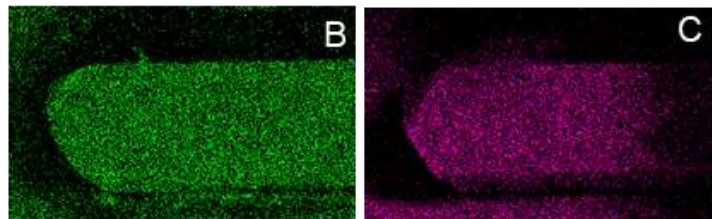
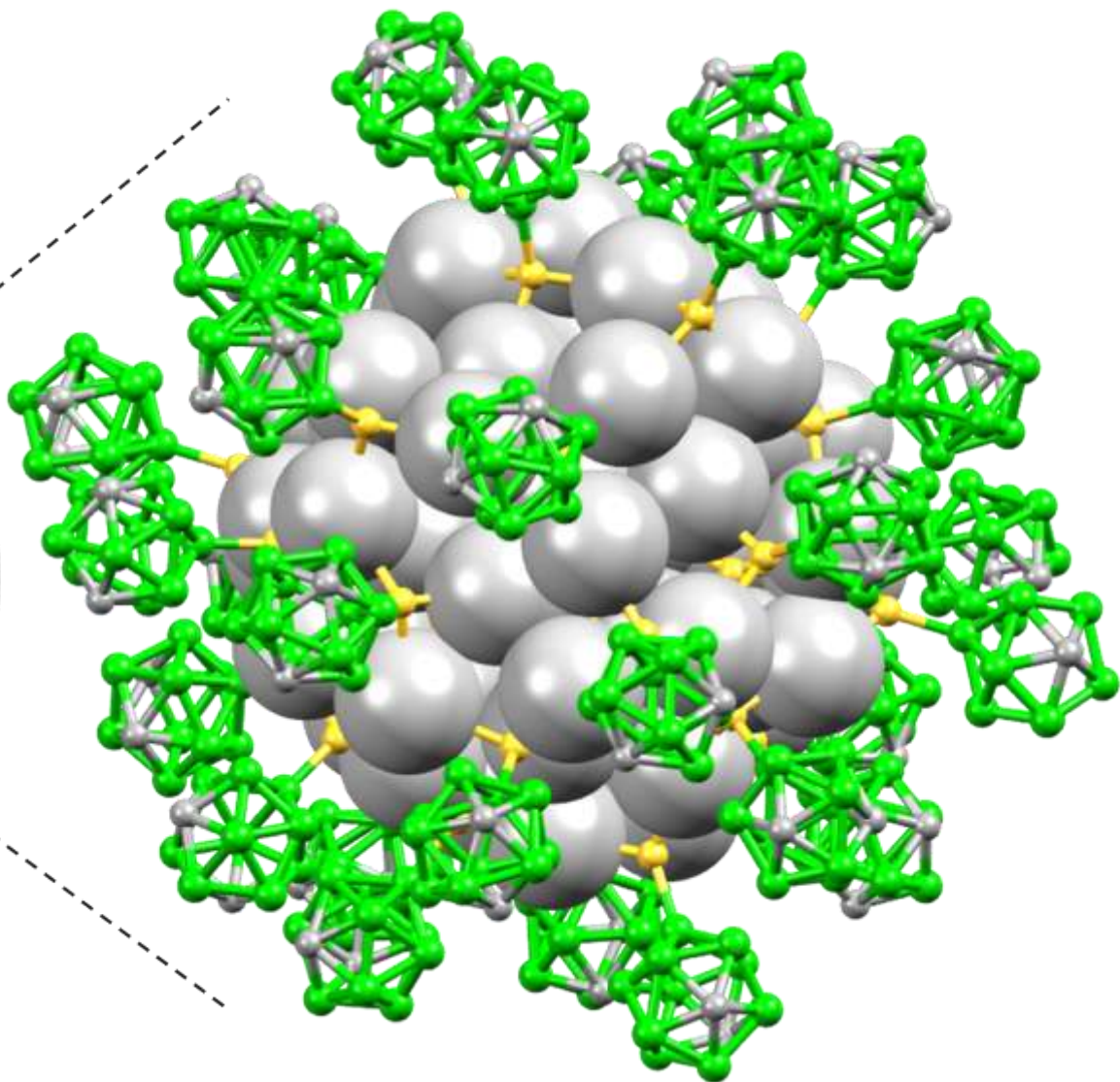
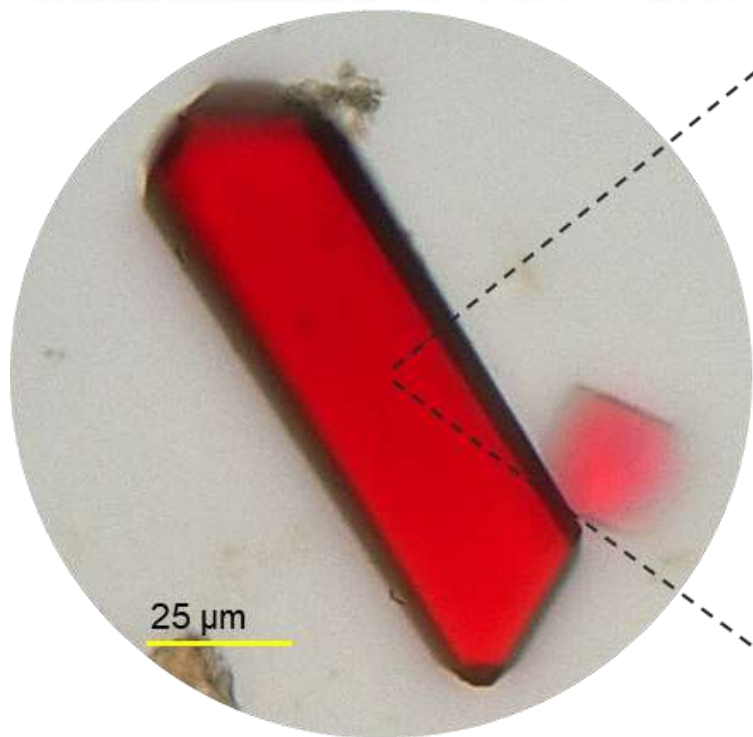
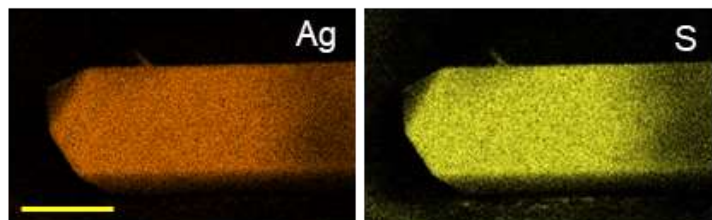


$Ag_{13}@Cu_4$



$Au@Ag_{12}@Cu_4$

$[Ag_{62}S_{12}(CBT)_{32}]$ Nanocluster



Largest molecule with carboranes so far....
36

Can Water Microdroplets Make Soil?

A path to sustainable nanotechnology

Spoorthi et al., Science 384, 1012–1017 (2024) 31 May 2024

A scale of 1000

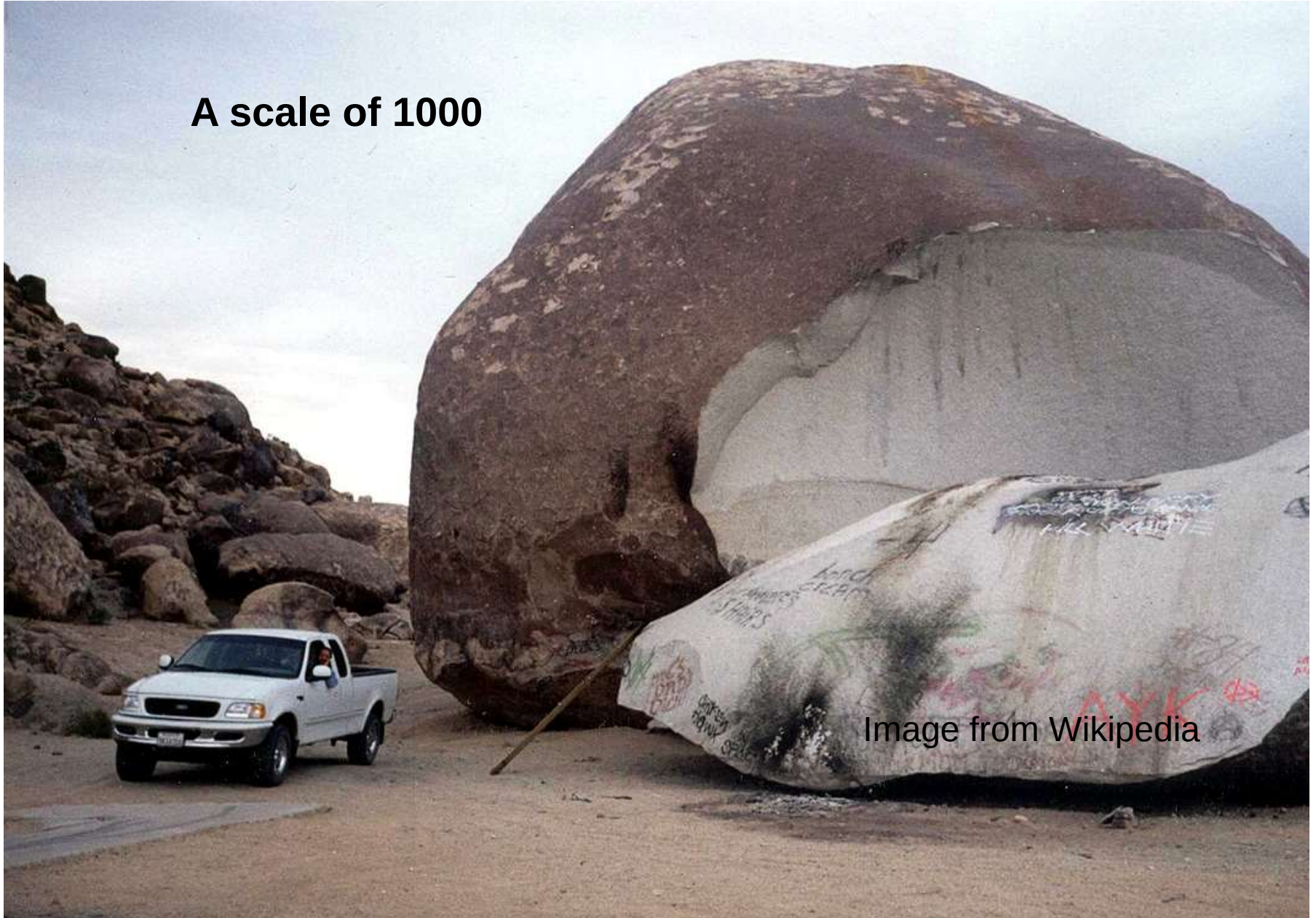


Image from Wikipedia



Thanks to ChatGPT

Weathering in Nature

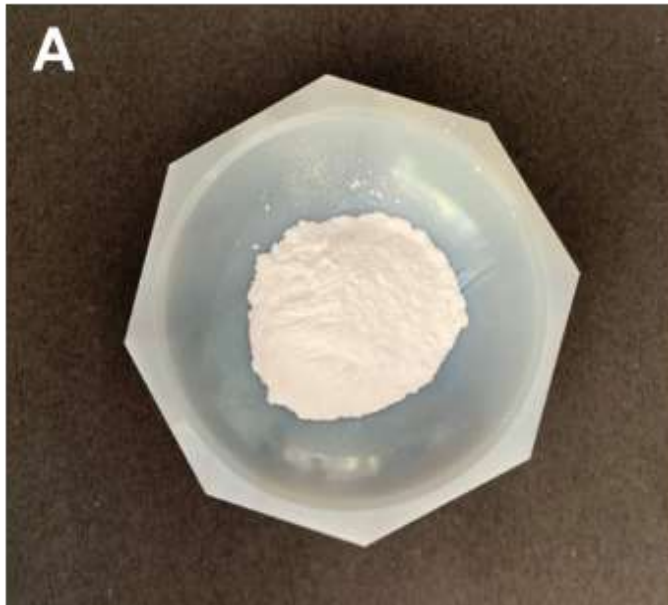


Sand, the Ubiquitous Material

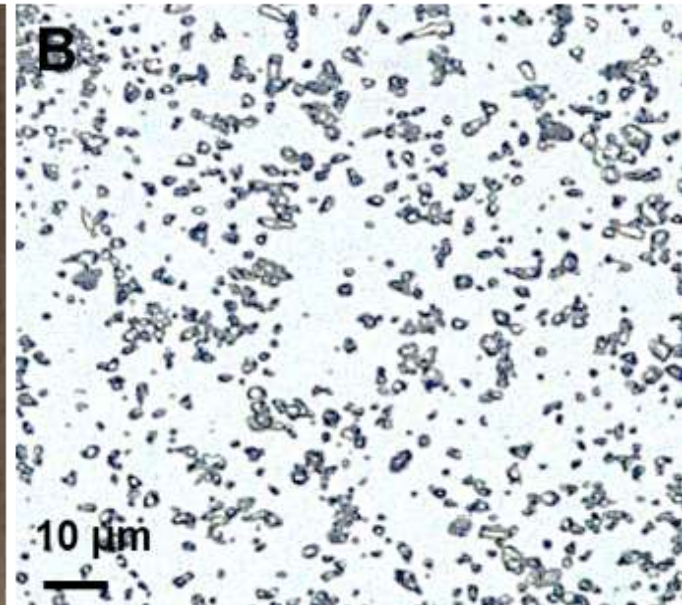


Images from Wikipedia



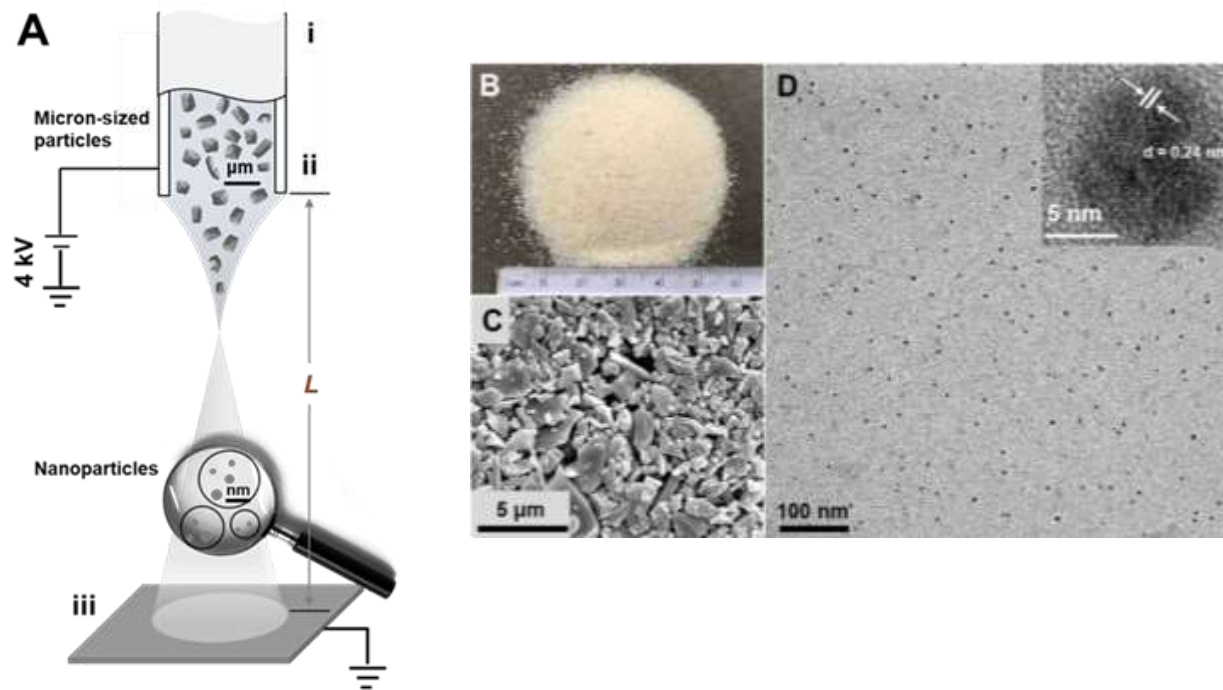


Ground silica



Optical image of silica

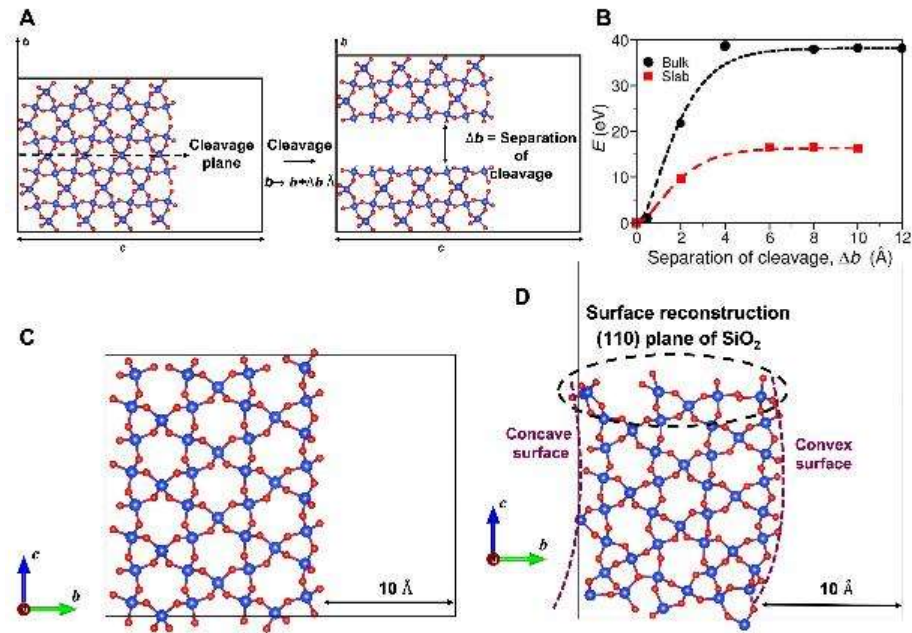
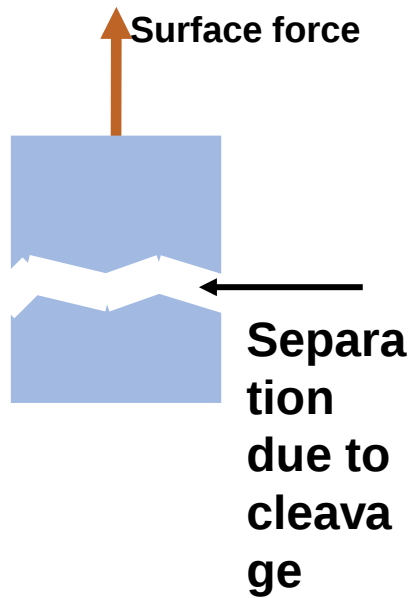
Weathering of Minerals in Microdroplets



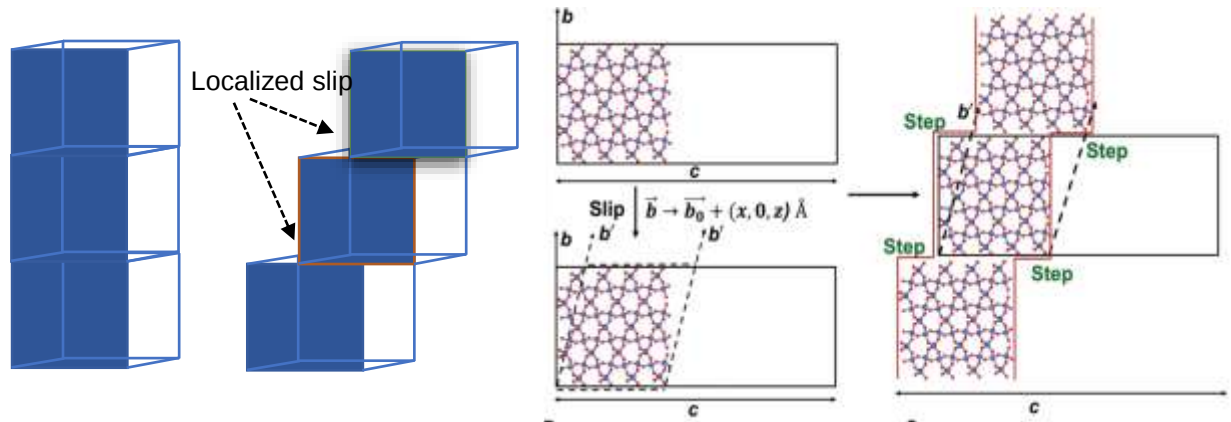
Spoorthi, et. al., *Science*, 2024

Mechanism: Cleavage

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



Mechanism: Slip



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

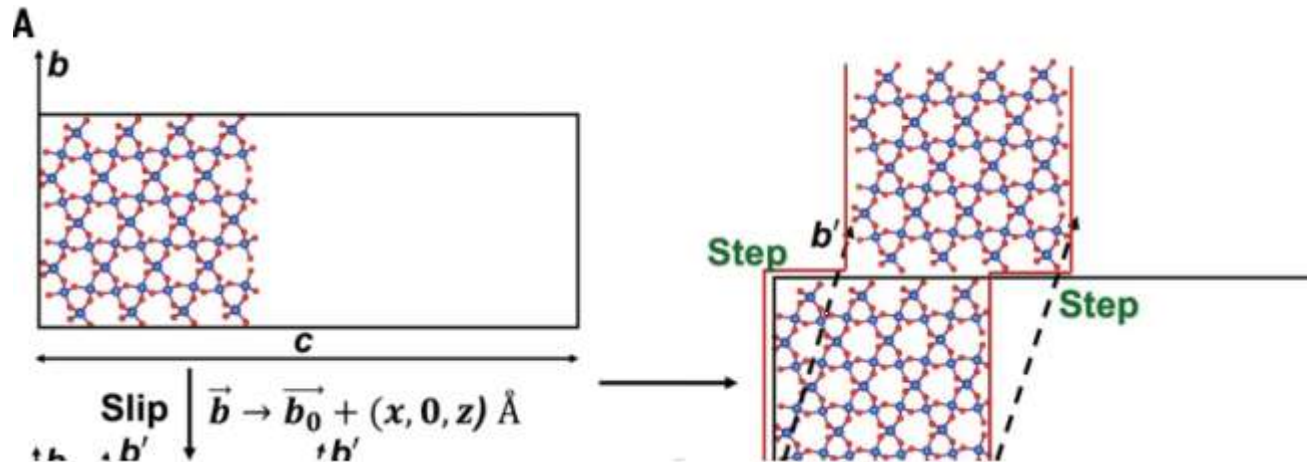
Stacking fault

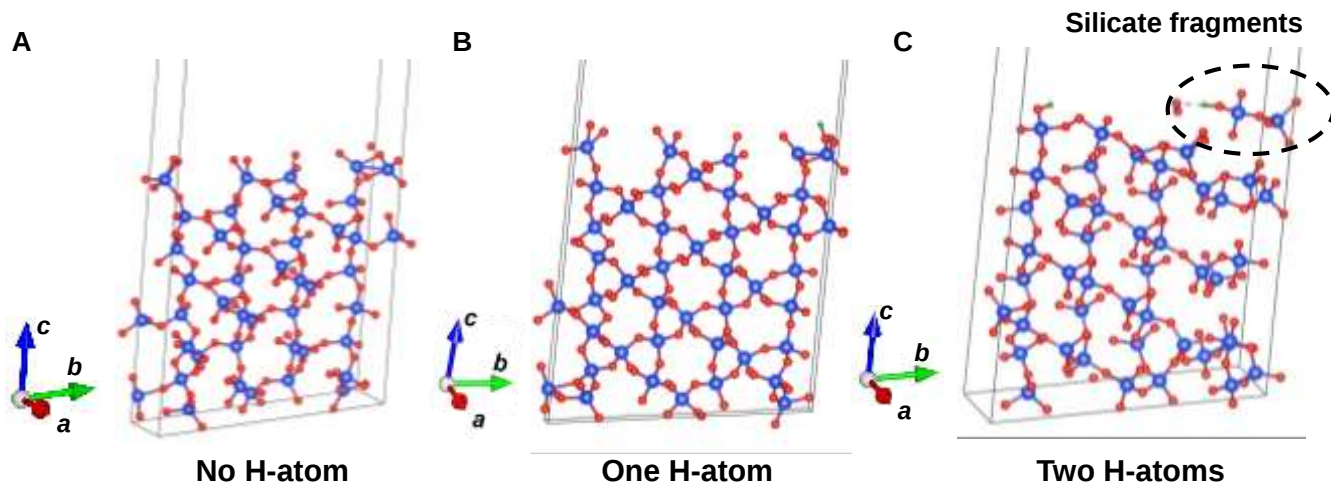
$$\vec{b} \rightarrow \vec{b}_0 + (x, 0, z)$$

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

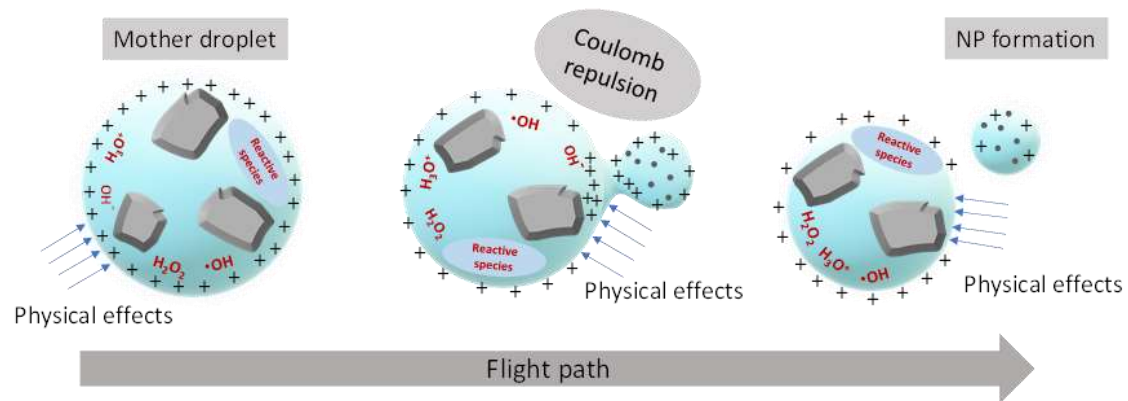
SFEs of (010) direction with (0, 0), (0, 0.5), (0.5, 0) and (0.5, 0.5) slip configurations on the (110) plane of SiO₂

SFE (J/ m ²)	Slab					
	x	z	w/o H- atom	1 H- atom	2 H- atoms	E
	0.0	0.0	0	0	0	0
	0.5	0.5	-1.21	-0.93	-0.88	-1.20
	0.5	0.0	1.20	1.18	0.90	1.12
	0.0	0.5	-0.07	0.89	-0.83	-0.09





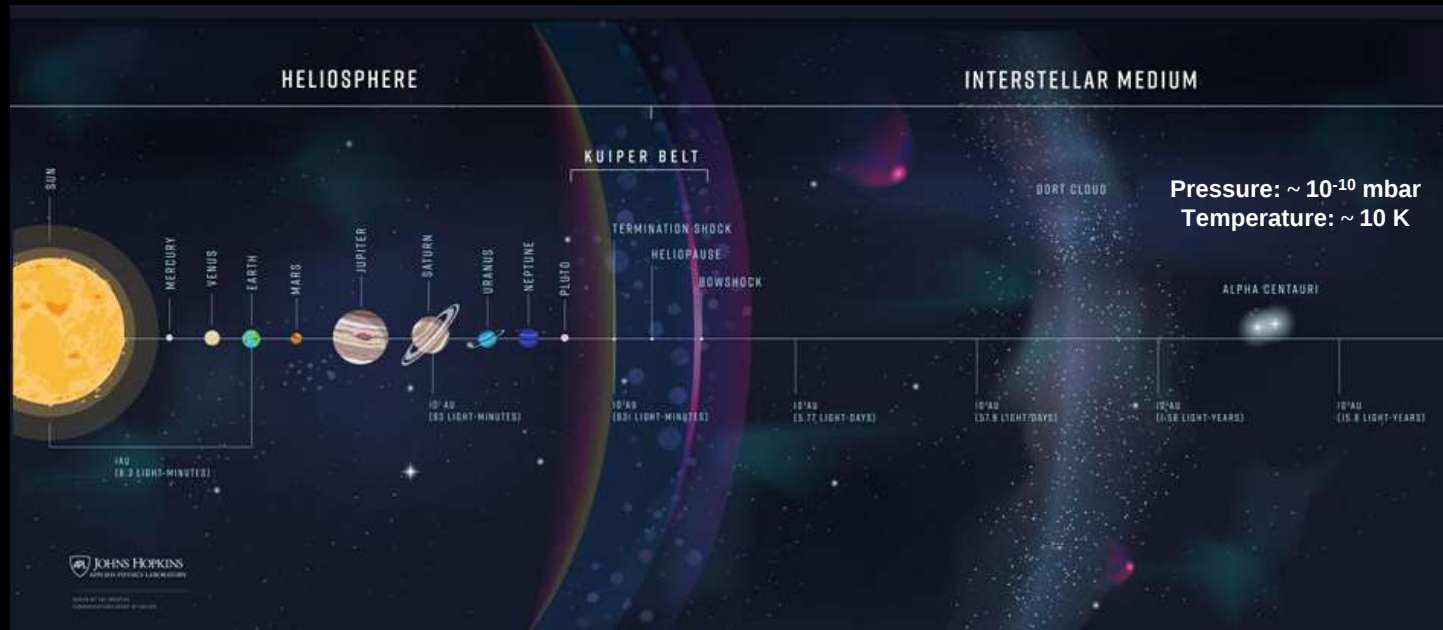
Mechanism of nanoparticle formation



Can Clathrate Hydrates Exist in Space?

Exploring astrobiology

Interstellar medium



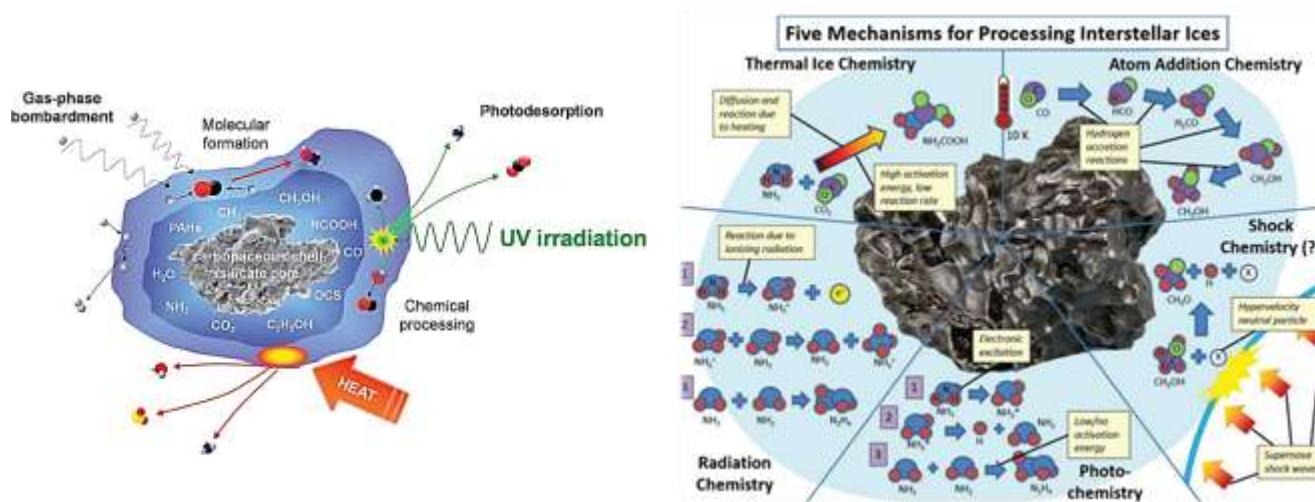
Diffuse clouds: $T \sim 100$ K, $n \sim 100$
molecules per cm^3

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

<https://spaceref.com/science>

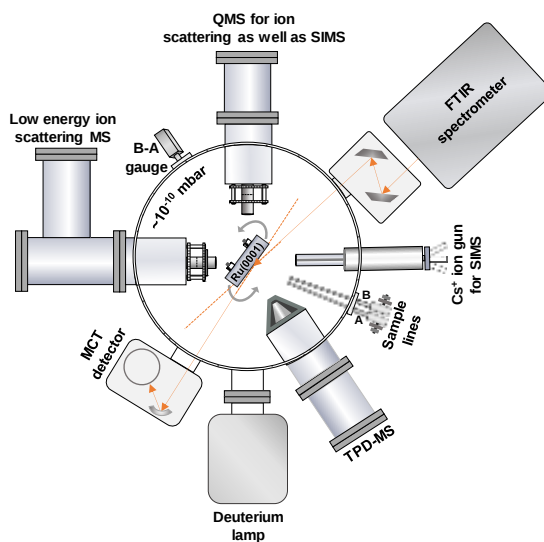
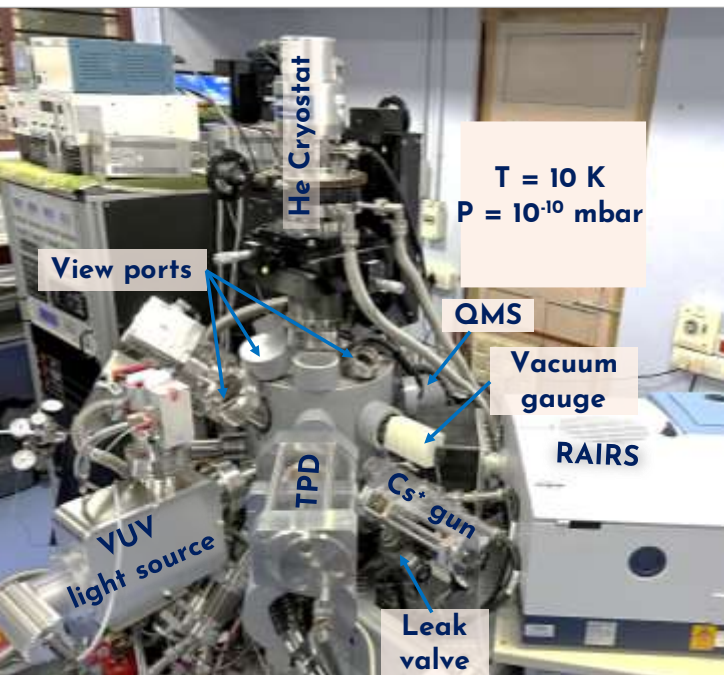
Interstellar ices



Silicates and carbonaceous material – 0.01-0.5 μm

Arumainayagam, C. R. *et al.*, *Chem. Soc. Rev.*, **2019**, 48, 2293–2314

Instrumentation

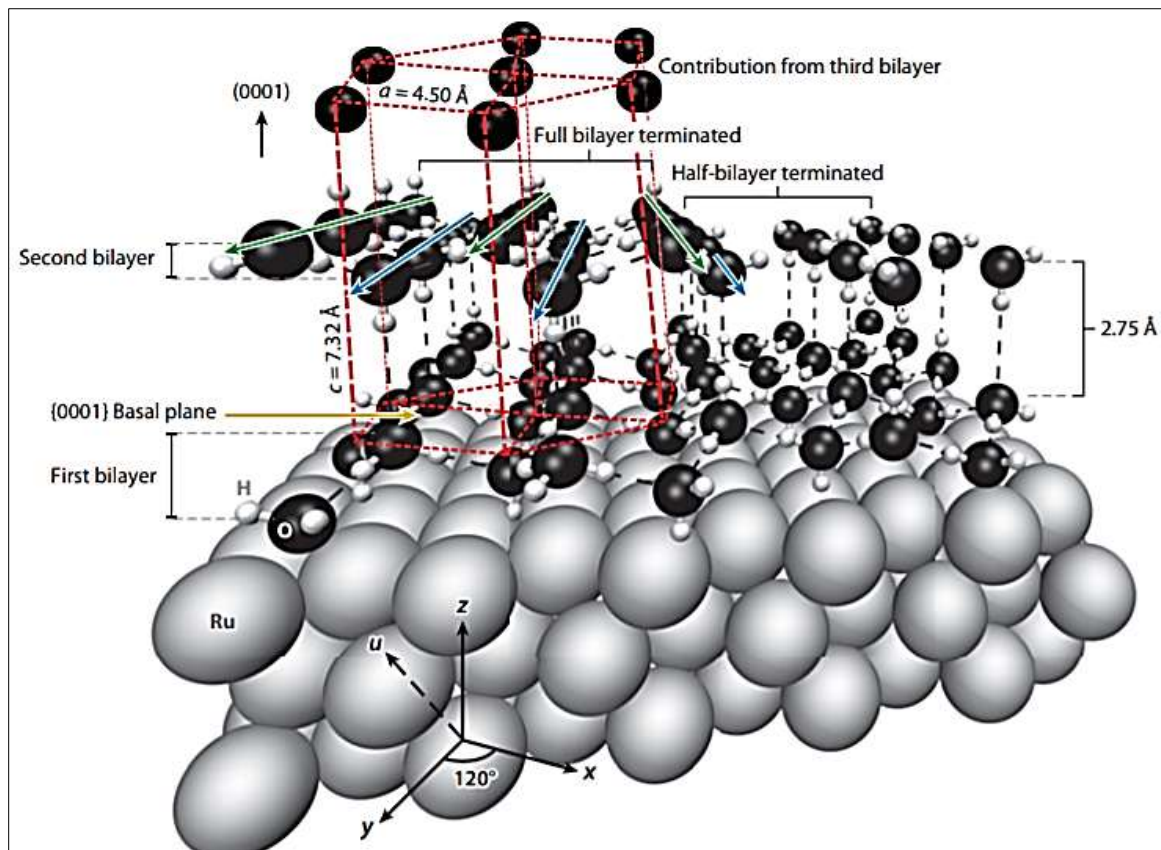


115-400 nm



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

Viswakarma, G. et al., *J. Phys. Chem. Lett.*, **2023**, *14*, 2823–2829



Formation and Transformation of Clathrate Hydrates under Interstellar Conditions

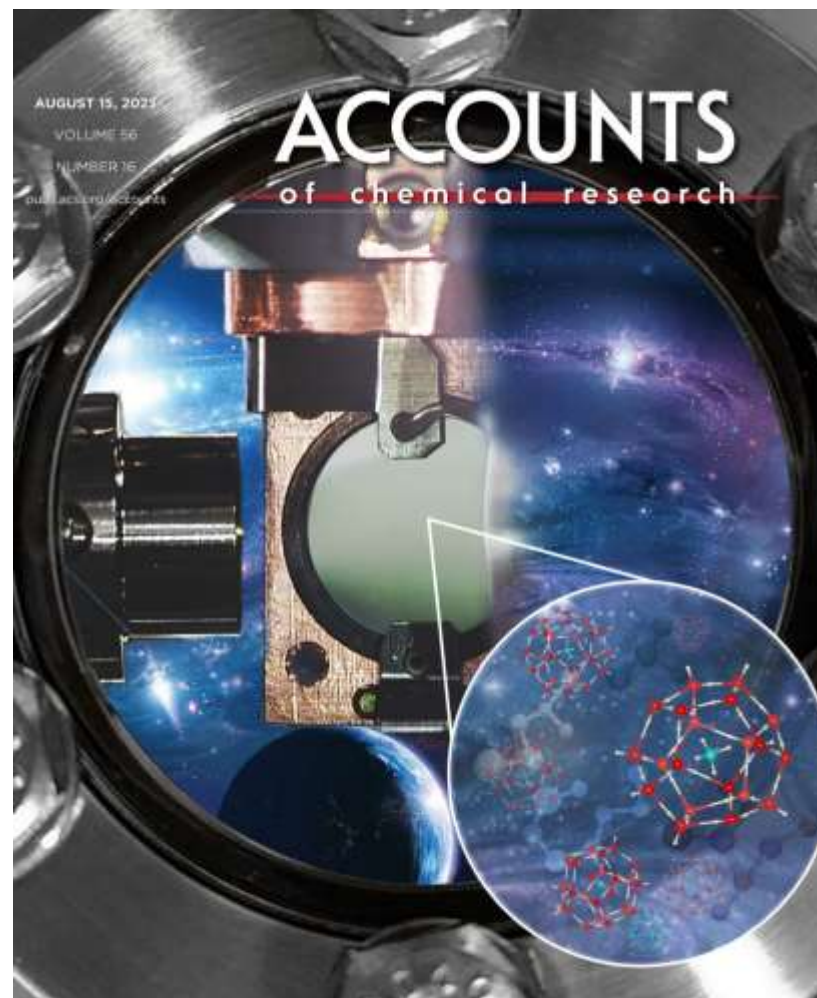
Jyotirmoy Ghosh, Gaurav Vishwakarma, Rajnish Kumar,^{*} and Thalappil Pradeep[†]



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



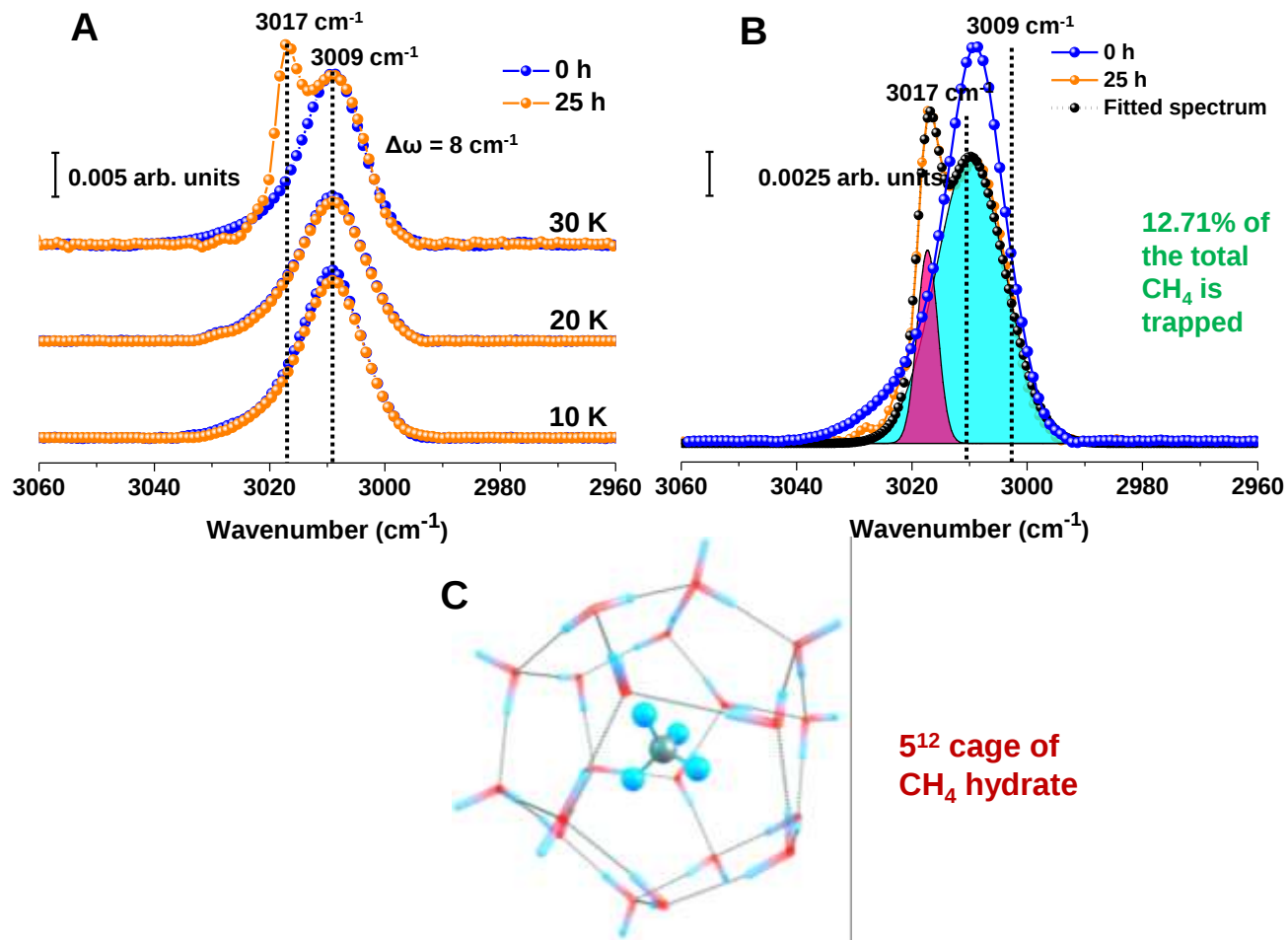
Read Online



Clathrate hydrates in interstellar environment

Ghosh, J. et al., *Proc. Natl. Acad. Sci. U.S.A.*, **2019**, *116*, 1526-1531

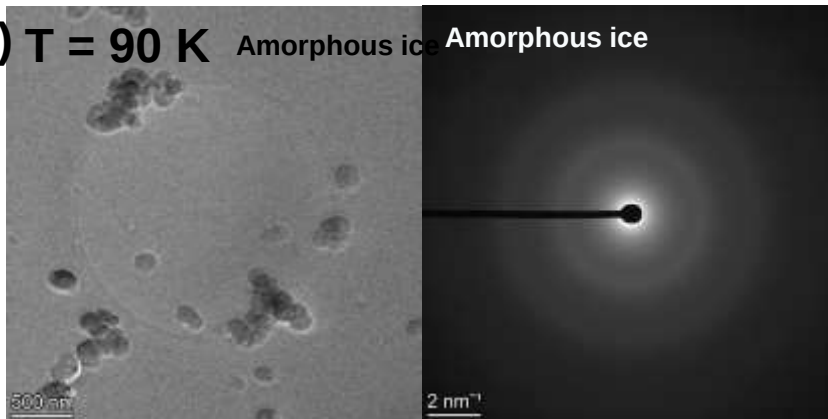
Clathrate hydrates in interstellar environment



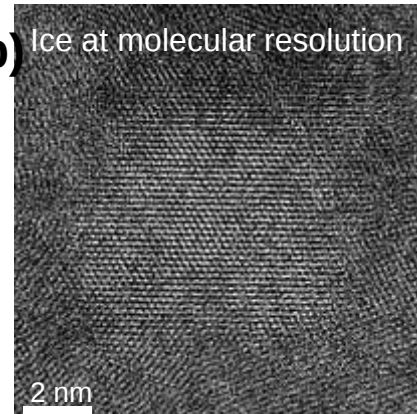
Ghosh, J. et al., *Proc. Natl. Acad. Sci. U.S.A.* **2019**, 116, 1526-1531

Observing growth of crystalline ice from amorphous ice

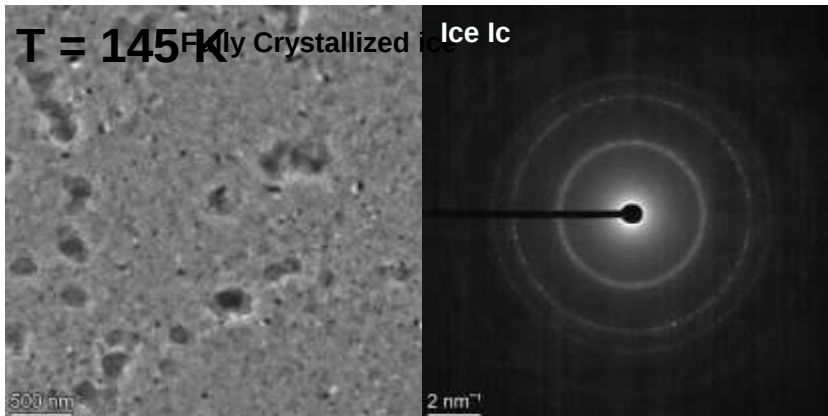
(a) $T = 90\text{ K}$ Amorphous ice



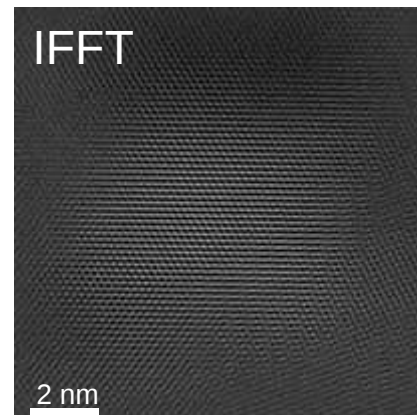
(b) Ice at molecular resolution



$T = 145\text{ K}$ Fully Crystallized ice

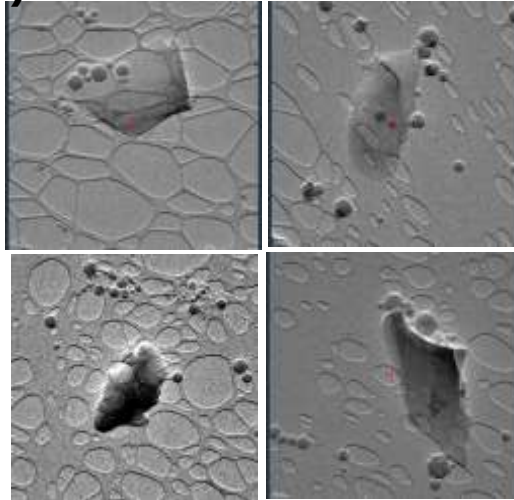


IFFT

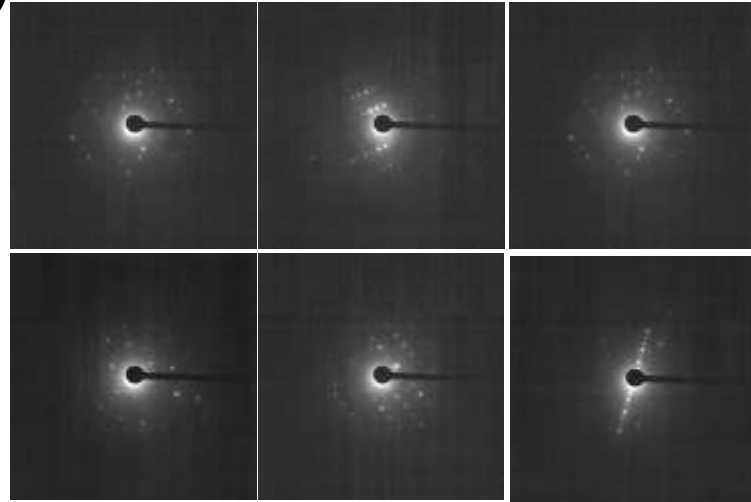


Electron diffraction of nanometer-scale crystals of clathrate hydrate

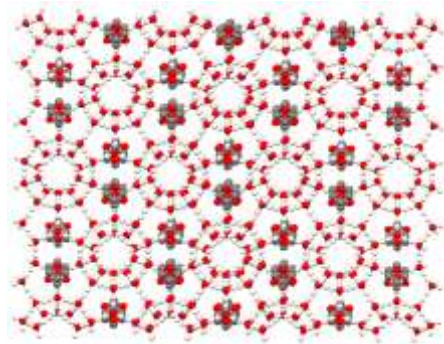
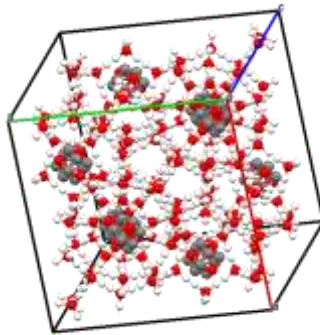
(a) THF-CH₄ Clathrate hydrate crystal



(b) 3 D electron diffraction



(c)



Crystal structure





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

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MS Theses: Ananthu Mahendranath, Ramesh Kumar Soni

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



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