

# THE SCIENCE NEWSLETTER

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### A Chain Full of Carbon

It can be hard and shiny; it can be flaky and soft; it can even look like a football. Carbon, the backbone of life on Earth, is one of the most versatile elements in the periodic table. It can form allotropes (structurally different forms of the same element) depending on its hybridisation states and atomic arrangements. These allotropes include the semiconducting layers of graphite, the insulator diamond, and fullerenes.

Cyclo[n]carbons — carbon allotropes built solely from n carbon atoms covalently linked in a ring — have enticed chemists for many years. Until now, it was considered almost impossible to isolate or structurally characterise these cyclo[n]carbons due to their high reactivity, although evidence for their existence was found in the gas phase.

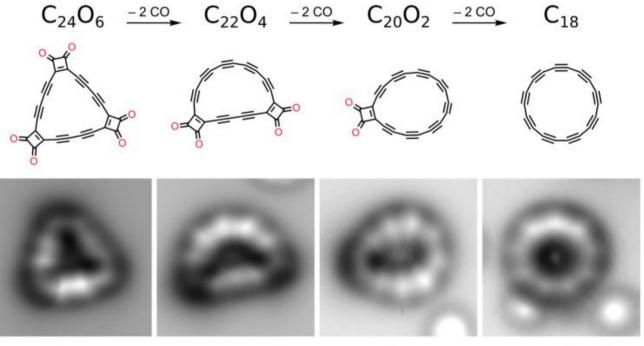


Fig. 1: From left to right, precursor molecule  $C_{24}O_6$ , intermediates  $C_{22}O_4$  and  $C_{20}O_2$  and the final product cyclo[18]carbon  $C_{18}$  created on surface by dissociating CO masking groups using atom manipulation. The bottom row shows atomic force microscopy data using a CO functionalized tip, obtained on an inert surface (bilayer NaCl on a Cu single crystal). [Image credits: IBM Research]

In an astounding first, a team of researchers from the University of Oxford and IBM Research (Zurich) have synthesised and characterised a pure ring of 18 carbon atoms. The team generated a cyclo[18]carbon on an inert surface at temperatures of nearly 5K (-268°C) and investigated the species using high-resolution atomic force microscopy. The chemists started with a carbon oxide precursor,  $C_{24}O_6$ , which has a triangular shape. By applying voltage pulses to the tip of the atomic microscope, they were able to remove pairs of CO-groups from the precursor, eventually removing all 6 CO-groups to form cyclo[18]carbon (see fig. 2), with fixed positions of alternating single and triple bonds.

Theoretical results were ambiguous about whether or not cyclo[18] carbon would have this kind of a structure. The alternating single and triple bond structure is supposed to give carbon chains and rings the properties of semiconductors. The high reactivity of the cyclo-carbon has opened up new avenues for synthesising other carbon allotropes and carbon-rich structures, which can be used as components for molecular electronics and nanotechnology.

While the researchers are yet to see if the molecule will remain stable when lifted off from the surface, these findings have given rise to new fields of investigation in cyclo-carbons, and show promising applications in the near future.

#### Miniature Mastermind

The 'Travelling Salesman Problem': a notorious mathematical puzzle that has been challenging masterminds for centuries, has met with a most peculiar contender—the amoeba.

The TSP states that there is a salesman who has to visit different cities by taking the shortest path possible and has to avoid visiting the same city twice. So far, the easiest known method to solve this is to try out all possible paths. The exponential increase in time taken to solve this problem as the number of cities increases makes it an extremely cumbersome task. There-

fore, this puzzle becomes an optimisation problem.

An amoeba was made to move in a petri-dish with agar (nutrient medium) at various locations which mimicked cities in the TSP. Amoeba instinctively avoids light, a characteristic which was exploited by illuminating some channels to ensure that the protozoan doesn't visit the same spot twice. The researchers concluded that the amoeba naturally chose the shortest path and found that the time taken by it was not an exponential function but rather a linear function of the number of locations (cities). Though they were unsuccessful in explaining the reason behind the amoeba's efficiency, their work encourages us to appreciate the omnipresent beauty of life. Thus, the amoeba has proven to be the quintessence of the prominent saying, 'Appearances can be deceptive.'





## An Interview with Dr Amal Medhi

Earlier this month, Anvesha got a chance to interview Dr Amal Medhi of the School of Physics here at IISER TVM. Dr Medhi works in several areas centred around condensed matter physics. Dr Medhi spoke to us about IISER TVM's first supercomputer cluster, PADMANABHA. Here are some excerpts from Dr Medhi's (AM) interview with Subrabalan M (SM) and Gokul Prabhu of batch '17:

#### SM: Prof. Medhi, what is a supercomputer? How is it different from an ordinary PC?

**AM:** Computational speed has hit a limit in terms of processor speed. The only way to breach this limit is to run multiple processors in parallel, in what is known as parallelisation. A typical modern-day laptop's processor, for example, will have around four cores working in parallel. A supercomputer runs a much larger number of processors in parallel. These processors are distributed among multiple nodes. A node can be thought of as a desktop or workstation, with each node typically having thirty processing cores. All the processors have to run in parallel, so they must be connected through a specialised network architecture since connecting them conventionally via ethernet will slow the computer down.

SM: What factors were taken into consideration while deciding to set up the supercomputing facility here?

AM: Many of our research work relies on high-performance computing. The faculty and research groups currently working at IISER, and possible new faculty might need a supercomputer to work with.

So, according to an estimate of computing power required and the budget in hand, we decided on this supercomputer, PADMANABHA. It has around 2500 GPU processing cores. The total computing capacity is measured in teraflops (Tflops), where flops stands for floating-point operations per second. Our cluster has a capacity of 120 teraflops. It ranks within the top 20 supercomputers in terms of computing capacity in India.

#### SM: How does our supercomputer compare to others in India and abroad?

AM: As of 2019, the world's number one supercomputer, named Summit, is stationed in the US and has over 2 million processing cores and around 10<sup>5</sup> teraflops of processing power.

India's top supercomputer is owned by the Indian Meteorological Department. It has 1 lakh processing cores and four thousand teraflops of processing capacity. Compared to this, our cluster is pretty small in size, but it is sufficient for our institute.

#### SM: Why a supercomputer?

**AM:** In my research, which is in the realm of computational condensed matter physics, I use techniques like the Quantum Monte Carlo. If I have to run a calculation of a physical system containing a hundred atoms to study the ground-state wave function of this system on my laptop, a program to calculate a single parameter will run for ten days or more. A supercomputer on the other hand can handle the same calculations in about an hour. In biology, studies in areas like genomics typically involve the processing of terabytes of data, which necessitates the usage of a supercomputer.

### SM: Maintaining a supercomputer of this scale probably comes with its own set of demands; what goes into the maintenance and upkeep of a supercomputer cluster?

AM: There is more to maintaining a supercomputer cluster than just the processors; having a large number of processors consumes a lot of power and generates a lot of heat. Even when the cluster is running no program, it consumes 20 kVA of power and dissipates an equal amount of heat. There is a significant increase in power consumption while at 100% utilisation, which necessitates a specialised cooling solution. Furthermore, a dedicated UPS system needs to be put in place for use during power outages. A specialised housing has been constructed with supporting infrastructure and sensors for various kinds of failures, like fires and leaks; this is called a datacentre.

#### SM: What kind of software does the cluster run? Why do most contemporary supercomputers run Linux? Why not Windows or macOS?

**AM:** Linux is the go-to operating system for computational uses. One reason behind this, is that Linux is more secure than Windows. Another reason is that you can do things faster on Linux. Many high-performance applications and softwares are specially developed on Linux systems for Linux systems.

#### SM: Can you tell us more about your current project and your field of interest?

**AM:** My area of research is condensed matter theory. Nearly every sphere of research has adopted the use of machine learning these days, and condensed matter theory is no exception. We have been using machine learning to detect phase transitions and study wave functions of condensed matter systems.

To give you an idea, it is possible to solve the equations for a single free particle in a box, but it becomes difficult to do so for a system of two electrons interacting with each other. A condensed matter system by default consists of particles in numbers of the order of  $10^{23}$  in magnitude; solving Schrödinger's equation for such a system is a near impossible endeavour.

How, then, are the quantum mechanical properties of a condensed matter system studied? We cannot solve Schrodinger's equation directly, but there are other ways by which we can extract the properties of such systems. One application of machine learning is based on neural network architecture. We can use a neural network to represent the wave function of a many-body interacting system.

My work also involves using neural networks to study the wave function of a many-body interacting system. Apart from this, I work on things like the theory of various electronic phases in condensed matter, which tells us why metals, insulators, topological insulators, superconductors and magnets are what they are. I often use numerical techniques for these explorations.

# SM: Condensed matter is a hot area of research currently. I am quite sure many students are interested in the same. What would you expect from a student interested in working with you, and what advice would you give him/her?

AM: Usually, condensed matter physics doesn't appeal to many students. Condensed matter physics is a tough subject; you need to know quantum mechanics, statistical mechanics and several other branches that are involved here. Often, in condensed matter, the theories that are dealt with aren't exact, and contain many approximations. The learning curve is very steep and it takes a long time to start getting deep into theory. After reaching the level of familiarity required to start exploring its depths, the subject becomes fascinating. Regardless of the area a student wants to work in, he/she has to show involvement and should enjoy whatever they are doing. Perseverance is key.

### SG: It has been a pleasure talking to you about supercomputers and condensed matter physics, sir. Thank you for your time. Do you have a message you'd like to give to the students?

**AM:** Thank you. I have an essential piece of information to share. In our supercomputer, the individual processors run at a lower speed than those on a laptop. For example, on an average computer, the processing core will run at around 3 GHz. In comparison, our supercomputer runs at around 2.6 GHz. As a result, a serial program runs slower on the supercomputer than an average laptop. One needs to run a parallel program/application to take full advantage of the supercomputer. One must keep that in mind. All the best!



#### Paper Review: There's Plenty of Room at the Bottom, by RP Feynman

Richard Feynman's famous talk, titled 'There's Plenty of Room at the Bottom,' is often credited with conceptualising the basic notions of nanotechnology. He delivered this seminal lecture at an American Physical Society meeting at Caltech in 1959. It addressed questions such as: 'How small a machine could one build? How tiny could one write?'

Feynman envisioned the creation of a new field that dealt with the manipulation and control of things at a microscopic scale. This lecture gave birth to the idea of tiny machines building even tinier machines. This one talk contained all the elements of inspiration for kick-starting developments in synthetic chemistry, molecular engineering and quantum computers.

It began with the realisation that it is possible to write all 24 volumes of the *Encyclopaedia Britannica*, on the head of a pin. Imagine being able to shoehorn all the information that mankind has ever gathered, into the pages of this newsletter! All we have to do, then, is find a way to write in a font that is small enough.

How then, do we write that small? The sputter deposition technique we use today comes close to achieving this feat. A large number of electrons or ions are directed onto a clean surface using electric fields. These accelerated particles either engrave characters on the surface or remove superfluous material around atoms to forge letters. The advent of scanning tunnelling microscopy in the 1980s paved the way towards the realisation of these ideas. One cannot help but marvel at how prescient Feynman's thoughts were.

Storing data physically and reading it on demand seemed to be the crux of the problem. Back when the scientific community had not yet thought of biological structures as machines, he recognised that data storage at nanoscales was already apparent in biological systems. It was remarkable to have identified DNA, only six years after its discovery, as an information-encoding structure.

This talk reveals a fantastically creative mind capable of envisioning that which is yet to come. Though the speech did not have a tremendous impact back then, by the 1990s, it came to be considered the earliest endorsement of nanotechnological research. Sixty years on, some of Feynman's ideas may sound dated, but they nonetheless remain relevant. Give it a read if you want to witness the spectacle of a genius giving free rein to his imagination!

-- Abhay Hegde, BSMS B'16 <u>Read the paper here</u> <u>Image Source</u>



#### The Truth about the Amazon Fires

Scientists conclude that the fires in the Amazon were man-made, and many claim fires were ultimately spawned by Brazilian President Bolsonaro's anti-indigenous agenda.

A total of 72,843 fires were recorded in the Amazon this year alone, the highest number ever recorded in history. Surprisingly, climate change is not to blame for this. After conducting multiple studies, scientists at Brazil's National Space Research Institute claim that there is no meteorological abnormality that could have propelled the forest fires.

'There is nothing abnormal about the climate this year or the rainfall in the Amazon region, which is just a little below average,' says National Space researcher Alberto Setzer. 'The dry season creates favourable conditions for the spread of fire, but starting a fire is the work of humans, either deliberately or by accident.' Indigenous communities find it hard to believe that the fires were accidental. The reports have been directed at cattle ranchers and profit-motivated companies (government and private) who have been instigating the fires with petrol bombs. Over a million indigenous people and at least a 100 uncontacted tribes have been affected.

The streets of Brazil were filled with angered activists, their voices echoed by thousands across the world who surrounded Brazil's embassies in protest against the fires and the government's inaction. After receiving pressure from the international community, the South American governments ramped up their fire-fighting initiatives. The fire continues to ravage the Amazon despite the governments' best efforts.

Smoke from the forest fires in the Amazon could be seen from space, blacking out the sun in livelihoods over a thousand miles away.

-- Kratika Mazde, BSMS B'18 Image Source





## The Humble Ballpoint

One fine day, László Bíró, a newspaper editor, noticed how the ink used in newspapers dried quickly and did not smudge. Acting upon his frustration of having to refill fountain pens and cleaning the smudges they caused, he ended up inventing the ballpoint pen in 1931.

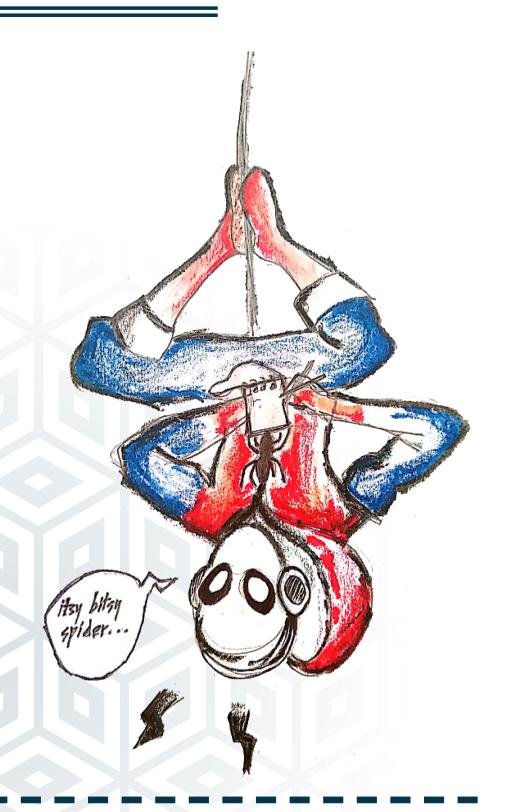
As the name suggests, ballpoint pens use a 'ball' commonly made of brass or steel to roll the ink stored in the barrel of the pen out on paper. The ink used in ballpoint pens is usually a paste containing 25-40% dye suspended in an oil-based solvent. The solvent is usually benzyl alcohol, which blends with the dye to create a smooth paste that dries quickly.

Did you know that a standard ballpoint pen will fail you if you try writing with it upside-down?

This is because the ink in a standard ballpoint pen isn't pressurised and only flows down because of gravity, the pen being upside-down will inhibit the ink's movement to the nib.

In recent years, there have been different modifications in the ballpoint pen, one of them being the use of pressurised cartridges to write upside-down. The pressurised reservoir forces a thicker ink to the nib, and the reservoir being sealed, eliminates leakages.

-- Akshita M, BSMS B'19 Art by Aiswarya P S, BSMS B'18



We hope you enjoyed this month's edition of Exhibit: A!

If you are interested in contributing any content, artwork, or want your research featured here, please get in touch with us at:

anveshacontent@gmail.com

Send your suggestions to: <a href="https://forms.gle/pBzJW7GSv7bC5r7RA">https://forms.gle/pBzJW7GSv7bC5r7RA</a>

Have any science-related questions you'd like answered? Send them to us and we'll get our best minds on it!

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