A*STAR

RESEARCH

Issue 42 | July – August 2024

NEARING QUANTUM HORIZONS

A*STAR frontiers in the national push for a quantum computing advantage

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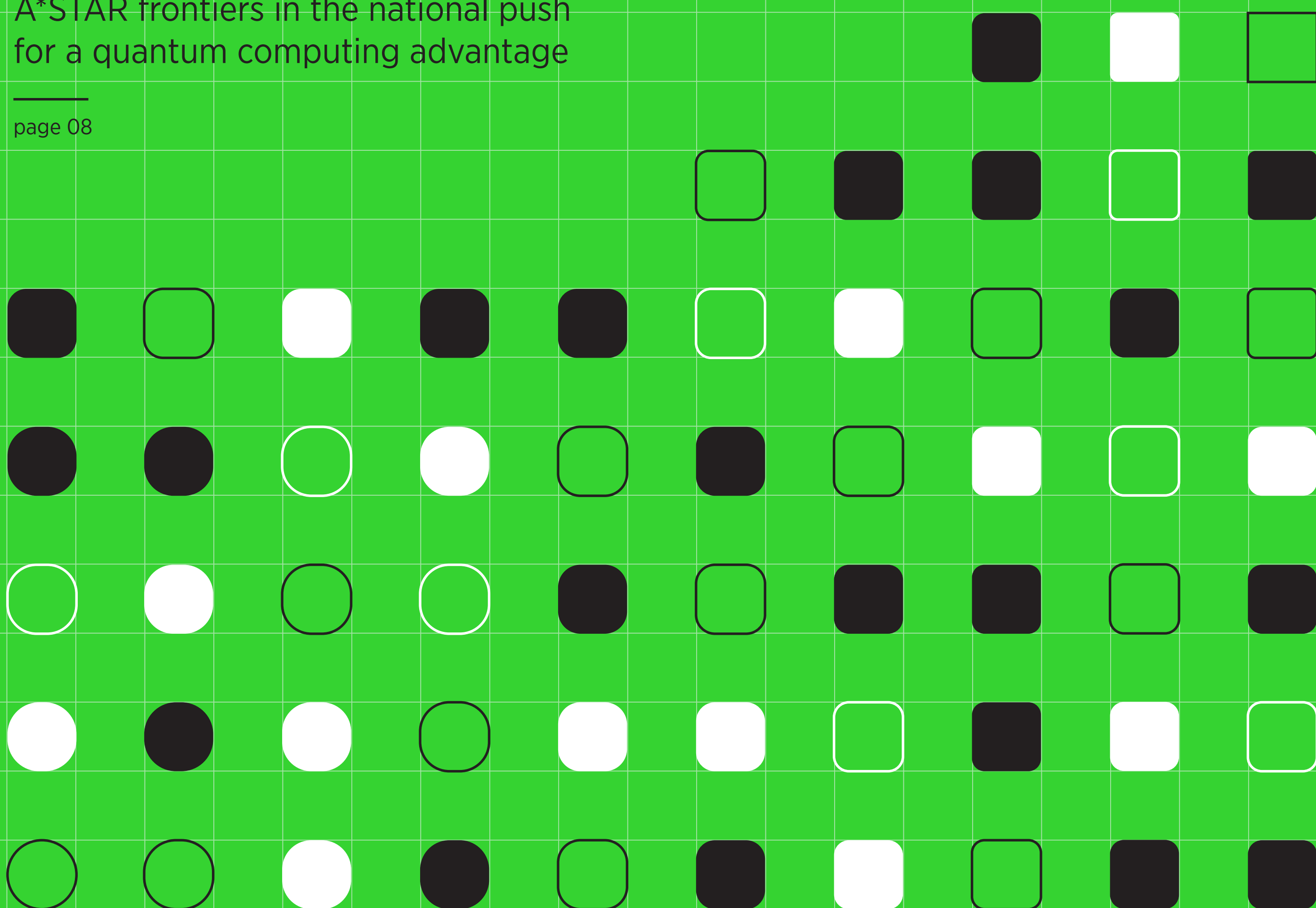

DECODING CANCER'S MOLECULAR DANCE

How spatial omics and AI reveal new disease insights

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BRINGING QUBITS TO CHEMISTRY

The promise of quantum circuits for molecular models

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EDITORIAL

Agency for Science, Technology and Research

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The Agency for Science, Technology and Research (A*STAR) is Singapore's lead government agency dedicated to fostering world-class scientific research and talent for a vibrant knowledge-based economy.

A*STAR actively nurtures public-sector research and development in biomedical sciences, physical sciences and engineering, and spurs growth in Singapore's key economic clusters by providing human, intellectual and industrial capital to our partners in industry and the healthcare sector.

A*STAR currently oversees the following research institutes, consortia and horizontal technology coordinating offices, and supports extramural research with universities, hospital research centres and other local and international partners:

- A*STAR Infectious Diseases Labs (ID Labs)
- A*STAR Institute for Human Development and Potential (A*STAR IHDP)
- A*STAR Skin Research Labs (A*SRL)
- Advanced Remanufacturing and Technology Centre (ARTC)
- Bioinformatics Institute (BII)
- Bioprocessing Technology Institute (BTI)
- Experimental Drug Development Centre (EDDC)
- Genome Institute of Singapore (GIS)
- Horizontal Technology Coordinating Offices (HTCO):
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  - Artificial Intelligence, Analytics and Informatics (AI³)
  - Epidemic Preparedness (EP)
  - Robotics
  - Social Sciences and Technology (SST)
  - Urban and Green Technology (UGT)
- Institute of Sustainability for Chemicals, Energy and Environment (ISCE²)
- Institute of High Performance Computing (IHPC)
- Institute for Infocomm Research (I²R)
- Institute of Molecular and Cell Biology (IMCB)
- Institute of Microelectronics (IME)
- Institute of Materials Research and Engineering (IMRE)
- National Metrology Centre (NMC)
- Singapore Immunology Network (SIgN)
- Singapore Institute of Manufacturing Technology (SIMTech)
- Singapore Institute of Food and Biotechnology Innovation (SIFBI)

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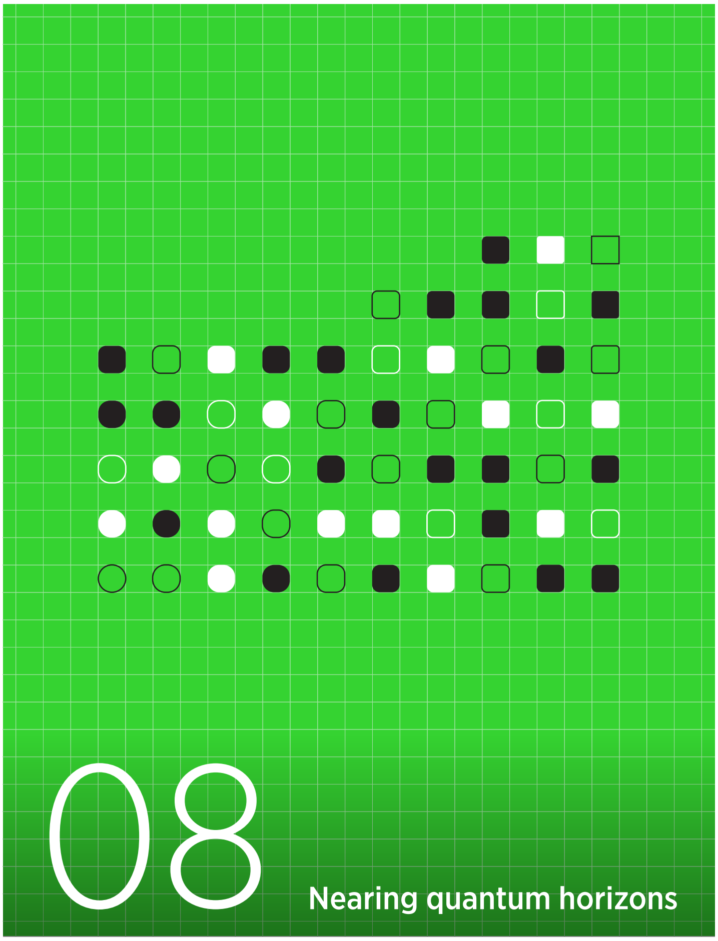

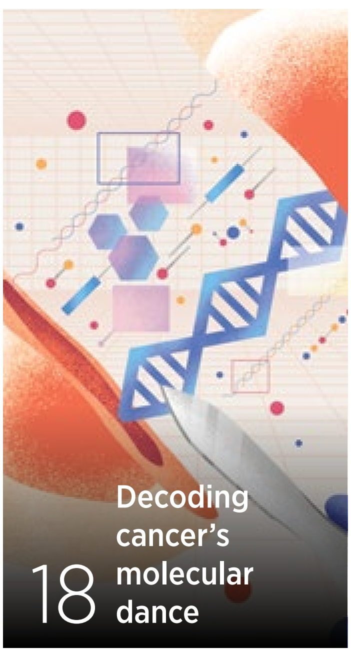

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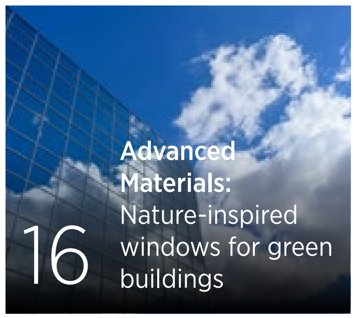

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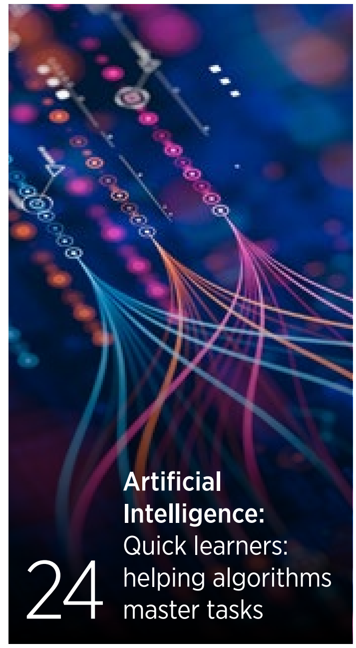

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EDITORIAL NOTES

Over eight decades since the first digital computer emerged, computers have changed our world by accelerating calculations vital for innovation. However, a new paradigm in computer architecture—one based on quantum mechanics, rather than electronics—promises to take the computing age further by solving problems beyond the scope of classical machines.

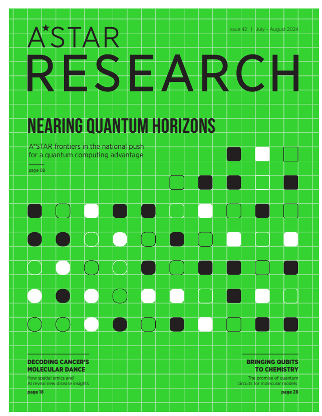
In this issue's cover story, 'Nearing quantum horizons (p. 8)', we dive into research taking place at A*STAR in quantum software and hardware that aim to harness quantum computing's advantages. From simulations to hybrid systems, the agency is at the forefront of explorations that support Singapore's aspirations as a hub for quantum technologies.

Whether powered by quantum or classical systems, artificial intelligence (AI) remains an exciting tool for clinicians aiming to make sense of health and disease. In our first feature, 'Decoding cancer's molecular dance (p. 18)', Assistant Principal Investigator Mai Chan Lau discusses how her team combines decades of histopathological knowledge with AI-assisted spatial technologies to provide new insights on cancers.

One promising advantage that quantum computing offers is in quantum chemistry, where its fundamental systems can more easily model the molecular physics of chemical reactions. In our second feature, 'Bringing qubits to chemistry (p. 28)', A*STAR scholar Karthik Shreekumar Panicker describes his current work in developing quantum circuits that capture the complex dynamics involved.

Beyond the quantum sphere, new developments in other fields continue to emerge from A*STAR research institutes. These include innovations such as smart windows that adapt to climate conditions, and cutting-edge photonic chip components. More on these can be found in 'Nature-inspired windows for green buildings (p. 16)' and 'To build a light-speed data highway (p. 34)'.

For more of the latest developments from A*STAR researchers, visit our website at **research.a-star.edu.sg**. You can also stay up-to-date by following us on X/Twitter at **@astar_research**, LinkedIn at **A*STAR Research** and Telegram at **A*STAR Research**.



On the cover
A grid of evolving icons symbolises the multiple possible states a qubit can represent: a foundational concept in quantum computing.

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MICROBIOLOGY

Superbug killers on native soil

A newly discovered antibiotic compound found in local soil can potentially combat some of the world's toughest drug-resistant bacteria.

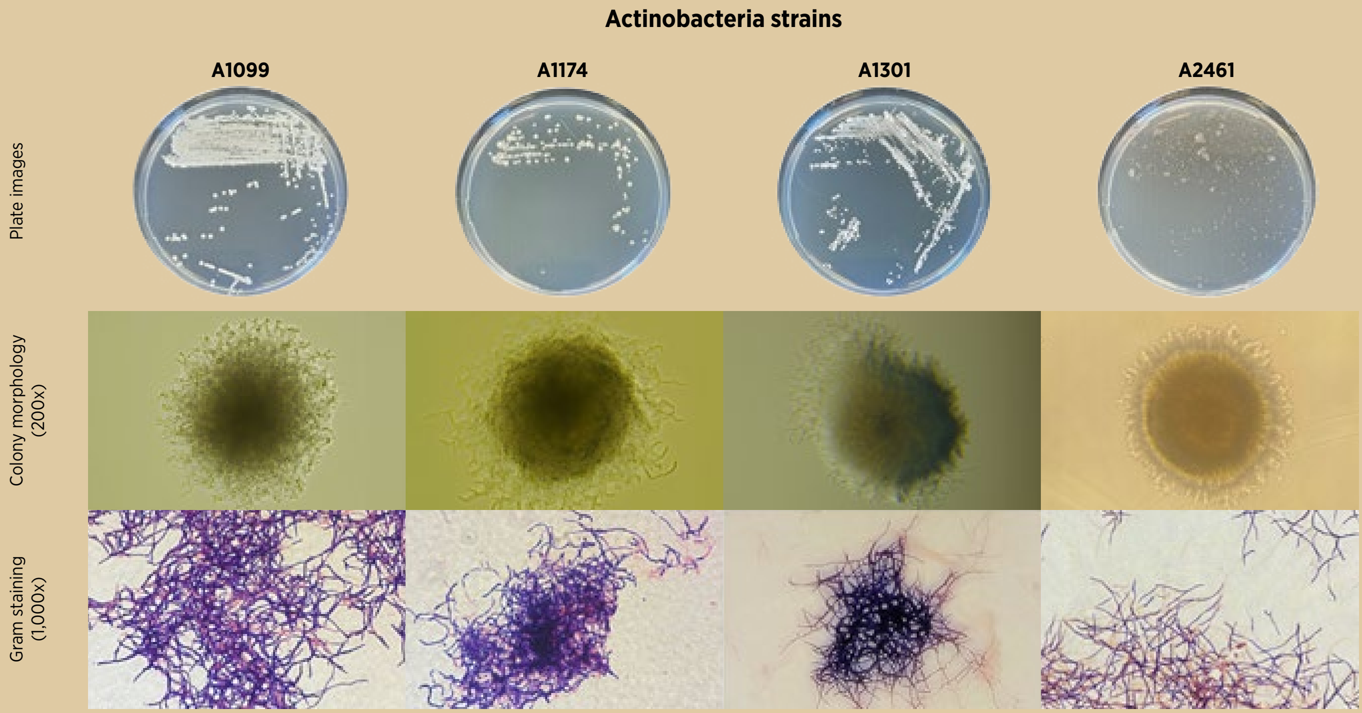
The solution to combating antibiotic resistance—one of the greatest threats to global health—might be right beneath our feet. As bacteria evolve genetic defences that render our existing antibiotics ineffective, microbiologists are urgently seeking new antimicrobial agents.

Elaine Jinfeng Chin, a Postdoctoral Researcher at A*STAR's Singapore Institute of Food and Biotechnology Innovation (SIFBI), has turned to the natural world for answers, specifically examining bacteria from Singapore's soil.

"Actinobacteria are a diverse group of bacteria that are known for producing bioactive compounds," said Chin. These microorganisms are like miniature factories, being responsible for about 45 percent of all bioactive compounds derived from microbes. They have also been pivotal in developing treatments for infections, cancer and inflammation. Yet despite their known potential, the actinobacteria indigenous to Singapore's soil are relatively uncharted.

To dig for answers, Chin and colleagues probed these microbial resources by cultivating selected

Photo credit: Nel Ranoko / Unsplash



Visual images of four actinobacterial strains that were isolated from terrestrial soil samples in Singapore and characterised to identify potential natural compounds with antimicrobial activity.

"The discovery of tetronomycin A provides hope for research to expand the repertoire of potential antimicrobial agents."

strains from A*STAR's diverse Natural Product Library under different culture conditions. This method, known as the OSMAC (One Strain Many Compounds) approach, is designed to activate different secondary metabolite gene clusters within the actinobacterial strains by altering their environmental and cultural conditions, said Chin.

The team then tested extracts from those strains against a range of pathogens that cause human diseases. The strains that showed potent antimicrobial activity were then cultivated on a larger scale. Extracts from them were then purified to isolate bioactive components.

Next, the researchers employed high-resolution mass spectrometry and nuclear magnetic resonance to shed light on the chemical structures of these compounds. They identified nine known antimicrobial compounds as well as a novel one—tetronomycin A, which proved effective against both *Staphylococcus aureus* (SA) and its more formidable variant, methicillin-resistant *Staphylococcus aureus* (MRSA).

Both SA and MRSA are notorious not only for the severe infections they cause in both healthcare and community settings, but for the resistance they have developed to many antibiotics.

"The discovery of tetronomycin A provides hope for research to expand the repertoire of potential antimicrobial agents," said Chin, highlighting its potential use in creating compound libraries for further antimicrobial efficacy evaluations.

Currently, the team is focused on deciphering tetronomycin A's mechanism of action and conducting structure-activity relationship studies to explore its viability as a novel antibacterial agent. ★

Researchers
Siew Bee Ng, Elaine Jinfeng Chin and Yoganathan Kanagasundaram, SIFBI

IN BRIEF
A*STAR researchers successfully isolate nine antimicrobial compounds from local soil bacteria strains, including a novel tetronomycin A that effectively inhibits *Staphylococcus aureus* and MRSA bacteria.

1. Chin, E.-J., Ching, K.-C., Tan, Z.Y., Wibowo, M., Leong, C.-Y., *et al*. Natural products from Singapore soil-derived *Streptomycetaceae* family and evaluation of their biological activities. *Molecules* **28** (15), 5832 (2023).

Photo credit: Dose Juice / Unsplash

CARDIOLOGY

To the heart of fasting benefits

A study in mice shows intermittent fasting can improve heart health by altering key molecular and cellular pathways.

We've been told to eat more heart-healthy foods like olive oil, but the latest nutritional advice is focusing on not just what we eat, but *when* we eat. Lifestyle changes like intermittent fasting (IF)—which limits eating to specific times of the day—are emerging as promising strategies to not only boost heart health, but protect against heart disease and peripheral vascular diseases such as atherosclerosis.

"Cardiovascular diseases (CVDs) represent the foremost cause of mortality in our society," said Jayantha Gunaratne, a Senior Principal Investigator at A*STAR's Institute of Molecular and Cell Biology (IMCB) and lead of the Translational Biomedical Proteomics lab.

While IF has been shown to lower CVD risk factors in both animals and humans, its molecular effects on heart cells were unclear. To solve this puzzle, Gunaratne teamed up with Thiruma Arumugam from Australia's La Trobe University to lead a multinational, multi-institutional effort to map out the molecular and cellular changes in the hearts of mice following different IF regimens.

Using quantitative mass spectrometry, the researchers tracked the heart proteins of mice undergoing fasting periods of 12–16 hours and every other day (EOD) fasting, and compared them to mice with unrestricted access to food. They also used RNA sequencing to identify any subtle changes in gene expression.

A comprehensive analysis of the data revealed which proteins and genes were most affected by the fasting regimens. They followed up with additional experiments to validate how these changes impacted heart function.

Gunaratne's team found that IF modified key biological pathways involved in metabolism, cell signalling and epigenetic remodelling. These changes were more significant during longer fasting periods, such as the 16-hour and EOD regimens. The functional studies also showed that IF improved how the heart handled stress compared to the control group.

This study not only supports the view that IF is good for heart health but also provides the most detailed look yet at the molecular changes it triggers in heart cells, according to Gunaratne.

"The findings expose pivotal molecular hubs corrected during IF, opening avenues for developing new medications to address various CVD issues," said Gunaratne.

Moving forward, the two research groups remain in collaboration to explore how to target the therapeutic opportunities uncovered in this research.

"We're also focusing on a comprehensive study of IF's impact on the molecular rewiring of vital organs such as the brain, liver and kidneys, as well as its implications for various diseases," Gunaratne added. ★

Researcher
Jayantha Gunaratne, IMCB

IN BRIEF

Using advanced analytical techniques, researchers report beneficial molecular changes in mice during longer periods of intermittent fasting, offering new insights for future cardiovascular interventions.

1. Arumugam, T.V., Alli-Shaik, A., Liehn, E.A., Selvaraji, S., Poh, L., *et al.* Multiomics analyses reveal dynamic bioenergetic pathways and functional remodeling of the heart during intermittent fasting. *eLife* **12**, RP89214 (2023).

PSYCHIATRY

Supporting mothers from the start

The term ‘postpartum depression’ may be misleading, as researchers discover maternal depressive symptoms often begin during pregnancy.

For many families, the joyous arrival of a new baby is overshadowed by an invisible struggle: postpartum depression. Although the term suggests it begins after childbirth, the reality of when and how maternal depression manifests has remained elusive.

It is vital for both mother and child that this knowledge gap be addressed, as doing so can shape public health policies that effectively support families during this crucial time, said Michelle Kee, a Principal Scientist at A*STAR Institute for Human Development and Potential (A*STAR IHDP), previously known as the Singapore Institute for Clinical Sciences (SICS).

“Previous studies, including those conducted in Singapore, have underscored the important role that maternal mood plays during pregnancy to influence a child’s neurodevelopmental outcomes,” Kee added.

Kee and Michael Meaney, Programme Director of Translational Neuroscience at A*STAR IHDP, collaborated with researchers from the National University of Singapore and KK Women’s and Children’s Hospital in Singapore; McGill University, University of Montreal and University of Calgary, Canada; and Yale School of Medicine, US; to launch a comprehensive multi-year study to gain deeper insights into postpartum depression.

The team recruited seven participant cohorts from Singapore, Canada and the UK to study the course and stability of depressive symptoms from pregnancy to two years post-childbirth across varied ethnic and geographic groups.

Participants underwent psychological tests and self-reported their depressive symptoms at various stages, from the beginning of pregnancy to two years after giving birth. The research team analysed this self-reported data, which was measured using well-established depression scales, applying advanced statistical methods such as item response theory and K-means clustering to categorise women with similar depressive symptom patterns.

Three distinct groups were identified: women with consistently low, mild and high levels of depressive symptoms. These patterns remained stable throughout the perinatal period for nearly all participants.

The study also found that variations in depressive levels frequently start during pregnancy and persist into the postpartum period. “Our findings contradict common misconceptions perpetuated by influential guidelines that maternal depression only manifests after childbirth,” Kee explained, noting that this challenges the suitability of the term ‘postpartum depression’.

These observations corroborate clinical experiences of the early onset of maternal depressive symptoms, now supported by empirical data from Kee and colleagues. The researchers also noted the need for more studies to confirm these results in other socioeconomic settings, particularly in low- and middle-income countries.

By determining the onset and trajectory of maternal depression, the researchers hope that their findings can refine public health guidelines, enabling mothers to recognise symptoms earlier and gain access to the necessary support.

Kee’s team is currently developing a preconception screening tool to identify individuals at risk for maternal mental health issues. ★

Photo credit: Omurden Cengiz / Unsplash

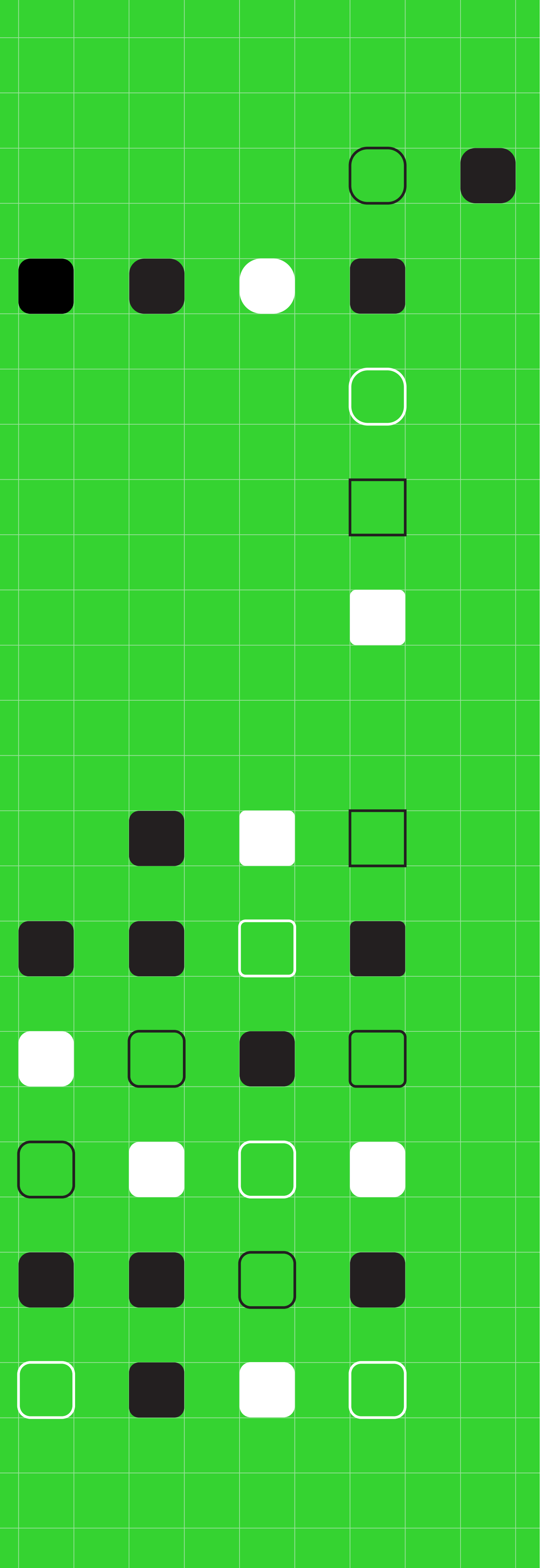
Researchers
Michelle Kee and Michael Meaney, A*STAR IHDP

IN BRIEF

A multi-year study with participants from three continents found that depressive symptoms often start during pregnancy and remain stable post-childbirth, challenging existing public health policies and highlighting the need for early detection and support for maternal depression.

1. Kee, M.Z.L., Cremaschi, A., De Iorio, M., Chen, H., Montreuil, T., *et al*. Perinatal trajectories of maternal depressive symptoms in prospective, community-based cohorts across 3 continents. *JAMA Network Open* **6** (10), e2339942 (2023).

NEARING QUANTUM HORIZONS



From full-stack software to quantum chips, A*STAR research initiatives are developing the tools to harness the power of quantum mechanics for modern-day computing challenges.

A hole punched in a card, or the lack thereof; a switch turned on or off; the numbers zero or one. These can all represent the binary digit, or 'bit': the most basic unit of information in today's digital world. Using long strings of varying bits, the electronic chips in our smartphones compactly store entire libraries and instantly make calculations that take hours by hand.

However, a very different paradigm of computing is emerging: one built on the quantum bit, or 'qubit'. Rather than the electric signals of bits, which can only represent one of two states, qubits are encoded into quantum states of subatomic systems, such as photons or the electronic states of atoms. This allows a qubit to have multiple possible states: a versatility that's foundational for quantum computers built on radically different principles from 'classical' machines widely used today.

"Quantum computing ushers in a new paradigm, alongside classical computing, that can solve a wide range of computational problems significantly faster, such as those encountered in chemistry and drug discovery, as well as in logistics and financial optimisation," said Keng Hui Lim, Assistant Chief Executive of A*STAR's Science and Engineering Research Council.

At A*STAR, research institutes like the Institute of High Performance Computing (IHPC), the Institute of Materials Research and Engineering (IMRE) and the Institute of Microelectronics (IME) are working not only to develop the foundational tools needed to make quantum computers a practical reality, but also to identify their advantages over classical counterparts.

"In partnership with Singapore's quantum research ecosystem, A*STAR's research takes a holistic approach to develop end-to-end, full-stack software solutions for quantum algorithms and applications, as well as quantum materials and devices to build scalable quantum computers," said Lim.

A NATIONAL STRATEGIC FOCUS

As part of that approach, A*STAR collaborates with national initiatives that drive quantum computing research, such as the National Quantum Computing Hub (NQCH). A joint initiative between IHPC, the Centre for Quantum Technologies (CQT) and the National Supercomputing Centre (NSCC) Singapore, NQCH supports the development of quantum computing software, middleware and hardware. The platform also works with industry to explore quantum solutions for real-world challenges, and hosts programmes for talent development in an emerging field.

Another key initiative is the National Quantum Federated Foundry (NQFF), which builds and provides access to capabilities needed to design, fabricate and characterise quantum devices. To support local research needs in quantum hardware, NQFF taps into and augments an existing network of cleanrooms across Singapore. The platform draws on IMRE's state-of-the-art device design and characterisation facilities, as well as device fabrication facilities at IME, the National University of Singapore (NUS) and Nanyang Technological University (NTU).

Both NQCH and NQFF are supported by the Quantum Engineering Programme (QEP), which aims to establish a competitive quantum engineering research community in Singapore.

SIMULATIONS IN THE QUANTUM CODE

At NQCH, Jayne Thompson, Group Manager of IHPC's Quantum Algorithms and Physics team, delves into quantum software by exploring how quantum algorithms can model and simulate complex, real-world physical systems.

"When we design quantum algorithms, they should harness the properties of quantum systems to do computations with less resources than any possible classical method," said Thompson. "This can include completing problems faster, using far less working memory or input data, or delivering more accurate heuristics than what is feasible on classical machines."

These advantages are possible due to a quantum phenomenon known as superposition, where a qubit is in multiple states (different configurations) at the same time.

"A quantum computer reaches the final answer faster by passing through many states in superposition," said Thompson. "Through careful engineering, we harness the quantum interference between those states to amplify the desired solution."

Superposition makes quantum computers a powerful computational tool to model and simulate classical systems like time-series events, where "we can simulate many possible futures," said Thompson. "In tandem with other quantum algorithms, this can speed up time-series analysis tasks—for example, risk analysis for tail events, which occur rarely but make huge impacts."

Such tail events include black swan-type events which can send financial markets crashing. One project by Thompson's group involves analysing S&P 500 data to predict the probability of rare events, and quantify the risk they pose to investment portfolios. Another includes computational fluid dynamics problems used to describe traffic networks and models of epidemic spread in populations.

QUANTUM TOOLS FOR QUANTUM PROBLEMS

As quantum computers are built on quantum mechanics, they also have a natural advantage when simulating quantum systems, such as chemical reactions or drug-protein interactions at the nanoscale.

"To simulate a quantum system on a classical computer, we need to use extremely high-dimensional data," said Thompson. "That storage quickly becomes prohibitively costly; it's also almost impossible to update those stored states under the simulation model. These scaling issues rapidly force researchers to make approximations when modelling these systems with classical architectures."

Conversely, the qubits of quantum computers can more compactly describe those states for digital simulation; by modelling atomic-scale behaviour with atomic-scale hardware, computations can be easily scaled up to classically intractable levels.

Quantum chemistry is a focus area for IHPC Principal Scientist Adrian Mak, whose team has been designing quantum algorithms for the field with CQT Principal Investigator Dimitris Angelakis and colleagues.

"By understanding the wave-like properties of electrons and how they affect atoms and molecules, we can better understand the electronic structures of atomic and molecular systems," said Mak. "This allows us to predict their geometries, spectra and reaction mechanisms, which then helps us to design new chemical reactions and materials."

Mak, Angelakis and colleagues recently produced an algorithm that calculates correlation energy—the measure of how much an electron's movement is affected by other electrons in the same quantum system—using quantum circuits with two-qubit gate depths. Capable of scaling linearly as more qubits are added, the team has successfully demonstrated the algorithm's use in cloud-accessed quantum computers.

"We've also developed a quantum algorithm that can encode a multi-electron state using quantum circuits with polylogarithmic scaling of depth, with respect to system size," said Mak. "Both these projects were supported by QEP 2.0."

NQCH efforts in this area led to the release of Qibochem, a plugin for quantum computational chemistry that works with NQCH's open-source quantum computing platform, Qibo. "Qibochem avails quantum computing for chemistry to the public without a need to intimately understand all the quantum details involved," said Mak.

BUILDING THE HARDWARE

Each qubit in a quantum computer presents a complex manufacturing challenge. To encode information in a single nano-sized particle, how do you keep it stable, measurable and free from interfering forces?

Working with NQFF, IME Principal Scientist Hongyu Li's group aims to fabricate hardware that meets requirements posed by different quantum computing architectures, such as trapped ion and superconducting qubits. The team is focused on packaging and process integration: designing functional quantum chips and fleshing out the steps to fabricate them.

"To understand the superconducting testing process, we worked closely with IMRE's cryogenic testing lab and CQT testing labs based at NUS and NTU," said Li. "IMRE also provided support in characterising materials and developing processes for film deposition."

From 2017 to 2021, Li's group worked with IMRE's Quantum Technologies for Engineering (QTE) department to develop the fabrication process and packaging approach for a strontium ion (Sr^+)-based 3D surface ion trap design that can hold over 200 ions.

"Since 2022, we've been developing a barium ion (Ba^+)-based ion trap with NQFF Director Manas Mukheerjee in a QEP-supported project," said Li. "As Ba^+ ion trap chips need high voltage RF—over 300 volts—this project needs multiple wavelength waveguides, as well as grating coupler integration under metal plates. Other ion trap chip integration processes are also in development."

Li's team is also creating hardware that can function at the very low temperatures needed for stable qubits. "With CQT Principal Investigator Rainer Dumke, we're developing cryogenic through-silicon via (TSV) applications within resonators and RF characterisation; as well as approaches to confine top quit chips to cryogenic interposer distances," said Li.

In another project under A*STAR's DELTA-Q Strategic Research Programme, Li's group and that of IMRE Senior Principal Scientist Johnson Goh developed a cryogenic interposer that copes with different transition temperatures.

Work by Li's group has attracted attention from the quantum hardware industry. "We recently submitted a joint proposal to an Australian start-up on cryogenic packaging, and are in discussion with a Europe-based company for a project using our cryogenic interposer designs," said Li.

"A quantum computer reaches the final answer faster by passing through many states in superposition. Through careful engineering, we harness the quantum interference between those states to amplify the desired solution."

— Jayne Thompson, Group Manager (Quantum Algorithms and Physics) at A*STAR's Institute of High Performance Computing (IHPC)

THE BEST OF BOTH WORLDS

With quantum computers well-suited to weighty computations and classical computers likewise to hefty data loads, a promising research direction involves pairing both architectures together.

"Hybrid computing systems leverage the strengths of classical high-performance computing (HPC) for general tasks such as big data processing, and quantum computing for highly complex and intensive computations," said Yi Su, IHPC Executive Director and NQCH Co-Principal Investigator. "This approach holds great promise for problems that pose both 'big data' and 'big compute' challenges."

At NQCH, IHPC Senior Principal Scientist Hoong Chuin Lau and his research group are working with IBM and Japanese universities such as Tokyo University, Tokyo Institute of Technology and Tsukuba University to identify useful hybrid classical-quantum techniques in logistics and transportation.

"The logistics sector collects a huge amount of data from orders and deliveries: locations, times, volumes and types of goods, order status, routes used, and so on," said Lau, also a Professor of Computer Science at Singapore Management University. "The challenge is deriving good predictions—like estimated delivery times—from all this data, and developing good stochastic optimisation models for tasks like order despatch and route planning."

While classical HPC can handle big data, it often struggles with using it to compute optimised solutions to logistics problems, such as the most efficient routes for a fleet of delivery vehicles, or the best combination of goods to load in a container, especially when their inputs are uncertain. Lau and colleagues are examining how hybrid quantum algorithms like VQE and QAE can help bridge the computational gaps.

Hybrid computing is also of interest to researchers like Chandra Verma, Senior Principal Investigator at A*STAR's Bioinformatics Institute (BII), who see their potential to support AI-powered drug discovery.

"We've already seen the first example of a quantum machine learning (QML) framework for small molecules that outperforms its classical counterpart," said Verma. "There's potential to develop hybrid QML models that achieve low generalisation errors, even with limited training data available—as is the case with small molecule libraries."

BII has recently begun to explore quantum computing applications in drug discovery problems such as protein conformations, peptide design and RNA folding.

"We're also looking at quantum-enhanced, artificial intelligence (AI)-powered assays to monitor T cell response in infectious disease control and immunotherapy, as well as quantum-deep learning models that enhance immunotherapy response prediction," added Sebastian Maurer-Stroh, BII Executive Director.

A PRACTICAL QUANTUM HORIZON

While research communities worldwide are racing to bring the first scalable and practical quantum computers beyond the lab, it remains important to consider the technology's potential strengths without introducing a sense of hype, said Ping Koy Lam, A*STAR Chief Quantum Scientist.

"Quantum computing is still a very nascent research area; currently, quantum computers are aimed at deep problems that require a lot of computing time on classical computers," said Lam. "As quantum computers are expected to have very small input bandwidths for the foreseeable future, it's hard to predict the roles they might play in big data problems."

> ***"Hybrid computing systems leverage the strengths of classical high-performance computing for general tasks such as big data processing, and quantum computing for highly complex and intensive computations."***
>
> — Yi Su, Executive Director at A*STAR's Institute of High Performance Computing (IHPC) and Co-Principal Investigator at the National Quantum Computing Hub (NQCH)

"At present, quantum computing's strengths lie in 'big compute, small data'; problems with relatively small data sizes, but very high computational complexity," added Yi Su. "For large-scale data processing tasks, classical computing remains more practical and efficient with current technologies. However, hybrid computing offers opportunities to target 'big data, big compute' problems in future."

To continue exploring quantum's technological capabilities, A*STAR continues to support research efforts across multiple fields in Singapore's quantum ecosystem. In 2023, A*STAR launched the Quantum Innovation Centre (Q.InC) to advance use-inspired basic research within the agency's scientific community and to focus on translational research for real-world impact. Powered by expertise and facilities from IHPC, IME, IMRE and the National Metrology Centre (NMC), Q.InC aims to develop next-generation translational quantum technologies, as well as talents in quantum science and engineering, supplementing NQCH and NQFF efforts.

Beyond pursuing an advantage over classical systems, Q.InC is also exploring novel quantum hardware applications in quantum photonics, quantum materials and quantum sensing.

"A*STAR plans to work with the research ecosystem including university and industry partners to push the state of the art, and develop breakthrough solutions for real-world use cases," said Keng Hui Lim. "Such collaborations are necessary to advance quantum computing research, and contribute to Singapore's National Quantum Strategy."

Other National Quantum Strategy programmes with A*STAR support include the National Quantum Processor Initiative to build local capacities for quantum processor design and fabrication; as well as the National Quantum Software Programme to support research in positioning, navigation and timing; biomedical sensing and imaging; and remote sensing applications. ★

FUTURE PROSPECTS: OTHER RESEARCH PERSPECTIVES

"Quantum computers could help combine various sources of health data—genomics, proteomics, clinical records—by processing them in parallel and modelling their complex statistical relationships. This could help speed up drug response predictions and molecular diagnosis of complex diseases."

— Dennis Wang, Senior Principal Investigator and Bioinformatics Platform Head, A*STAR Institute for Human Development and Potential (A*STAR IHDP)

"These systems may have synergistic effects with AI. For instance, the data used to train AI models are often probabilistic and costly to evaluate; in such settings, quantum computing-based simulations may provide improved estimates with fewer evaluations. Moreover, quantum circuits are similar to deep neural networks in that they can approximate high-dimensional functions from large data sets, but a promising advantage is that they often need fewer parameters."

— David Bossens, Senior Scientist, Centre for Frontier AI Research (CFAR)

"With the Port of Singapore aiming to deal with 65 million twenty-foot equivalent units (TEUs) of cargo annually in future, optimisation algorithms on classical computing facilities may not be able to handle the complex optimisation problems involved with so many dynamic factors and players in making sure port operations are at their most efficient and sustainable. Quantum computing may enhance AI-based solutions by speeding up optimisation and parameter convergence in this area."

— Xiuju Fu, Senior Principal Scientist and Director (Maritime AI Research Programme), Institute of High Performance Computing (IHPC)

DIGITAL HEALTH

Pulse checks on lingering symptoms

Smartwatch data points to a connection between physical activity and prolonged COVID-19 symptoms among healthcare workers.

Wearable technology has the power to transform everyday fitness trackers into powerful tools that do more than just count steps. Scientists are now harnessing these gadgets to detect subtle signs of diseases, potentially spotting health issues before symptoms even emerge—keeping a digital finger on the pulse of our well-being.

Varsha Gupta, a Senior Scientist at A*STAR Institute for Human Development and Potential (A*STAR IHDP), previously known as the Singapore Institute for Clinical Sciences (SICS); and Bioinformatics Institute (BII), noted that healthcare monitoring became crucial during the COVID-19 pandemic as researchers found a connection between physical activity and prolonged COVID-19 symptoms in healthcare workers.

"The temporal patterns of markers from smartwatches can provide a deeper understanding of the dynamic nature of lifestyle-health associations, enabling us to identify intervention points and novel insights."

"COVID-19 symptoms were taking observably differing lengths of time to resolve. At the same time, movement and social distancing restrictions may have had an impact on daily life physical activity patterns," Gupta said. This observation prompted the team to investigate whether recorded physical activity levels were linked to COVID-19 symptoms.

Together with Senior Principal Scientist Dennis Wang (from A*STAR IHDP and BII), Gupta collaborated with researchers from the University of Sheffield, UK and Stanford University, US, on a year-long study of staff at the UK's National Health Service (NHS). The team analysed data from NHS healthcare workers who recorded their symptoms via an app and tracked their physical activities with Apple watches starting from April 2020.

Gupta explained that collecting data in real-life settings introduces variability because participants have different daily routines and sometimes forget to wear their watches. As a result, the team had to implement rigorous data cleaning processes to handle self-reported data, removing outliers and duplicate entries.

Using a data-driven approach, the researchers applied unsupervised machine learning techniques to identify the evolution of COVID-19 symptoms and physical activity patterns among the participants. They discovered a correlation between the distances participants walked or ran and the duration of their COVID-19 symptoms: those with prolonged symptoms generally showed reduced physical activity from the infection's onset.

These findings highlight the persistence of symptoms in mild COVID-19 cases, as well as what Gupta sees as a promising future for wearable technology in shaping healthcare. "The temporal patterns of markers from smartwatches can provide a deeper understanding of the dynamic nature of lifestyle-health associations, enabling us to identify intervention points and novel insights," said Gupta.

These findings also suggest that future studies should consider differences in device brands, user lifestyles and varying diseases to fully harness the technology's potential, Gupta added. The team is continuing their research, working with international partners to explore further how health markers relate to physical activity across different settings. ★

Researcher
Varsha Gupta, A*STAR IHDP and BII

IN BRIEF
By applying unsupervised machine learning to smartwatch data, researchers discover a correlation between decreased physical activity and prolonged COVID-19 symptoms, highlighting how wearable technology can improve disease monitoring and management.

1. Gupta, V., Kariotis, S., Rajab, M.D., Errington, N., Alhathli, E., *et al.* Unsupervised machine learning to investigate trajectory patterns of COVID-19 symptoms and physical activity measured via the MyHeart Counts App and smart devices. *npj Digital Medicine* **6**, 239 (2023).

Photo credit: Alexander Sinn / Unsplash

BIOTECHNOLOGY

Nature's solution to plastic pollution

Enzymes from soil bacteria can effectively break down some of the toughest plastic pollutants, offering a promising approach to tackling plastic waste.

As nature's 'recyclers', actinobacteria reside in the soil, secreting enzymes to break down their surroundings and returning nutrients to the soil to sustain the cycle of life. Scientists have uncovered something surprising about these microscopic powerhouses: their enzymes can also degrade some of the most stubborn pollutants on Earth.

Enzymes such as cutinases and hydrolases from actinobacteria can be harnessed to break down polyethylene terephthalate (PET)—a plastic commonly used in water bottles and packaging that is notoriously difficult to recycle. These enzymes reduce PET into simpler, non-plastic molecules that can be further processed or biodegraded.

A multidisciplinary team led by Yee Hwee Lim and Fong Tian Wong worked to explore how these unique bacteria might bridge gaps in existing PET recycling technologies. The team consisted of colleagues across science and engineering and biology disciplines from A*STAR's Institute of Molecular and Cell Biology (IMCB) and Institute of Sustainability for Chemicals, Energy and Environment (ISCE[2]).

"We drew inspiration from this bacterial family to expand our research into PET degradation, leveraging our expertise and a newly developed in-house platform for protein construction and testing," said Wong.

The researchers delved into actinobacterial genomic data, targeting enzymes from *Microbispora*, *Nonomuraea* and *Micromonospora*. The team identified, engineered and tested these enzymes to evaluate their ability to decompose PET.

Analyses of the enzymes' by-products confirmed that they not only effectively reduced PET into smaller fragments, but transformed it back into its original monomers, which can then be used for making new PET (completing the cycle) or upcycled into other products.

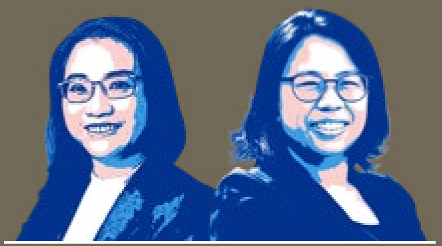
"Although these genera are known for breaking down complex molecules in diverse environments, this is the first example demonstrating that they also contain enzymes that can depolymerise PET," said Wong.

The team found that a selection of enzymes can degrade PET at mild temperatures and neutral pH—conditions that are less energy-intensive than traditional mechanical recycling methods and more environmentally friendly than chemical processes. "By breaking down plastics to monomers, bio-based recycling not only aligns with eco-friendly practices but also simplifies the production chain, filling the gaps left by current recycling technologies," Wong remarked.

Wong highlighted that these enzymes and their host organisms, actinobacteria, may be pivotal in real-world sustainability efforts by offering energy-efficient and non-toxic bio-based solutions that utilise water-based and low-temperature processes. They can also facilitate long-term waste management strategies, such as the integration of anaerobic digesters for handling mixed waste.

The researchers have patented their technology and are expanding their work through the Accelerated Design & Engineering Platform (ADEPT) for enzymes, which supports the rapid construction and testing of proteins, enabling advances in microbial and enzymatic solutions.

"Witnessing the incredible abilities of microbes and enzymes in action gives us hope for a more sustainable future," Wong concluded. ★



Researchers
Yee Hwee Lim, ISCE[2]
and Fong Tian Wong, IMCB and ISCE[2]

IN BRIEF
By screening and engineering enzymes from Actinobacteria, A*STAR researchers have identified a sustainable method for degrading persistent PET plastics, offering a greener alternative to current recycling practices.

1. Tiong, E., Koo, Y.S., Bi, J., Koduru, L., Koh, W., *et al.* Expression and engineering of PET-degrading enzymes from *Microbispora, Nonomuraea*, and *Micromonospora. Applied and Environmental Microbiology* **89** (11), e00632-23 (2023).

Photo credit: Omurden Cengiz / Unsplash

ADVANCED MATERIALS

Nature-inspired windows for green buildings

A versatile film that adjusts its transparency in response to temperature, pressure and moisture can enhance the energy efficiency of buildings, making them more sustainable.

Photo credit: Cbrett Sayle / Pexels

As architectural landscapes evolve, so do the windows that frame them. Tomorrow's windows may not just be mere panes of glass, but intelligent entities that dynamically adjust their optical and thermal properties to create a comfortable indoor environment and reduce the energy consumption of buildings.

However, creating materials as building blocks for smart windows that respond to thermal, mechanical and chemical stimuli while meeting aesthetic standards has proven challenging, according to materials science experts.

"In smart windows, the materials must maintain transparency, which narrows down the pool of suitable candidates," said Yujie Ke, a Scientist at A*STAR's Institute of Materials Research and Engineering (IMRE).

In their quest for solutions, Ke and Yuwei Hu, a corresponding author of the study, drew inspiration from nature. "We observed how a chameleon changes its colour by altering the crystal structure of its skin, which affects how it reflects light," Ke said. "Similarly, skeleton flowers change transparency in response to moisture."

In collaboration with researchers from Nanyang Technological University, Singapore; Beihang University and Beijing Institute of Technology in China; and North Carolina State University, US; Ke and IMRE colleagues developed an innovative film for smart windows. They aimed for a design capable of tri-mode stimuli response, integrating thermochromism (sensitivity to temperature changes), mechanochromism (reactivity to mechanical stress), and hydro-/solvato-chromism (responsiveness to water or solvent contact).

Leveraging a bio-inspired hierarchical structure and functional elastomers, they engineered a composite of vanadium dioxide and polydimethylsiloxane, layered over silica nanospheres. "These nanospheres introduce structural changes when stretched, enhancing light scattering, while the vanadium dioxide particles react to temperature, modulating light transmission," Ke said.

When incorporated into smart windows, the film can optimise a building's energy consumption by dynamically manipulating how light enters it. This would substantially reduce its reliance on heating and cooling systems, lowering overall energy expenses.

Moreover, this technology paves the way for customisable aesthetics. "Our method allows for the dynamic control of colours and patterns, adding an element of design flexibility that was previously unexplored in smart windows," said Ke.

"We observed how a chameleon changes its colour by altering the crystal structure of its skin [and] how skeleton flowers change transparency in response to moisture."

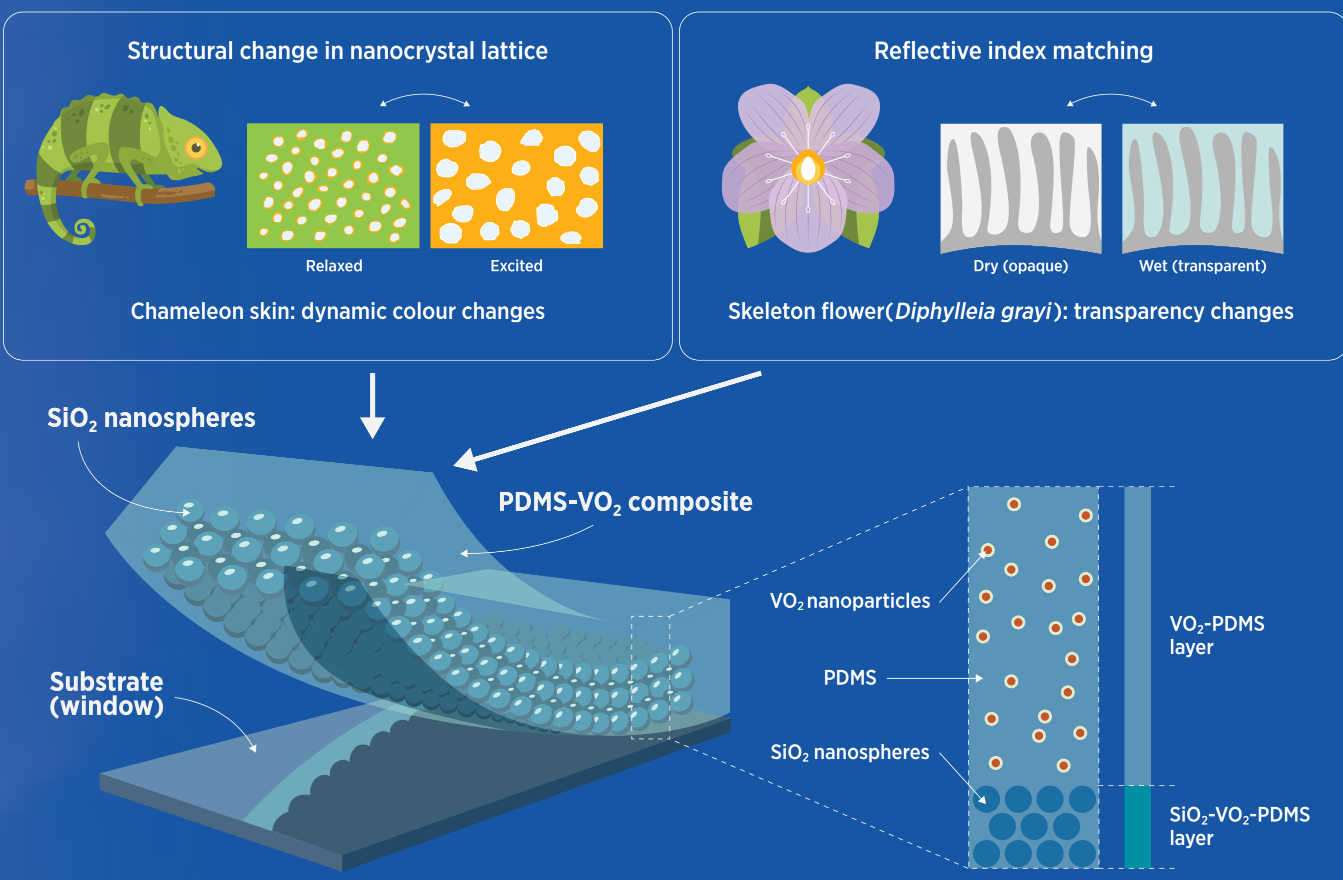
In simulations, the team's smart windows outperformed the energy efficiency of conventional single-layered and double-glazed windows used in cities like Barcelona, Melbourne and Auckland. Nevertheless, scaling up production might present a hurdle to widespread adoption, particularly for developers aiming for cost-effective solutions with rapid payback periods.

To meet market demands, the team has plans to improve the solar management performance of their smart windows, for which they have filed a provisional patent. By integrating features such as on-demand privacy and aesthetic enhancements, they aim to elevate the smart window design's value and expedite the payback period. ★

Researchers
Yuwei Hu and Yujie Ke,
IMRE

IN BRIEF
A smart window film made from a composite of vanadium dioxide, polydimethylsiloxane and silica nanoparticles facilitated tri-mode light regulation, showing potential to enhance the energy efficiency, privacy and aesthetic design of buildings.

1. Ke, Y., Li, N., Liu, Y., Zhu, T., Wang, S., *et al.* Bio-inspired, scalable, and tri-mode stimuli-chromic composite for smart window multifunctionality. *Advanced Functional Materials* **33** (46), 2305998 (2023).



Design of a novel window film capable of changing transparencies and colours based on heat, light and mechanical forces. Comprised of silica (SiO_2) nanospheres, vanadium dioxide (VO_2) and polydimethylsiloxane (PDMS), its structure is based on the colour-shifting nanocrystal lattices found in chameleon skins, as well as the intercellular spacing in skeleton flowers which change transparencies for dry and wet weather conditions.

DECODING CANCER'S MOLECULAR DANCE

Using artificial intelligence techniques, Mai Chan Lau maps the spatial relationships between tumour cells and immune cells to understand their effect on clinical outcomes.

Cells are bursting with information, from the 3.1 billion base pairs that make up the human genome to the multitudes of biochemical pathways that transform one protein into another. Even the way tissues look under a microscope can hold important clues when tackling diseases like cancer.

However, teasing out the clinically relevant details from a sea of information remains an ongoing mission for cancer researchers. A treatment's efficacy could be influenced by highly-activated genes in tumours, or by the changing functional states of immune cells. Excitingly, the advent of innovative computational tools is padding the cancer researcher's arsenal, enabling them to better study the disease across biological scales.

These tools include single-cell bioinformatics, which grants scientists like Mai Chan Lau a more intricate view of the dynamic molecular features, plasticity, development and behaviours of individual cells. Spatial omics technologies take that view a dimension further by shining a spotlight on these interactions in a physical tissue space—effectively framing molecular signals within locational contexts.

Backed by these emerging technologies, Lau concurrently leads her own group as an Assistant Principal Investigator at A*STAR's Bioinformatics Institute (BII) while heading the Singapore Immunology Network (SIgN)'s Computational Immunology Platform. By harnessing the power of artificial intelligence (AI), Lau and colleagues aim to improve cancer diagnostics and treatment by rummaging through elaborate molecular maps of cancer-immune interactions and translating them into clinically applicable insights.

In this interview with *A*STAR Research*, Lau reflects on the key people and experiences that shaped her career from trainee to supervisor, and highlights the importance of AI-enabled research in cancer immunology.

Q: TELL US ABOUT YOUR SCIENTIFIC JOURNEY.

My interest in biomedical research started during my undergraduate final year project at the National University of Singapore with Lakshminarayanan Samavedham. There, I developed neural network models—a form of machine learning—to predict appropriate drug doses for cancer treatment. This project fuelled my passion for AI, and I became convinced that mastering big data was crucial to advance AI research.

Subsequently, I decided to focus on high-performance computing based on graphics processing units (GPUs) for my PhD project under Rajagopalan Srinivasan. That experience solidified my technical skills and belief in the transformative power of AI in handling large datasets. As I was eager to apply my computing expertise to biomedical research, I was fortunate to then join SIgN, where I dove into single-cell bioinformatics in Jinmiao Chen's lab and received valuable mentorship from Bernett Lee.

During my second postdoctoral position with Shuji Ogino at Brigham and Women's Hospital in Boston, I realised that it isn't enough for an immune cell to have the appropriate functional states to target tumour cells. Rather, the physical proximity of these cells is equally crucial; they need to be in reach of their targets. As such, I turned to integrating knowledge from histopathology: the microscopic examination of tissues for disease diagnostics. These combined experiences in single-cell immunology and molecular pathology stimulated my interest in tumour-immune interactions.

Q: HOW CAN SPATIAL TECHNOLOGIES HELP TACKLE CANCER?

Simply put, spatial technologies reveal the spatial relationships of cells: how they interact with each other in disease contexts. They fill in key gaps by capturing the significant cell-cell interactions that influence cancer development, progression, drug response and resistance. Such unprecedented insights can help greatly refine biomarkers, enabling more accurate diagnosis and patient stratification. An understanding of cellular and spatial contexts can also create opportunities to identify new treatment targets.

When these advanced cellular and molecular-level insights are integrated with decades of established histopathological knowledge, their advantages are magnified—they can help optimise existing histological or single-molecule biomarkers, which paves the way towards better personalised cancer treatments.

Q: TELL US ABOUT YOUR WORK ON THE H&E2.0 PLATFORM.

While advanced spatial technologies show great promise for cancer immunology research, their high cost and specialised skill requirements significantly hinder their accessibility and potential clinical impact. To address this, I am working with Joe Yeong, my former mentor and a pathologist at the Institute of Molecular and Cell Biology (IMCB), to co-develop the H&E2.0 platform.

H&E2.0 has two aims: the first is to provide interactive, integrated visualisations of molecular signals—obtained from advanced spatial technologies—in haemotoxylin and eosin-stained (H&E) tissue samples at high-resolution views. For reference, H&E is a gold standard in histopathology; the platform's ability to seamlessly visualise data would be of great help to clinicians, histologists and pathologists that seek to interpret and appreciate new molecular insights of clinical interest.

The platform's second aim is to improve access to advanced spatial omics data for the research community, especially for those in resource-limited settings. To that end, we're training H&E-based generative AI models for H&E2.0, using spatial omics data acquired from the same H&E tissue sections as training ground-truth. By synthesising molecular signals from H&E tissue space, our platform also enables a seamless integration of data at multiple biological scales.

We think H&E2.0's visualisation capabilities provide essential interpretations that can bring AI-predicted biomarkers into clinical settings. In future, we intend to make AI-capable H&E2.0 a publicly available web tool through our collaboration with Minh Nguyen and Chandra Verma from BII.

> ***"H&E2.0's visualisation capabilities provide essential interpretations that can bring AI-predicted biomarkers into clinical settings."***
>
> — Mai Chan Lau, Head of Computational Immunology Platform at A*STAR's Singapore Immunology Network (SIgN) and Assistant Principal Investigator at Bioinformatics Institute (BII)

Q: HOW DID YOUR RESEARCH JOURNEY INFLUENCE YOUR LEADERSHIP STYLE?

My diverse experiences in different labs taught me the importance of focusing on the career growth of my team members and understanding their interests, whether they are oriented towards academia or industry. I strive to give them chances to develop leadership skills by allowing each of them to lead projects that align with their interests, such as bioinformatics tools, production pipelines or AI projects.

Recognising the importance of showcasing our work, I ensure my group has ample opportunities to present their research at various venues, giving them credit both verbally and in authorship. Most importantly, I aim to cultivate an open and receptive environment where every team member feels safe to provide feedback and share ideas.

Mai Chan Lau

Head of Computational Immunology Platform, Singapore Immunology Network (SIgN); and Assistant Principal Investigator, Bioinformatics Institute (BII), A*STAR

Q: HOW HAS A*STAR SUPPORTED YOU AS AN EARLY-CAREER RESEARCHER?

As I have just started my own lab, A*STAR's support has been invaluable in providing crucial access to various resources. These include computing facilities and mentorship from senior BII and SIgN group leaders, particularly BII Executive Director, Sebastian Maurer-Stroh; and SIgN Executive Director, Kong-Peng Lam. The agency has also facilitated interactions with management; at a Group Engagement Session, I had the chance to discuss grant mechanisms with Huck Hui Ng, the Assistant Chief Executive of Research and Talent Development.

In turn, mentoring students through A*STAR-funded internships has enabled me to expand my research more effectively and enhance my leadership skills. In addition, platforms like the *A*STAR Research* publication and Science Brew—organised by Andy Hor, Deputy Chief Executive (Research), and his team—have given me opportunities to publicise my work. These experiences have been important in my growth as a researcher and a leader.

Q: WHAT ADVICE CAN YOU SHARE WITH ASPIRING SCIENTISTS?

My key motivation for staying in research—for nearly 10 years, to date—is a genuine passion for my work and a strong belief in its potential societal impact. I think that one crucial trait for a successful researcher is the ability to recover from failures and rejections. It is important to recognise that it takes time to learn and grow through feedback from others. Embracing this learning process is essential for long-term success in research. ★

TRANSPORTATION

Smart simulations calm commuter chaos

A new simulation platform helps assess the impact of public transport disruptions in cities like Singapore, ensuring smoother commutes even during major incidents.

A single train breakdown during rush hour can send a smoothly-running flow of commuters into a tailspin. Frantic crowds hurry for buses and taxis, only to be frustratingly met by snaking queues.

Densely-populated cities like Singapore need contingency plans to ensure their high volumes of commuters can seamlessly transition between transport modes when major systems, such as rail lines, are disrupted. These plans can include regular and accurate communication with commuters; effective service rerouting; and rapid deployment of alternative transport modes like bridging buses.

"Transport simulation software can be used to evaluate different scenarios, such as the impact of mitigation measures on commuter travel time during a train line disruption, or estimated levels of congestion at stations," said Vasundhara Jayaraman, a Lead Research Engineer at A*STAR's Institute of High Performance Computing (IHPC). "Such simulations not only help city planners and governments understand how transportation changes impact traffic, commuter times and overall mobility, but can also be used to test policies like transportation subsidies."

Vasundhara and Rakhi Manohar Mepparambath, a Senior Scientist at IHPC's Systems Science Department, were part of a team that developed a simulation platform calibrated with real-world data from Singapore. Through a co-simulation approach, SUMMIT (Singapore Urban Multi-Modal Integrated Transport Simulator) integrates train, bus and taxi simulators to facilitate seamless commuter transitions between transport modes. The platform also uses a message-passing framework codenamed 'Fabric' to synchronise simulations and manage transitions.

Vasundhara explained that SUMMIT's co-simulation approach with Fabric integrates different independently developed and calibrated models to allow efficient, flexible and scalable commuter behaviour simulations. The platform does not rely heavily on primary surveys, as it uses existing data from sources such as GPS and farecards.

Rakhi shared that most other existing simulation projects that also model train disruption scenarios did not calibrate the simulated commuter behaviours using real-world data from actual disruptions. "SUMMIT is calibrated using real-world datasets such as those from past train-line disruption events in Singapore. It can turn around a full-day simulation of bus, train and taxi systems at a city-wide scale relatively quickly, completing multiple simulation evaluations within hours," added Rakhi.

By running scenarios using SUMMIT, the team found that while bridging bus services can generally reduce station crowd sizes during train disruptions, overall commuter travel times could still increase due to over-demand at bus stops. Simulations also showed that early dissemination of disruption information can reduce negative impacts on commuters significantly, as commuters could plan earlier for travel journeys to avoid heavily congested areas.

By improving contingency planning, the SUMMIT platform—a project supported by the National Research Foundation and the Land Transport Authority of Singapore—can enhance commuter satisfaction and the reliability of public transport systems, the team concluded. ★

Researchers
Vasundhara Jayaraman and Rakhi Manohar Mepparambath, IHPC

Nasri Bin Othman and Wyean Chan, IHPC

IN BRIEF
Using real-world data from Singapore's train, bus and taxi systems, SUMMIT's multi-modal simulation approach revealed the importance of timely information dissemination to improve urban transport planning and disruption response.

1. Othman, N.B., Jayaraman, V., Chan, W., Loh, Z.X.K., Rajendram, R., *et al*. SUMMIT: A multi-modal agent-based co-simulation of urban public transport with applications in contingency planning. *Simulation Modelling Practice and Theory* **126**, 102760 (2023).

Photo credit: Calvin Teo / Wikicommons

WASTE MANAGEMENT

Plastics turning over a new leaf

Researchers transform common plastic waste into exceptional water-repelling materials, inspired by the natural properties of lotus leaves.

The lotus leaf, celebrated across cultures as a symbol of purity, owes its self-cleaning abilities to a phenomenon known as superhydrophobicity. Lotus leaves repel water so effectively that droplets skitter off, taking dirt and impurities with them. Inspired by this, materials researchers have turned to a similar strategy to address a pressing environmental issue: polypropylene (PP) recycling.

PP is ubiquitous in everyday items like plastic bags, yet despite its prevalence, barely one percent of it is recycled each year. The remainder accumulates in landfills, where it slowly degrades, releasing hazardous gases and contributing to pollution. Traditional PP recycling methods are resource-intensive and often fall short on a large scale.

Xiukai Li and Yugen Zhang from A*STAR's Institute of Sustainability for Chemicals, Energy and Environment (ISCE^2) have pioneered a more sustainable approach to upcycling PP, enhancing its properties to add value. "PP is difficult to dissolve in most organic solvents, making traditional recycling methods like dissolution less effective," the researchers explained.

"Polypropylene is difficult to dissolve in most organic solvents, making traditional recycling methods like dissolution less effective."

Their study aimed to transform PP into microspheres that emulate the hierarchical nanostructures of lotus leaves, creating a superhydrophobic material. "Adapting the nanostructures inspired by lotus leaves posed challenges in achieving uniformity and stability in the synthesised microspheres," said Li and Zhang.

Rising to the challenge, the team subjected waste PP to a catalytic oxidation process, then dissolved it in various solvents to create microspheres. Their method not only enhances PP's hydrophobicity, but also does so in a way that is both cost-effective and scalable.

"Theoretically, our oxidised PP should be more hydrophilic," the researchers remarked, yet their results showed that the microspheres were exceptionally water-repellent: with a contact angle reaching up to 164 degrees, they mirrored the superhydrophobic properties of natural lotus leaves. Their performance versus similar materials exceeded the researchers' expectations.

Moreover, this process proved effective with PP waste from a diverse array of sources, including medical waste and food packaging. "The synthesis process is simple and can be applied to waste PP from diverse sources, offering a versatile solution for a wide range of applications," the researchers added, highlighting its potential in environmental remediation for oil spill clean-ups, the development of water-repellent textiles and self-cleaning surfaces.

Encouraged by these promising results, the team has filed a patent application for their microspheres and is actively seeking industry partnerships to further explore the technology's potential. ★

Researchers
Yugen Zhang and Xiukai Li, ISCE^2

IN BRIEF

A scalable process to upcycle polypropylene waste into superhydrophobic microspheres that mimic lotus leaves offers potential for applications such as oil spill remediation and water-repellent textile production.

1. Li, X., Wang, J., Yi, G., Teong, S.P., Chan, S.P., *et al.* From waste plastic to artificial lotus leaf: Upcycling waste polypropylene to superhydrophobic spheres with hierarchical micro/nanostructure. *Applied Catalysis B: Environmental* **342**, 123378 (2024).

Photo credit: Clement Falize / Unsplash

ARTIFICIAL INTELLIGENCE

Quick learners: helping algorithms master tasks

Researchers find that pre-training AI models on a global scale boosts their performance in machine learning tasks, particularly in scenarios with limited training data.

Have you ever wondered how facial recognition on a smartphone works with just a quick scan of a user's face? The secret lies in a machine learning technique aimed at enabling models to perform tasks proficiently with a very limited amount of training data, known as few-shot learning (FSL).

"FSL empowers artificial intelligence (AI) models to leverage their existing knowledge to learn new concepts with just a few examples," explained Ruohan Wang, a Senior Scientist at A*STAR's Institute for Infocomm Research (I^2R).

In FSL, the primary hurdles include accumulating knowledge within the model and applying it towards new tasks. To tackle both, many researchers turn to meta-learning, which involves training an AI model on a diverse collection of tasks to enhance its adaptability.

"Many researchers held a traditional view that AI models must directly learn how to reuse knowledge by being trained on many disparate tasks," Wang noted. However, subsequent research revealed that focusing knowledge accumulation at a global level can significantly enhance an AI model's robustness.

"For instance, if you have scattered data from many different tasks, it would be advantageous to merge these tasks into a unified task and then train an AI model on this amalgamated data," said Wang.

Task merging simplifies meta-learning into pre-training and decouples knowledge accumulation from how the model intends to transfer such knowledge. Empirically, the benefits of pre-training are widely recognised for FSL, yet the theoretical reasons behind its success remain fuzzy.

Recognising this knowledge gap, Wang and researchers from the University College London, UK, delved into the inner workings of pre-training, demonstrating that pre-training is essentially a form of meta-learning that enhances how quickly the model learns and improves.

Despite pre-training's advantages, one of its practical limitations is that real-world datasets seldom come pre-labelled on a global scale, which makes it challenging to implement the method effectively.

An example of a three-way-two-shot classification task used for few-shot learning. An algorithm is trained across multiple training tasks. In each training task, the algorithm is presented with a support set of six images: three classes of animals, with two examples provided for each class. The algorithm is then tasked to predict what class of animal each image in a subsequent query set belongs to. After, the model's ability to generalise to new, unseen classes is evaluated using a test task, in which the model is presented with three new classes that do not overlap with those used in the training tasks.

"For instance, if you have scattered data from many different tasks, it would be advantageous to merge these tasks into a unified task and then train an AI model on this amalgamated data."

To tackle this, Wang's team developed Meta-Label Learning (MeLa), a system where the model independently infers global labels from available tasks before undergoing pre-training. Specifically, the MeLa algorithm effectively identifies hidden global labels that align with local task specifications, while also grouping diverse task data based on their similarities.

The team also employed data augmentation techniques to enhance the diversity and volume of training data for more robust meta-representations. In experiments, their approach outperformed other existing meta-learning models, which affirmed the team's findings.

With their new insights into the mechanics of pre-training and how MeLa can facilitate it under less-than-ideal conditions, the team is now focusing on foundation models. These models, which are vast repositories of accumulated knowledge, present an opportunity to pioneer methods that transfer knowledge to a variety of AI applications. ★

Researcher
Ruohan Wang, I²R

IN BRIEF
Researchers developed a pre-training and Meta-Label Learning system which boosts algorithm performance by enabling efficient global label inference across tasks.

1. Wang, R., Falk, J.I.T., Pontil, M. and Ciliberto C. Robust meta-representation learning via global label inference and classification. *IEEE Transactions on Pattern Analysis and Machine Intelligence* **46**, 1996-2010 (2024).

Photo credit: Chaosamran Studio / Shutterstock

ROBOTICS

Robot teams chart new paths

A new training strategy enables robots to efficiently collaborate and learn in dynamic environments, improving their performance in real-world tasks.

A group of friends sit around a table to piece together a jigsaw puzzle, but imagine if the image on the puzzle changed every time someone made a move. This is reminiscent of what happens in multirobot systems—where groups of robots try to learn and adapt to their environment simultaneously.

This phenomenon, known as 'nonstationarity', refers to the challenge each robot faces in learning from its surroundings to make better decisions. As robots learn and modify their actions, their collective impact changes the robots' environment unpredictably.

Hongliang Guo, a Scientist at A*STAR's Institute for Infocomm Research (I^{2}R), painted a picture of the complications nonstationarity causes: "In the worst-case scenario, although the robots have visited every part of an environment, a moving target in that environment may still not be detected."

Robots often rely on traditional learning methods such as deep Q-networks and policy gradient methods, which excel in static and predictable environments. However, Guo explained that these methods face challenges in dynamic settings because they assume stable conditions while robots are in the process of learning to navigate and complete tasks.

To counter this, Guo and researchers from the University of Electronic Science and Technology of China; and the Massachusetts Institute of Technology, US; proposed a solution involving a rule called a cross-entropy regularisation policy gradient (CE-PG). This strategy helps robots in a multirobot system spread out and learn more effectively in variable environments, encouraging them not to cluster in one place but to explore different areas.

Initially, robots were trained centrally with shared information but executed their tasks independently using the learned policies. This setup avoids real-time policy adjustments that can destabilise learning. Subsequently, CE-PG aided in dispersing the robots, ensuring coverage of different areas during tasks.

Through a series of test simulations and real-world experiments, the researchers showed that the CE-PG approach successfully overcomes the issue of unpredictable changes by ensuring that robots stick to their initial strategies during tasks. In all cases, the CE-PG scheme found the moving target, outperforming or matching standard policy gradient and deep Q-network techniques, especially in maintaining robustness against individual robot failures.

"Multirobot search teams could look for a missing child in a mall environment, or for lost luggage at the airport."

This method can significantly enhance the efficiency and reliability of multirobot systems in real-world applications such as search and rescue, surveillance and exploration. Guo suggested some practical applications: "Multirobot search teams could look for a missing child in a mall environment, or for lost luggage at the airport."

The decentralised execution aspect of the team's method also means it scales well with the number of robots involved, potentially enabling larger and more complex multirobot operations. "Our next step is to devise CE-PG+, which is applicable to 'unknown' environments, without prior topological information," said Guo. ★

Researcher
Hongliang Guo, I^{2}R

IN BRIEF

A new training method known as cross-entropy regularised policy gradient (CE-PG) enhances multirobot performance in unpredictable environments by ensuring each robot consistently follows its assigned role, offering potential advancements in fields like search and rescue.

1. Guo, H., Liu, Z., Shi, R., Yau, W.-Y. and Rus, D. Cross-entropy regularized policy gradient for multirobot nonadversarial moving target search. *IEEE Transactions on Robotics* **39** (4), 2569-2584 (2023).

Photo credit: Alexander Sinn / Unsplash

INDUSTRIAL ENGINEERING

Keeping tabs on moving parts

Machine learning-based predictions intelligently analyse complex sensor data to enhance equipment maintenance and reliability.

Photo credit: Eduardo Buscariolli / Unsplash

In 2003, an electrical glitch in a power grid sparked one of the most extensive blackouts in history—the Northeast Blackout, affecting 50 million people across North America. This incident highlighted the need for predictive analytics to anticipate equipment malfunctions within such critical infrastructures.

Predicting the remaining useful life (RUL) of machinery and systems is vital across many sectors, including manufacturing and aviation, and involves gathering and analysing data to forecast future equipment failures using advanced machine learning (ML) techniques.

Yucheng Wang, a Senior Research Engineer at A*STAR's Institute for Infocomm Research (I^2R), noted that while newer ML methods like graph neural networks (GNNs) are being used to account for interactions among different sensor data, such as temperature and pressure, they often neglect local correlations. This oversight restricts how these models are built and ultimately limits their accuracy when predicting equipment lifespan.

To address these challenges, Wang and I^2R colleagues worked with researchers from Nanyang Technological University, Singapore, to develop a new approach named LOGO (LOcal–GlObal correlation fusion). This framework integrates both immediate (local) and long-term (global) sensor data correlations into GNNs, enhancing their predictive accuracy. LOGO meticulously constructs models to represent sensor interactions from both perspectives, then uses these models to capture dependencies that evolve over time and across different sensors.

LOGO divides sensor data into smaller segments or 'patches', each processed to form sequential micro-graphs. Known as multi-patch segmentation, this action allows for the detailed analysis of local correlations, while global correlations are processed separately. An adaptive fusion mechanism then integrates these insights, ensuring each patch reflects a comprehensive spectrum of data.

The research team demonstrated the method's efficacy in numerous tests, which markedly outperformed traditional models and significantly reduced prediction errors to promise substantial cost savings and improved reliability. LOGO's success may enhance operational efficiency across various industries.

"This algorithm can be applied to aircraft engines to detect whether the engines need maintenance or repairs," Wang noted.

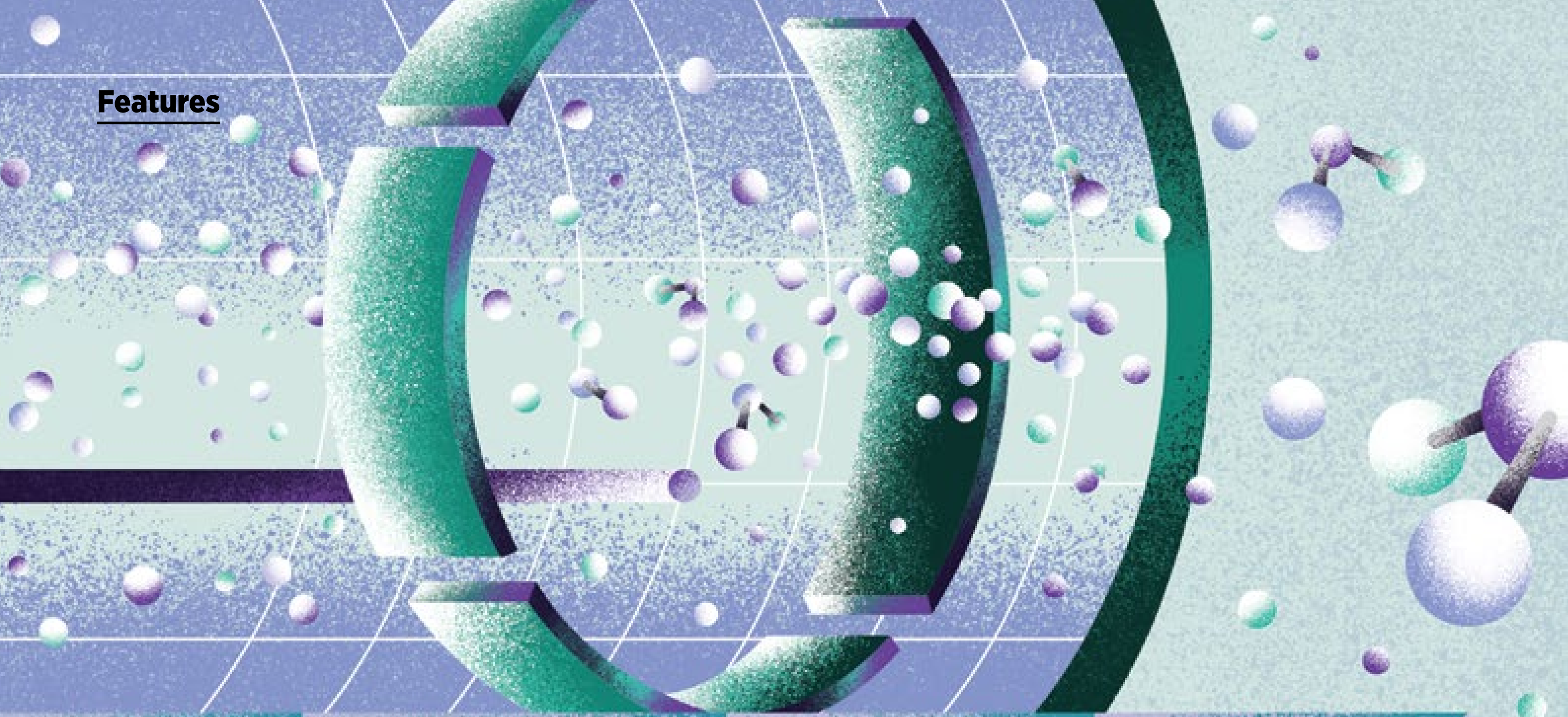
Looking ahead, the team aims to refine their process further. "The graph construction and GNN processes require a large number of samples for training. To address this and improve the model, we plan to incorporate data-efficient algorithms, such as self-supervised learning techniques," Wang said. ★

Researchers
Yucheng Wang and Zhenghua Chen, I^2R

Min Wu and Ruibing Jin, I^2R

IN BRIEF
LOGO, a novel machine learning framework, leverages multi-sensor data to significantly enhance remaining useful life (RUL) predictions and reduce prediction errors across industries like aviation.

1. Wang, Y., Wu, M., Jin, R., Li, X., Xie, L., *et al.* Local-Global correlation fusion-based graph neutral network for remaining useful life prediction. *IEEE Transactions on Neural Networks and Learning Systems* (2023).



BRINGING QUBITS TO CHEMISTRY

By designing quantum circuits to simulate the complexities of chemical reactions, A*STAR scholar Karthik Shreekumar Panicker aims to support new discoveries in chemistry, materials and medicine.

Computer simulations have transformed our approach to understanding nature. Digital models of our world not only provide faster and cheaper ways for researchers to explore new frontiers, but also enable them to validate theories that are difficult to test in laboratory settings. Today, insights from computational models aid scientists at scales large and small: from predicting extreme weather events to identifying new medicinal molecules.

However, even today's most advanced supercomputers can struggle to accurately replicate how the simplest molecules behave in chemical reactions. To efficiently model such reactions on classical computing architectures, scientists often rely on approximations of the physical properties involved, which can fail to fully capture the complex interactions of individual atoms and molecules.

Researchers like A*STAR National Science Scholar Karthik Shreekumar Panicker believe that quantum computing offers researchers a way to model real-world chemistry with greater precision. Rooted in the principles of quantum mechanics—the science of the tiny—quantum computers have the potential to simulate the energetics of atoms and subatomic particles with a higher degree of confidence. Such systems can benefit fields other than chemistry; quantum-powered insights can speed up the discovery of new drug candidates, catalysts and materials.

Piqued by a mutual interest in quantum physics and computational chemistry, Panicker aims to use his cross-disciplinary experiences to support the expanding field of quantum chemistry and the promise it offers for natural science. In this interview with *A*STAR Research*, Panicker shares some highlights from his scientific journey to date, his motivations in the dynamic world of science, and advice for other early-career researchers.

Q: WHAT BROUGHT YOU TO YOUR CURRENT RESEARCH FOCUS?

It all began in secondary school, when I had the opportunity to work on a computational chemistry research project. I was introduced to the world of theoretical research in chemistry: an eye-opening experience that I thoroughly enjoyed. However, I decided to follow my passion for physics and majored in it for my bachelor's degree. After graduating, I knew I wanted to pursue a PhD in the field of quantum sciences, though I was unsure of the specifics involved.

Fortunately, during my one-year research assistantship at A*STAR, I received a lot of support and advice from experts in the field and my peers. My work during that year was in the field of quantum optics at IMRE under Victor Leong. This was my first hands-on research experience in quantum physics, and I got to explore and discuss new ideas in and around the subfield.

These insightful discussions helped me discover my true interest in quantum computing for chemistry, bringing my research full circle. Throughout this journey, the National Science Scholarship helped me gain valuable experience in diverse fields, allowing me to make informed decisions about my future.

Q: WHAT MAKES QUANTUM COMPUTING AN EXCITING FIELD TO EXPLORE?

The field has been quietly making strides over the years. Within the next decade or so, quantum computing is expected to mature enough to be able to make significant contributions to society. One major anticipated benefit from the technology is its ability to simulate chemical reactions on a more exact level, given that atoms and molecules operate on inherently quantum mechanical principles. This could revolutionise fields like drug discovery, materials design and so on.

It is also exciting to be part of an actively growing area of research that openly encourages new ideas. Considering my interests and background, pursuing this field for my PhD was a natural choice.

Q: TELL US ABOUT YOUR CURRENT WORK.

ChatGPT has captivated the world in recent times. At the University of Toronto, I'm currently working under Alán Aspuru-Guzik to harness its underlying model to design quantum circuits that can accurately simulate molecules in chemistry. Quantum circuits are specialised computational pathways that use the principles of quantum mechanics; where classical circuits rely on bits, which can only exist as one of two values ('0' and '1'), quantum circuits use qubits, which can exist as multiple values. It is this fundamental difference that allows quantum computers to be able to solve certain problems much faster than classical computers.

To date, precise molecular modelling has been prohibitively expensive on conventional computers. Finding a scalable way to do this on quantum computers would be a breakthrough.

Karthik Shreekumar Panicker

A*STAR National Science Scholar

> **"Within the next decade or so, quantum computing is expected to mature enough to be able to make significant contributions to society."**
>
> — Karthik Shreekumar Panicker, A*STAR National Science Scholar

Q: WHAT ARE SOME OTHER RESEARCH PROJECTS YOU'VE WORKED ON AT A*STAR?

I have predominantly worked on physics research projects throughout my time with the agency, albeit in different areas. It all started with a research project about thin-film solar cells which aimed to improve the fabrication processes involved. It was an integral experience that taught me about how communication and research is carried out within a large institute.

My research attachment with IMRE was about the use of integrated photonics for single-photon detectors. I learned a lot of hard skills during that year about how to set up a scientifically sound experiment, including the extremely hands-on task of creating all the necessary parts from the ground up. Over the years, I've gotten to develop different skills due to the different experiences I had. Perhaps this breadth of experience encouraged me to pursue interdisciplinary areas of research for my PhD.

Q: AS AN EARLY-CAREER RESEARCHER, WHAT EXCITES YOU ABOUT YOUR JOURNEY AHEAD?

The ever-evolving world of science makes it challenging to predict its future when I graduate. Science will continue answering questions while sparking new ones in the process. This can be equal parts nerve-wracking and thrilling. However, as a quantum computing researcher, I find Singapore's commitment to invest in quantum technologies particularly exciting.

Q: WHAT ADVICE WOULD YOU GIVE THOSE PURSUING THEIR OWN STEM CAREERS?

I think it can be succinctly expressed by an Oscar Wilde quote, which Stephen Fry summarised as: "If you know what you want to be, then you inevitably become it—that is your punishment. But if you never know, then you can be anything."

It's okay not to have your career path figured out at 18. Even most PhD graduates don't end up working on the exact problem they wrote their thesis on. In my opinion, it's best to have a broader understanding of your choices and learn to view problems from different perspectives. ★

MATERIALS SCIENCE

Spinning wonders of future computing

Complex magnetic particle arrangements, called skyrmions, can transform computing by making data storage and processing more efficient and energy-saving.

Nanometre-scale compass needles, known as skyrmions, are magnetic textures in certain materials. Their low-energy creation, manipulation and erasure make them ideal for future computing technologies, especially biomimetic computing.

Anjan Soumyanarayanan, a Research Scientist at A*STAR's Institute of Materials Research and Engineering (IMRE), has been exploring the potential of skyrmions in a study with lead author Xiaoye Chen; IMRE Lead Research Engineer, Hui Ru Tan; and other researchers of IMRE's Spin Technology for Electronic Devices (SpEED) team, as well as the National University of Singapore.

Chen explained that conventional computers use transistor-based hardware to simulate neural networks for artificial intelligence tasks. Meanwhile, biomimetic computing uses specialised hardware that replicates the behaviour of biological brain cells.

"This allows a computer to natively perform neural network inference tasks without using an emulation layer, offering superior speed and efficiency compared to present-day computers," said Chen.

Despite their potential, skyrmions face stability hurdles. While they form compact structures under an external magnetic field, they become unstable and stretch into stripe-like formations when the field is removed, losing essential characteristics needed for computing applications.

To counter this, the team posited that integrating two distinct types of magnetic interactions within specially engineered magnetic layers can maintain skyrmion stability under ambient conditions without an externally applied magnetic field.

The team used wafer-scale techniques, transmission electron microscopy (TEM) and detailed simulations to tweak skyrmion behaviour in custom magnetic structures. They overcame hurdles by developing methods to quantify interlayer exchange coupling (IEC), a critical but not directly measurable parameter.

Ultrathin magnetic films are at the resolution limit of TEM imaging. "Distinguishing magnetic textures, like skyrmions, from structural defects is challenging. We developed custom imaging recipes and computational analysis techniques to address this," Tan said.

Initial attempts to regulate skyrmions by altering the thickness of a single magnetic layer to manipulate IEC were unsuccessful due to the skyrmions' high sensitivity. This prompted the exploration of IEC with a second magnetic layer, a strategy not previously considered by the community. The team discovered that fine-tuning this layer provided much more precise control over skyrmion numbers.

"With two chiral layers coupled together by the second IEC, fluctuations in one chiral layer can be restored by the second layer," Chen explained. "This greatly improves the stability of skyrmions in chiral bilayers, which host the second IEC."

Controlling skyrmions without a magnetic field enables scalable, energy-efficient computing technologies. Meanwhile, extending IEC beyond traditional materials can create exotic 3D textures by coupling layers with different or complementary properties.

"Our work opens up the third dimension of magnetic films as a playground for materials exploration," said Soumyanarayanan, adding that this breakthrough enabled the creation of the world's first all-electrical skyrmionic magnetic tunnel junction—an advanced, high-efficiency memory device that reads and writes data using purely electrical signals. ★

Researchers
Anjan Soumyanarayanan, Xiaoye Chen and Hui Ru Tan, IMRE

Photo credit: Faisal al-adabi / Shutterstock

IN BRIEF
A new method using double magnetic layers to stabilise and control skyrmions without applying a magnetic field enables faster, lower-energy computing.

1. Chen, X., Tai, T., Tan, H.R., Tan, H.K., Lim, R., *et al*. Tailoring zero-field magnetic skyrmions in chiral multilayers by a duet of interlayer exchange couplings. *Advanced Functional Materials* **34** (1), 2304560 (2024).

CHEMISTRY

Smart models decode liquid mysteries

A*STAR researchers develop machine learning models that quickly and accurately simulate chemical reactions involving complex liquid interactions.

Predicting how chemical reactions unfold used to rely on trial and error at the lab bench. Computational modelling has transformed this, driving innovation in fields from pharmaceuticals to environmental engineering by reducing development time and costs while enhancing precision and efficiency.

Some reactions, particularly those involving liquids, remain exceptionally difficult to predict. Benjamin Chen and Xinglong Zhang, Scientists at A*STAR's Institute of High Performance Computing (IHPC), highlight the complexity of predicting the behaviour of liquids in chemical reactions. "There is not one 'best' arrangement of liquids," they explained. "An ensemble of arrangements may be present as the solvent molecules fluctuate over time."

These infinite arrangements mean that there are high computational costs to adequately sample the representative structures in a liquid reaction via molecular dynamics simulations. For instance, quantum-mechanical calculations require about 10 minutes per time step. "This translates to the entire calculation requiring 20 years," said Chen and Zhang.

While implicit solvation models are faster and less expensive for simulating solvent interactions, they're often inaccurate, missing critical details like hydrogen bonding and molecular disorder. To address these shortcomings, the team proposed using machine learning interatomic potentials (MLIPs). These models learn from existing data to swiftly and accurately simulate complex chemical systems at the atomic level.

"MLIPS, unlike quantum-mechanical calculations, do not have to solve Schrödinger's equations and obtain the wavefunction of the system," said Zhang and Chen, noting that this makes MLIPs up to 10,000 times faster, reducing the time for one million timesteps from 20 years to 24 hours.

The researchers tested different MLIPs to identify the most effective one for studying interactions between water and different materials. They validated their accuracy by comparing the results with traditional calculations and real-world data, focusing on bulk water and water-metal interfaces.

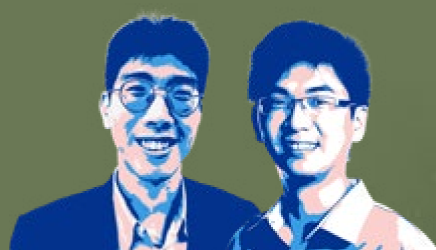
Their approach, which combined machine learning with active learning, proved successful in conducting detailed and realistic studies of liquid catalysts over extended time and length scales. Active learning continuously refines MLIPs with only the most relevant data, making simulations both faster and more accurate without needing vast initial datasets.

"We showed that our simulations are nearly as accurate as first-principles simulations, which are the current gold standard," said Chen and Zhang.

The researchers believe MLIPs will allow the study of more complex and larger systems. Such advanced models will be crucial for accurately representing real-world catalysts in different environments, such as nanoconfined solvents or dynamically changing catalysts, which can lead to the development of more efficient chemical processes.

Chen, Zhang and colleagues are currently collaborating with researchers at the University of Alabama, US, to optimise the use and training of MLIPs further. ★

Photo credit: Sonika Agarwal / Unsplash



Researchers
Benjamin Chen and Xinglong Zhang, IHPC

IN BRIEF
Machine learning interatomic potentials (MLIPs) combined with active learning successfully simulate complex liquid interactions in chemical reactions, achieving nearly the same accuracy as traditional first-principles methods but up to 10,000 times faster.

1. Chen, B.W.J., Zhang, X. and Zhang, J. Accelerating explicit solvent models of heterogeneous catalysts with machine learning interatomic potentials. *Chemical Science* **14**, 8338–8354 (2023).

PHOTONICS

To build a light-speed data highway

Advanced photonic processors boost machine learning efficiency by handling vast data streams in parallel, with potential benefits for enhanced patient monitoring and cloud computing.

The unsung hero behind multimedia experiences is a tiny electronic chip—often no bigger than a credit card—that brings productivity and entertainment to life. Found in smart devices and computers, the graphics processing unit (GPU) performs numerous simultaneous calculations to render images and videos seamlessly.

"Being able to process more data in each clock cycle means you can run algorithms faster and with higher energy efficiency," explained Bowei Dong, a Principal Investigator at A*STAR's Institute of Microelectronics (IME). This capability stems from hardware-based 'accelerators': specially designed architectures that handle multiple data streams in a single step (parallelism). It's an essential feature for the complex, data-heavy demands of machine learning (ML).

Everyday computers used in homes and offices that rely on traditional electronic architectures falter under high parallelism, struggling to double their capacity every few months. In response, Dong and his colleagues have proposed an innovative solution: adding an extra dimension to data processing to boost parallel processing capabilities.

Think of how adding more lanes to a congested highway, each designated for a different vehicle type, allows for smoother, faster travel without bottlenecks. Similarly, advanced photonic processors can use multiple channels—like lanes—to manage several data streams on a single chip. These processors exploit the colour of light and numerous parallel optical fibres, integrating them into a data-processing photonic tensor core.

"The access to many degrees of freedom is the reason why photonics can achieve higher parallelism than electronics."

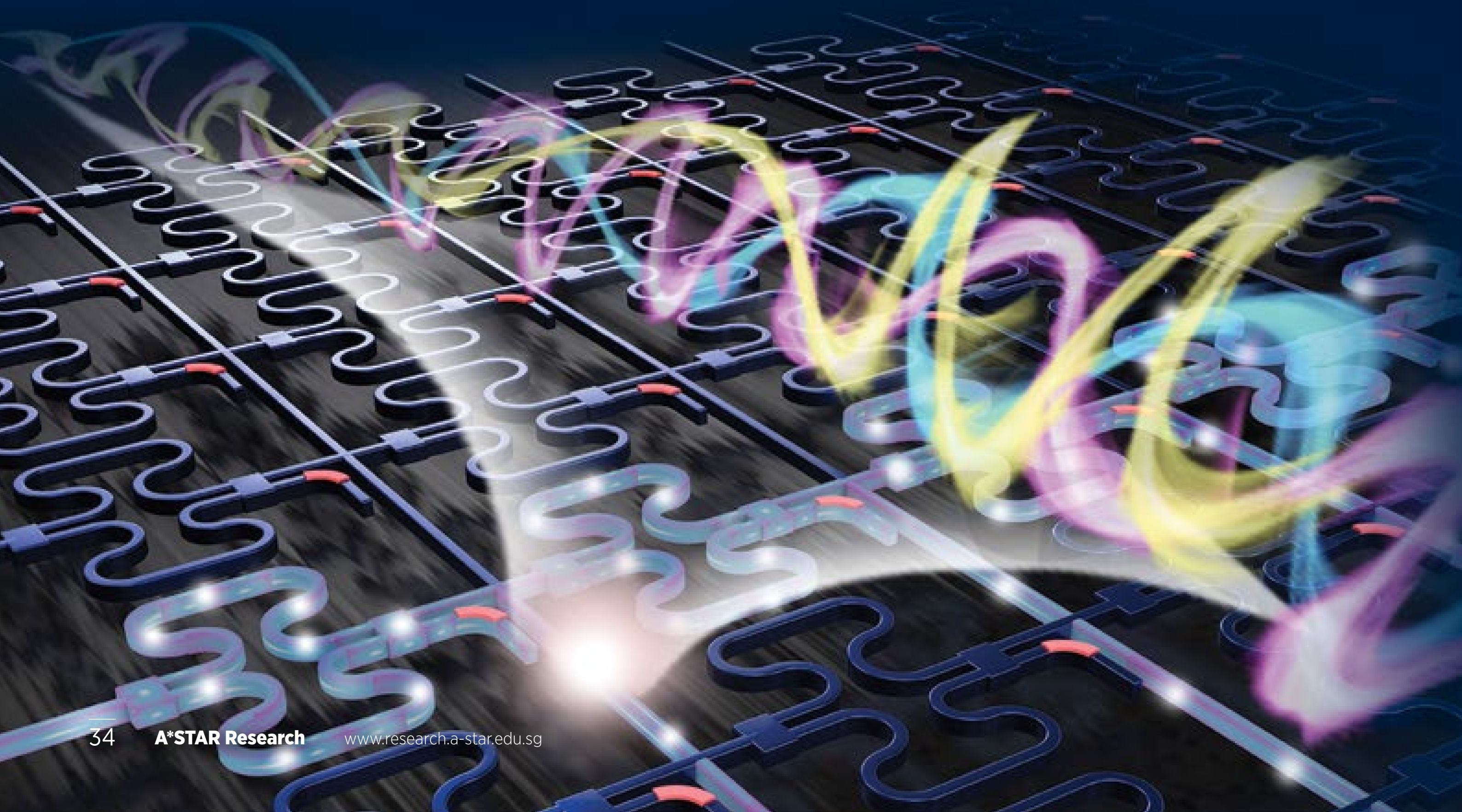
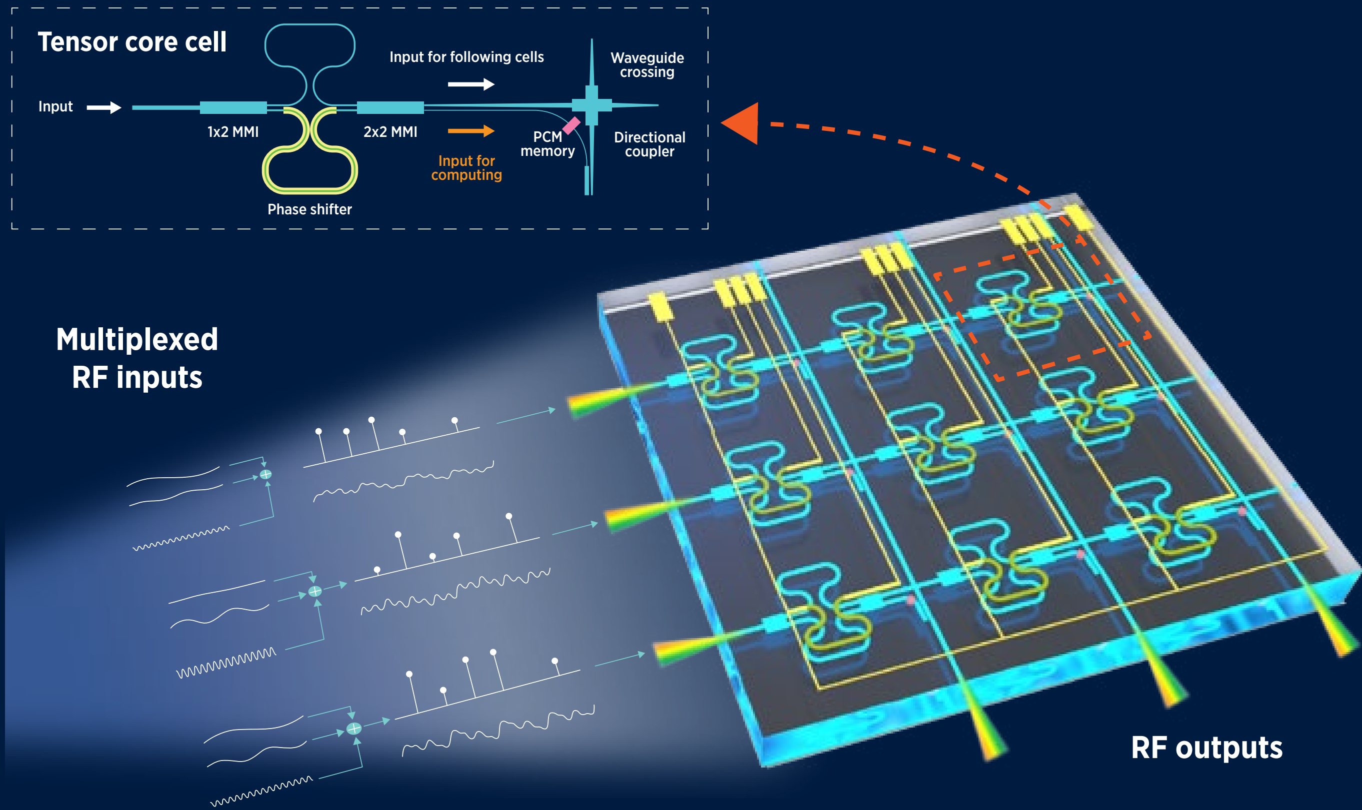


Photo credit: Bowei Dong / A*STAR Research



The architecture of a photonic tensor core for in-memory computing. Multiple radiofrequency (RF) components are multiplexed into a single optical wavelength as it enters the tensor core, which processes them in parallel. In the tensor core, each cell (inset image) contains a tuneable power splitter; a phase-change memory (PCM); two multimode interferometers (MMI); a waveguide crossing for interconnects; and a directional coupler.

"The access to many degrees of freedom is the reason why photonics can achieve higher parallelism than electronics," said Dong.

Building on this architecture, Dong and collaborators from the University of Oxford and University of Exeter in the UK; and University of Muenster, Germany; introduced a third data channel using radio-frequency (RF) multiplexing, enhancing the photonic tensor core's capacity to process even more information concurrently.

The team showcased the superiority of their system using real-time heart activity recordings, processing clinical electrocardiogram (ECG) data from 100 patients. Their advanced processor handled the data with a parallelism of 100, two orders of magnitude higher than current methods. By applying an ML model to this data, the system also identified patients at risk of sudden death with 93.5 percent accuracy.

This breakthrough offers exciting real-world benefits: beyond improved real-time patient monitoring, it has broader applications in the Internet of Things (IoT)—a network of interconnected devices—and in edge cloud computing, which processes data closer to where it's generated for faster results.

The team plans to build on this promising schematic by exploring methods to encode information onto additional light channels. "Meanwhile, we will also explore new electronics-photonics integration to improve the performance of each individual computing channel," said Dong, pointing to a future where hardware evolves to meet the colossal computational demands of ML. ★

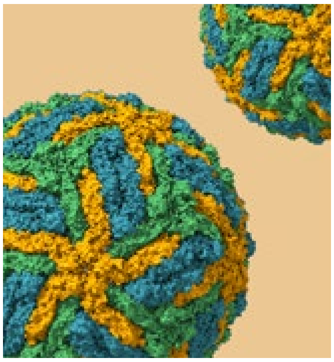
Researcher
Bowei Dong, IME

IN BRIEF
Researchers develop a photonic processor using three-dimensional data processing, incorporating radio-frequency modulation alongside spatial and wavelength multiplexing to achieve 100-fold parallelism.

1. Dong, B., Aggarwal, S., Zhou, W., Ali, U.E., Farmakidis, N., *et al.* Higher-dimensional processing using a photonic tensor core with continuous-time data. *Nature Photonics* **17**, 1080-1088 (2023).

SNEAK PEEK

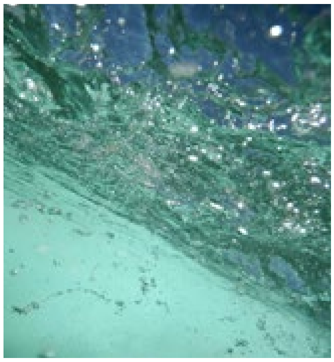
*A brief look at upcoming research highlights in the next issue of A*STAR Research*



VIROLOGY

HIDDEN POCKETS EXPOSE ANTIVIRAL HOTSPOTS

High-resolution simulations uncover dynamic regions on the surface of dengue-like viruses, offering added guidance for new drug designs.



CATALYSIS

REFINING RECIPES FOR GREEN HYDROGEN CATALYSTS

Machine learning models help zero in on optimal designs for water-splitting molecules to boost sustainable hydrogen production.

TRANSPORTATION

DEEP LEARNING FOR DEEP WATERS

Researchers develop a dynamic, context-aware maritime AI that helps vessels predict safer and more efficient oceanic routes.

MATERIALS SCIENCE

NANOARRAYS TUNE LIGHT ON THE DOT

A new optical nanoantenna design provides fine control over light emissions from quantum dots, honing their tunablilty for advanced optoelectronic devices.

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