

# AI for Science (AI4S) Funding Opportunity

The National Research Foundation (NRF) of Singapore will launch an **AI for Science (AI4Science) Grand Challenge Call** on 1 January.

Imperial Academics are eligible to apply through **Imperial Global Singapore**, our entity at the Singapore Campus for Research Excellence and Technical Enterprise (CREATE).

**OPPORTUNITY** - To co-lead a **\$10M-15M, 3-4 years** AI for Science programme with Singapore partners.

## PORTFOLIO

Imperial Global Singapore currently hosts 2 major CREATE grants:

- INCYPHER - \$20m research centre on safety and security of medical devices
- SOSV - \$15m research centre on decarbonisation with green ammonia using solid oxide fuel cells

## NOTES

PIs typically expected to spend 20% or more of time in Singapore

Impact on Singapore - research must have impact on Singapore plus global impact

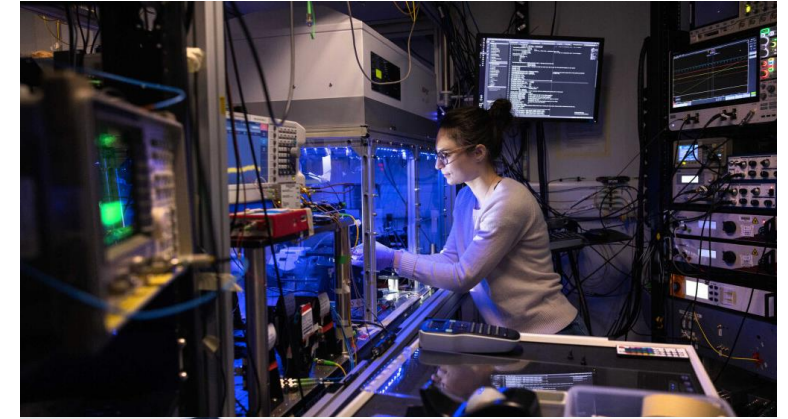
# IMPERIAL GLOBAL SINGAPORE

A formal legal entity in Singapore  
at **CREATE** – Campus for Research  
Excellence and Technical Enterprise.

**CREATE** hosts interdisciplinary research  
centres from top global universities.

**Initial Programme** – \$20m research centre  
on safety and security of medical devices.

Vibrant  
science and  
technology  
ecosystem



# IMPERIAL GLOBAL SINGAPORE

## Funding opportunities for Imperial Global Singapore

### CREATE Grand Challenges Funding Calls

- Periodic calls framed around a grand challenge involving Singapore partners as well as other CREATE international partners (S\$10M–15M)

### CREATE Responsive Mode

- Short White Papers can be developed in collaboration with Singapore partners for ambitious research programmes (~S\$25M) or smaller pilot or proof of concept programmes aligned to Singapore's needs.
- Important to understand the local ecosystem and Singapore's needs before applying.

### Intra-CREATE calls

- Periodic thematic funding calls for CREATE entities to undertake collaborative research in Singapore (S\$2-\$5M). Partners to include Singapore institutions and international institutions within the CREATE.



# AI for Science (AI4S)

## What is AI for Science?

Use of AI to *accelerate scientific inquiry and discovery*, by automating and expanding the scale of hypothesis generation, experiments, and data analysis.

## Why AI for Science?

Enables discoveries that would not otherwise be possible

e.g. AI can mine vast amounts of data to uncover patterns beyond human capabilities.

Much greater speed and efficiency

e.g. a much greater part of research could be done computationally, and maximizing the yield of downstream wet-science experimentation.

# AI for Science

## What to Expect / Consider

- Two rounds of **Grand Challenge** (January 2025, 2026) and **Catalytic** (Mid 2025, 2026).
- Call will have a short window, probably ~6 weeks.
- First stage will be a ~10 page 'white paper', followed by an opportunity to present.
- Proposals must include Imperial and one or more local partner – priority should be to partner with universities (e.g. NUS, NTU) over A\*STAR or others.
- Can include other CREATE partners (MIT, TUM, CNRS, ETH, Cambridge, SJTU, Berkeley, Illinois), but may dilute funding.
- Impact on Singapore - research must have impact on Singapore and its peoples' needs – global impact is not enough.
- Alignment with Singapore government goals - research should align with Singapore government strategy, e.g. [RIE 2025](#), [Smart Nation](#), [AI Strategy](#).
- Should fill a 'gap' in Singapore capabilities and not overlap with other projects funded in Singapore.
- Residency in Singapore for investigators is required, typically 20% of time for leads.

The AI4S funding initiative will fund basic research projects which will advance the development of AI methods and tools for scientific research and leverage these AI solutions to make a transformative step-change in scientific discovery.

Research projects will be funded through 2 grant schemes:

- The 'Challenge' grant scheme, which will support larger programmes with clearly articulated potential for impact in areas of Singapore's strategic priorities. *Expected launch in Q1 2025.*
- The 'Catalyst' grant scheme, which will support smaller projects in areas proposed bottom-up by the community. *Expected launch in Q3-Q4 2025.*

Project Teams are expected to be multidisciplinary, and should have at least two co-Lead PIs, who possess relevant expertise in AI and a scientific domain, respectively.

CREATE entities and international PIs are invited to participate in collaboration with local researchers.

# Flow-through of AI methods & approaches across Fundamental Research, AI4S, & Applied Research

## Fundamental Research (Research in AI)

*Build peaks of basic AI research excellence*

## AI4Science (AI4S)

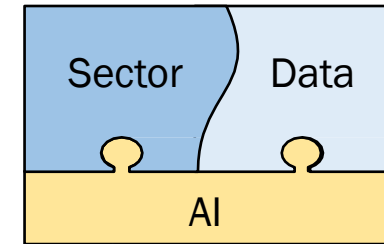
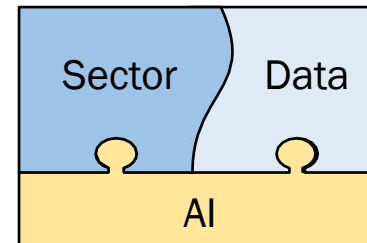
*Use of AI to accelerate scientific inquiry and discovery*

## Applied Research (AI4X)

*Apply AI to drive major use cases to advance priority sectors*

Responsible, Resource  
Efficient, Gen Purpose  
& Emerging AI

Challenge Programmes,  
Catalytic Projects



- Enhancing AI (e.g. reasoning, efficiency, explainability, trust)
- Expand applicability of AI, mitigate risks, data/computational efficiency
- Pushing boundaries for analyses of classical / quantum data

Imperial College London

- Targets the broad field of scientific research and discovery
- Extract scientific knowledge and generalizable understanding
- Focus on identifying patterns, generating theories, new research questions
- Crucial for ensuring transparency, reliability of scientific findings, knowledge generation

- Implementation for specific tasks
- Solve practical problems and optimize workflows
- Discovery & Hypothesis generation is not primary focus

# AI4S Strategy for scoping AI4S research areas

## Grant Scheme

## Challenge

## Catalyst

Selected themes based on national strategic priorities

Open to bottom-up proposal

## Domain Verticals

|                                                     |                                                                    |                                                                        |                 |
|-----------------------------------------------------|--------------------------------------------------------------------|------------------------------------------------------------------------|-----------------|
| <b>Domain 1</b><br>e.g. Target/Bio-marker Discovery | <b>Domain 2</b><br>e.g. Modelling & Simulation for Climate Science | <b>Domain ...</b><br>e.g. Automated Synthesis of Materials & Molecules | <b>Domain n</b> |
| <b>Data 1</b><br>e.g. PRECISE                       | <b>Data 2</b><br>e.g. NEA                                          | <b>Data ...</b>                                                        | <b>Data n</b>   |

## Horizontals

AI models, methods, approaches  
Computation

|                            |                          |                            |
|----------------------------|--------------------------|----------------------------|
| Generative AI              | Foundation models        | Physics-informed models    |
| Geometric learning         | Transformers             | Literature-based discovery |
| High performance computing | Hybrid quantum computing |                            |

*\*Topics are indicative and not final, scoping in progress*

## Domain verticals

- Based on national strategic priority, or may be transformative areas proposed by the research community
- Key consideration is also availability of a unique high-quality datasets

## Cross-cutting horizontals

- AI models, methods, and approaches that are generalizable to a class of problems across domains.
- Developments in computation to support AI for research, including hybrid quantum compute.

# AI for Science

## Potential research capabilities to build

AI-aided data collection and augmentation

Generative, Science-based, Foundation Models and methodologies beyond deep learning

Multi-modal AI, LLMs for scientific discovery (incl. literature based discovery, self-driving labs)

Hybrid Quantum Computing

HPC research for AI



## Potential use cases



1. Propose to **establish an AI for Science Grand Challenge (GC)** to call for our local research community to tackle big scientific questions that they are already interested in, but using AI much more extensively.
2. NRF, together with stakeholder agencies, will **centrally assist with the provisioning of required datasets, accessing compute, as well as providing relevant AI expertise through AISG**, as part of the GC design.
3. The GC will involve a call for concept papers, followed by workshops, full proposal evaluations, and engaging up to 8 global partners along with local IHLs.
4. The **global talent base may be engaged through the CREATE setup**.

# Community efforts: to outline the transformative potential of AI4S across domains

- Scoping and convening of research community: AI4S Scoping Report (<https://ai4science.sg>), 1<sup>st</sup> Workshop (29 Feb)
- Thematic workshops for domain deep dives (Apr-Jun) ⑦ Whitepapers outlining (i) problem statements (ii) bottlenecks (iii) methodology (iv) transformative opportunity / target outcomes

| Domain                                  | Leads: Domain expert, AI expert, bilingual expert                    | Date   |
|-----------------------------------------|----------------------------------------------------------------------|--------|
| Complexity Science and Physics          | Duane Loh, Lock Yue Chew                                             | 5 Apr  |
| Earth and Climate Sciences              | Dale Barker, Sang-Ho Yun                                             | 12 Apr |
| Genomics                                | Joanne Ngeow, Mile Sikic                                             | 12 Apr |
| Biomedical Sciences                     | Sebastian Maurer-Stroh, Mile Sikic                                   | 18 Apr |
| Financial Services                      | Bo An, Huang Ke-Wei                                                  | 24 Apr |
| Chemical and Biological Manufacturing   | Saif Khan, Wu Zhe                                                    | 24 Apr |
| RNA Biology                             | Ashok Venkitaraman, Jinmiao Chen                                     | 25 Apr |
| Science, Software and Security          | David Lo, Reza Shokri                                                | 2 May  |
| Semiconductor manufacturing             | J Senthilnath, Li Xiaoli, Aaron Thean                                | 6 May  |
| Materials Science and Chemistry         | Kedar Hippalgaonkar, Kostya Novoselov                                | 8 May  |
| Digital Phenotyping and Interventions   | Robert Morris, Jimmy Lee                                             | 16 May |
| Hybrid Quantum Computing                | Dario Poletti, Jose Ignacio Latorre                                  | 16 May |
| Sustainability                          | Madhavi Srinivasan, Yeoh Lean Weng, Arvind Easwaran                  | 21 May |
| Healthcare and Imaging                  | Rosa Qi Yue So, Daniel Ting, Ngiam Kee Yuan, Tan Cher Heng, Rick Goh | 28 May |
| AI methods for Science (across domains) | B Low, YS Ong, Ng See Kiong, Li Qianxiao, + Domain Experts           | 7 Jun  |

# AI for Science

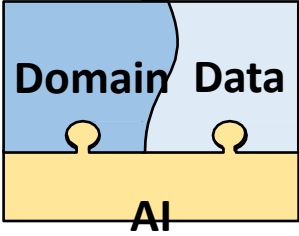
*AI for Science* unlocks discoveries through (a) science-inspired model architectures, (b) development of generalizable and interpretable models, and (c) autonomous hypothesis generation and testing (data-driven, including AI-powered labs)

| Feature                                 | <i>Research for AI</i>                                                                                | <i>AI for Science</i>                                                                                           | <i>AI for Applications</i>                                                                      |
|-----------------------------------------|-------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------|
| Scope                                   | Focuses on enhancing aspects of AI, such as reasoning, trustworthiness, and resource efficiency       | Targets the <b>broad field</b> of scientific research and discovery                                             | Focuses on implementation of AI for <b>specific tasks</b> within a particular field or industry |
| Goals                                   | To expand the applicability of AI, mitigate its risks, and address its data/computational efficiency. | Extract scientific knowledge and generalizable understanding                                                    | Solve practical problems and optimize workflows                                                 |
| Data                                    | Pushing boundaries for analyses of not only classical data, but also quantum data                     | Complex, multi-dimensional data                                                                                 | At present tailored to specific data types and formats                                          |
| Discovery and hypothesis generation     | Not a primary focus, as it relates to scientific discovery                                            | Plays a central role in <b>identifying patterns, generating theories</b> and exploring new research questions   | May not be a primary focus                                                                      |
| Explainability, repeatability and trust | Primary focus of R&D within this vertical                                                             | Crucial for ensuring <b>transparency and reliability</b> of scientific findings and <b>knowledge generation</b> | Varies, depending on application                                                                |

AI can augment the scientific method and transform scientific inquiry by automating and expanding the scale of hypothesis generation, experiments, and data analysis. Possibilities include:

- **Literature based discovery** mines existing research for hidden connections and encompassing domain expertise
- **Geometric learning** uncovers patterns in complex data such as protein structures
- **AI powered labs** with automated experiment design and evaluation accelerate the pace of discovery
- **Data augmentation** generates synthetic data for deeper model training
- **Transformers and language models** analyze DNA sequences and protein interactions
- **Self-supervised learning** extracts features from unlabeled datasets, accelerating research in climate modelling & drug discovery

# AI4S Structure & rationale

|                     | Type I: Challenge                                                                                                          | Type II: Catalytic                                                                                                                                                 |
|---------------------|----------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Objective</b>    | Programme funding aimed at achieving transformative step-change in a domain of national strategic priority. (\$10-15M)     | Project grants aimed at stimulating new collaborations between domain and AI researchers, creating a large base of activity in AI for research. (\$2-3M)           |
| <b>Organisation</b> | <div> <div>Research Cluster</div>  </div> | Organised as Research Clusters (RCs), co-led by KOLs in domain and AI. Development of AI models, methods, approaches that generalize across domains is encouraged. |
| <b>CREATE</b>       | Global partnerships                                                                                                        |                                                                                                                                                                    |

## Next Steps for interested PIs

Contact Imperial Global Singapore team:

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**Prof. Azra Ghani**, Academic Director, Imperial Global Singapore ([a.ghani@imperial.ac.uk](mailto:a.ghani@imperial.ac.uk))

*Note: CREATE Members are limited to 3-5 bids per institution. PIs are required to express interest with the Imperial Global Singapore team to ensure applications can be managed in line with funder guidance. A pre-selection stage maybe required dependent on demand/interest.*