

AI-for-Science (AI4S) Catalytic Grant Call 2025/26 – Awarded Projects

S/N	Project Title	Lead PI	Host Institution
1	Generative AI Meets Green Electrocatalysis: Flow-Matched Models for Condition Discovery towards C2 Selectivity	Li Haobo, Mengmi Zhang, Leow Wan Ru	NTU
2	Achieving Systematic Generalization via Cross-Domain Foundation Models for Theragnostic Inhibitor Discovery	Liu Bin, Bian Yatao	NUS
3	Advancing Generative Models for Materials: Unified AI and Mathematical Foundations	Xavier Bresson, Kostya Novoselov	NUS
4	Agri-TrAlt: AI Model-as-a-Service (MaaS) for Data-to-Decision Agriculture	Wei Yang Bryan Lim, Menachem Moshelion	NTU
5	Advancing AI Models for Protein-Protein Interaction and Binder Design with Applications to Force-Bearing Cytoskeletal Proteins	Yan Jie, Zhang Yang	NUS
6	GenAgent-Tx: A Multimodal Generative AI Agent for Therapeutic Development	Chan Guo Wei Alvin, Tan Nguan Soon	NTU
7	Quantum-Augmented Model Reduction to Discover More with Less	Mile Gu, Dacheng Tao	NTU
8	AI for Recycling: HYDRA - Hydrometallurgical Yield Discovery through Responsive Automation	Leonard Ng Wei Tat, Nripan Matthews, Ong Yew Soon	NTU
9	Unified AI solutions to enable scientific inference for next-generation gravitational-wave astronomy	Chua Jing Kang Alvn, Li Cheng	NUS
10	FLUX: Fusion Learning for Unified Cross-diagnostics – A Multimodal Foundation Model for Plasma Diagnostics and Forecasting	Chua Kunting Eddie, Lin Gu	A*STAR Research Entities (ARES)
11	AI for Discovering Materials with Outstanding Electromechanical Response	Yao Kui, Ooi Chin Chun	A*STAR Research Entities (ARES)