CONFERENCE PROGRAM

AI4X – ACCELERATE 2026

June 16–19, 2026

VENUE	Raffles City Convention Centre, Singapore
DAYS	4
TALKS	256 — *73 invited · 176 contributed · 7 sponsor*
POSTERS	173

RESEARCH TRACKS

- AI Agents and LLMs for Science
- AI for Chemistry
- AI for Materials Science
- AI for Physics
- ML Algorithmic Advances
- Unconventional Computing
- AI for Biology
- AI for Earth Science
- AI for Medicine and Healthcare
- AI for Society
- Self-Driving Labs

PROGRAM DATA AS OF 19 JUNE 2026, 00:04 (UTC+08:00)

TUESDAY, JUNE 16

DAY 1 — AT A GLANCE

TIME	OLIVIA	SOPHIA	MOOR	MORRISON	HULLET
08:00 – 09:00	REGISTRATION				
09:00 – 09:15	Kostya Novoselov & Alán Aspuru-Guzik: Opening *Chair: Shi Xuan Leong*				
09:15 – 09:45	Ulrich S. Schubert: Combining online characterization and synthetic robots – On the road to self-driving labs				
09:45 – 10:15	Tommaso Dorigo: The second AI revolution in fundamental science				
10:15 – 10:30	Tejs Vegge: MaterialsCommons for Europe – SDLs and FAIR workflows for federated discovery of advanced materials				
10:30 – 11:00	TEA BREAK *SPONSORED BY SEA GARENA*				
11:00 – 11:30	Curtis Berlinguette: Ada-Carbon: A self-driving laboratory to enable the lowest-cost pathway to scalable CO_2-to-fuels conversion *Chair: Jacqueline Cole*				
11:30 – 11:45	Maria K. Y. Chan: Seeing the invisible in materials with AI				
11:45 – 12:00	Lesley Schultz, Santha Santhakumar (TECAN & Acceleration Consortium): Accelerating Hit Optimization with Automated Parallel Synthesis				
12:00 – 12:15	BREAK				
12:15 – 12:45	Laura Matz: Unlocking Precision Medicine | The Digital Ecosystem Powering Tomorrow's Therapies *Chair: Kostya Novoselov*				
12:45 – 13:00	Maksym Plakhotnyuk, ATLANT 3D: The Autonomous Materials Foundry: The Physical Infrastructure for AI-Driven Materials Discovery with Direct Atomic Layer Processing (DALP®) Technology				
13:00 – 13:15	Tan Chorh Chuan: Launch of AI for Science: Accelerating Discovery Through AI				
13:15 – 14:45	LUNCH *SPONSORED BY JEOL ASIA PTE LTD*				
14:45 – 15:00	SELF-DRIVING LABS Bowen Li: AI-driven LNP design for mRNA delivery *Chair: Adam Gormley*	SELF-DRIVING LABS Beatrice Soh: Learning Stochastic Polymer Dynamics at the Single-Molecule Level with High-Throughput Experiments *Chair: Ulrich S. Schubert*	AI FOR CHEMISTRY Yanwei Lum: Physical Unified Device Architecture for AI-Assisted CO_2 Electrocatalysis *Chair: Berend Smit*	AI AGENTS AND LLMS FOR SCIENCE Jennifer Dodgson: Negative Space Learning: Where Survival is the Only Reward *Chair: Tejs Vegge*	ML ALGORITHMIC ADVANCES Luis Camuñas-Mesa: Neuromorphic Systems: Towards Sustainable AI *Chair: Willi Gottstein*
15:00 – 15:15	Shigeru Kobayashi: Development of a benchtop self-driving laboratory for electrocatalyst deposition and evaluation	Stephen Dale: High-index saddle dynamics for the automated mapping of reaction routes	Mathilde Franckel: Accelerating Ammonia Decomposition Catalyst Discovery with AI	Ngoc Duy Dinh: Large Language Model Agents Enable Autonomous Design and Image Analysis of Microwell Microfluidics	Andrey Ustyuzhanin: Directing Open-Ended Evolution in Artificial Life via Temporal Multi-Scale Structural Complexity
15:15 – 15:30	Naruki Yoshikawa: NIMO Controller: An accessible self-driving laboratory orchestrator based on the model context protocol	Florian Boser: PlateOpt: Bayesian Optimization for Organic Catalysis in Combinatorial Well Plates	Yue Yifei: Towards ab-initio quality description of porous materials: Developing general Machine-Learned Potentials to	Samuel Addington: Neurosymbolic Guardrails for World-Model Digital Twins: Securing AI-Driven Scientific Discovery and Autonomy	Maxime Goulet: Self-Driven Process Optimization in Pneumatic 3D Printing: From Static Ensemble Learning to Autonomous Bayesian Method

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			simulate physical and adsorption properties of Metal-Organic Frameworks		
15:30 – 15:45	Calvin Phan: AutoMEA - an automated electrolyser device for self-driving labs	Xiao Li: A Self-Driving Closed-Loop Workflow for Data-Efficient Kinetic Modeling and Op-timization of the Aldol Reaction	Ivan Kruglov; Liudmila Klimova: Diffusion-Driven Generation of Novel Crystalline Materials with Target Optical Properties	Yitian Huang: How Prompt Structural Framing and Cognitive Scaffolding Influence Performance in Generative AI Design?	Paola Driza: A Framework for Bayesian Optimization in Mixture Spaces
15:45 – 16:00	Han Hao: Integrating Multimodal Knowledge Mining and Autonomous Experimentation for Accelerated Electrosynthesis Discovery	Chen Jie: A systematic effort toward establishing an automatic end-to-end synthesis workflow for small molecules	Alastair Price: Atom-in-molecule based quantum machine learning of defect formation energies	Mengjia Zhu: Can We Automate Scientific Reasoning in Closed-Loop Experiments using Large Language Models?	Hongbin Zhang: Bayesian Optimization for the Inverse Problems in Materials Science
16:00 – 16:15	Ivory Wenyu Zhang: IvoryOS: An Interoperable Platform and Community for Self-Driving Laboratories	Wendi Cai: Automation and AI-Powered Prediction in Chromatographic Separation	Patrick Butler: AI-guided experimental design of zirconium MOPs with The World Avatar for sustainable photocatalysis	Yu Chinen: Evolving collaborative research ideas with multi-agent grounding in lab-specific contexts and literature	Yuki Takezawa: Meta Bayesian Optimization to Discover a Problem Worth Optimizing
16:15 – 16:45	TEA BREAK				
16:45 – 17:00	AI FOR MATERIALS SCIENCE **Yousung Jung: Designing Materials That Can Be Made** *Chair: Victor Posligua*	SELF-DRIVING LABS **Shoichi Matsuda: Data-Driven Materials Discovery for Rechargeable Batteries: High-Throughput Experimental Platforms and Closed-Loop Autonomous Optimization** *Chair: Keith A. Brown*	AI AGENTS AND LLMS FOR SCIENCE **Santiago Miret: How Autonomous Labs & AI Are Transforming Scientific Discovery** *Chair: Andrey E Ustyuzhanin*	AI AGENTS AND LLMS FOR SCIENCE **Mohamad Moosavi: Reasoning in the Language of Materials** *Chair: Ray Meng Gao*	ML ALGORITHMIC ADVANCES **Ivor W. Tsang: Building Physical AI Systems: From Geometry and Physics to Scientific Discovery** *Chair: Gianmarco Mengaldo*
17:00 – 17:15	Sergei Tatarin: Towards accelerating the discovery of efficient iridium(III) emitters using a novel database and machine learning based only on structural formulas	Sanna Jarl: Machine learning for in-situ composition mapping in a self-driving magnetron sputtering system	Marcel Mueller: La Agente Optima – orchestrated Bayesian optimization and active learning for accelerated in-silico compound discovery	Fengxu Yang: A Universal Autonomous Agent for Atomistic Simulation and Benchmarking Its Capabilities	Abdul Kadir: A Three-Level Feature Selection Framework for Android Malware Detection
17:15 – 17:30	Lulu Wang: Data-scarce synthesis-by-design of ferroelectric Dion–Jacobson 2D hybrid organic–inorganic perovskites	Matthew Osvaldo: When is Bayesian Optimization Beneficial? A Critical Assessment of Optimization Strategies in High-Throughput Organic Photovoltaic Manufacturing	Jiaru Bai: El Agente Gráfico: Structured Execution Graph for Scientific Agents	Ioana Zelko: DarkMatterFM: An Agentic Foundation Model for Multimodal Dark-Matter Inference with GPU-Accelerated Emulators	Leonardo Pesce: Exiaa: Explainable Injections for Adversarial Attack
17:30 – 17:45	SWITCH: SWITCH (EnterpriseSG) Talk	Fanjin Wang: Constrained composite Bayesian optimisation for rational synthesis of polymeric particles	Shruti Badhwar: SciAgent: Containerized Code Generation for Scientific Computing with Verification	Zonglin Yang: MOOSE-Chem2: Exploring LLM Limits in Fine-Grained Scientific Hypothesis Discovery via Hierarchical Search	Qian Yang: MultiTaskDeltaNet: Change Detection-based Image Segmentation for operando ETEM with Application to Carbon Gasification Kinetics
17:45 – 18:00	Emha Bayu Miftahullatif: High-Throughput In-Device Screening of Printable Lead-Free Halide Perovskite Memristors via Machine Learning-Driven Optimization	Lars Sonneveld: Autonomous Optimization of Perovskite Solar Cell Thin Films via Robotic Spin-Coating and Bayesian Optimization	Zijian Zhang: El Agente Forjador: Task-Driven Agent Generation for Quantum Simulation	Jingyu Feng: DIGIBAT: Bridging the gap between physical automation and AI in energy research	Bohui lyu: Code and Data are not all you need for reproducibility

WEDNESDAY, JUNE 17

DAY 2 — AT A GLANCE

TIME	OLIVIA	SOPHIA	MOOR	MORRISON	HULLET
09:00 – 09:30	Eun-Ah Kim: Learning Quantum Matter from Data: Data Centric AI for Scientific Discovery *Chair: Yong Tao Tan*				
09:30 – 10:30	Editors Panel - Scientific Publishing in the AI Era				
10:30 – 11:00	TEA BREAK				
11:00 – 11:30	Giacomo Indiveri: Bridging natural and artificial intelligence with mixed-signal neuromorphic circuits *Chair: Jennifer Dodgson*				
11:30 – 11:45	Ngiam Kee Yuan: CASCADE AI - An Agentic AI Variant-to-Disease Mechanism Discovery				
11:45 – 12:00	Aruhan Rui Shi: Macroeconomic Modeling and Forecasting with AI Tools				
12:00 – 12:30	Jun Jiang: Building a Global Infrastructure for AI-Driven Innovation				
12:30 – 14:45	Poster Session #1 / Lunch				
14:45 – 15:00	AI FOR MATERIALS SCIENCE **Antonio Helio Castro Neto: Machine learning for synthesis of real materials** *Chair: Yeong Wai Yee*	SELF-DRIVING LABS **Nasim Abdollahi: Self-driving lab for viscous nanoemulsions** *Chair: Yang Cao*	AI FOR CHEMISTRY **Pengfei Ou: Machine Learning Accelerated Simulations of Electrochemical Interfaces** *Chair: Yizhou Zhu*	AI FOR MEDICINE AND HEALTHCARE **Yimu Zhao: Accelerating Biological Discovery Through AI, Robotics, and Human Organ Mimicry** *Chair: Luis Camuñas-Mesa*	ML ALGORITHMIC ADVANCES **Dmitry Vetrov: Thermodynamical Analogies in Deep Learning** *Chair: Carlo Vittorio Cannistraci*
15:00 – 15:15	Zhuoying Zhu: Accelerating materials innovation through automated theoretical-experimental iterations empowered by AI-Chemist	Martin Seifrid: Toward Generalizable, Data-Efficient Self-Driving Laboratories for Organic Materials	Haobo Li: Active Learning Interatomic Potentials-Enhanced Molecular Dynamics for Grain Boundary Engineering in Anti-perovskite Solid Electrolytes	Alokendra Ghosh: Inferring Oocyte Cytoplasmic Material Properties from Cytoplasmic Streaming Movies Using Physics-Informed Neural Networks	Feixiang Ren: Towards Critical Branching Mechanism in Recurrent Neural Networks
15:15 – 15:30	Hirokuni Jintoku: Accelerating Nanocarbon Dispersion Research via Machine Learning and Automated Experimentation	Timothy McClure: An Integrated Platform for In Situ Electroanalytical–Driven Reaction Optimization	Autonomous Discovery of High-performance Ni–Mo Electrocatalysts for Green Hydrogen Production	Zhen Yuan Yeo: Inferring the hidden and long-range dengue transmission routes in Singapore	Ling Feng: Order-chaos transition in deep neural network and its application to the training process
15:30 – 15:45	Kensei Terashima: Automated Bulk Intermetallic Synthesis via Orchestrated Heterogeneous Laboratory Machines	Jeongwook Lim: Designing of Microfluidic Concentration Generator Module for Self-Driving Fluid Mixing System	Qi Jie Yeow: Large Language Model Assisted Optimisation of Photocatalytic Hydrogen Production	Giacomo Indiveri: Event driven neural network on a mixed signal neuromorphic processor for detecting EEG based epileptic seizure	Mengyi Chen: Scalable learning of macroscopic stochastic dynamics
15:45 – 16:00	Kazunori Nishio: Exploration of Ternary Thin-Film Lithium Solid Electrolyte Composites Using the Digital Laboratory for Enhanced Lithium-Ion Conductivity	Owen Melville: Resource-efficient Bayesian optimization for self-calibrating liquid handling	Yonatan Kurniawan: A reinforcement learning approach to generate equivalent circuit models for Electrochemical Impedance Spectroscopy	Poorva Pandya: Conceptualising Case Formulation as a Neurosymbolic AI Framework for Mental Health	Zhuoyuan Li: Learning non-equilibrium mesoscopic dynamics with Onsager principle
16:00 – 16:15	Haiwen Dai: Closed Loop Inorganic Material Discovery with Design-Test-Make-Analyze Paradigm	David Scott Lewis: ACHT-World: Causal World Models for Closed-Loop Self-Driving Laboratories	Yicheng Chen: Benchmarking Foundation Potentials against Quantum Chem-	Malik Saif: The Cognitive Clinical OS: Architecting Asynchronous Agentic	Zhichao Han: Learning Permutation-invariant Macroscopic Dynamics

TIME	OLIVIA	SOPHIA	MOOR	MORRISON	HULLET
			istry Methods for Predicting Molecular Redox Potentials	Reasoning for Real-Time Decision Support	
16:15 – 16:45	TEA BREAK				
16:45 – 17:00	AI FOR MATERIALS SCIENCE **Yeong Wai Yee: Machine Learning for 3D Printed Soft Robotics and Intelligent Systems** *Chair: Seunghwa Ryu*	SELF-DRIVING LABS **Daria Andreeva: Closed-Loop autonomous discovery of functional membranes and 2D Materials for resource recovery and energy applications** *Chair: Shoichi Matsuda*	AI FOR SOCIETY **Nancy F. Chen: Beyond Alignment: Grounding AI in Society** *Chair: Truyen Tran*	AI FOR PHYSICS **Marco Bernardi: Quantum Interactions in Materials: a New Frontier for AI** *Chair: Shyue Ping Ong*	UNCONVENTIONAL COMPUTING **Fernando Aguirre: CMOS-Integrated Silicon-Oxide Memristors: Reliability Characterization, SPICE-Based Circuit Simulation and potential application in neuromorphic computing** *Chair: Giacomo Indiveri*
17:00 – 17:15	Hangwei Qian: A Multimodal Conditional JEPA for Composite Materials	Yuuya Nagata: Closed-loop Optimization of Mono-functionalization via Suzuki-Miyaura Reaction	**Sulfikar Amir: Exploring Social Trust in AI**	**Yuehaw Khoo: Generative modeling and tensor-network**	Santhosh Sivasubramani: LLM-Powered Autonomous Agents for Spintronic Device Optimization: From Rule-Based to AI-Driven Design
17:15 – 17:30	Bo Hu: Test-Time Self-Evolution in Multi-Agent Systems for Materials Discovery	Nicholas Warren: Flow Chemistry as a Platform for Experimental Multi-objective Optimization of Heterogeneous Polymer Synthesis	**Nikita Kazeev: Align AI to our Aspirations, not our Flaws**	Jiadong Dan: Symmetry-Aware Deep Learning for Generalizable STEM Phase Classification	Santhosh Sivasubramani: Design Methodologies for Skyrmion-Based Circuits and Systems in AI-Driven Applications: Bi-Directional Integration
17:30 – 17:45	Ben Rowlinson: Data-Driven Property Prediction for Memristor Resistive Switching Layers	Ryo Tamura: NIMO: Universal Middleware for Closed-Loop Materials Exploration	Reena Shadaan: Ethical Nail Salons: A community-governed and SDL-facilitated approach to mitigate occupational chemical hazards in nail salons	Yue Yifei: Mapping diverse structures of liquid water and ice using variational autoencoders: A vector quantization approach to discover structural motifs in model latent spaces	Santhosh Sivasubramani: Ultra-low-energy skyrmion-based learning automata element for adaptive edge intelligence
17:45 – 18:00	Atish Dixit: EMOS: The Unified AI Platform for Electronic Materials Discovery	MCP-Enabled LLM Agents for Closed-Loop Optimization in Real-Time Physical Experiments	Eric J. W. Orlowski: AI & Culture Alignment: Interpretation over Measurement	Qianshu Ye: VLM4Physics: Equation Discovery Using Multi-modal Inputs	Jianlong Lu: Spectrum-Aware Quantum Control beyond Classical Spectral Access

THURSDAY, JUNE 18

DAY 3 — AT A GLANCE

TIME	OLIVIA	SOPHIA	MOOR	MORRISON	HULLET
09:00 – 09:30	Vivek Natarajan: General-purpose AI systems from Google DeepMind designed to accelerate scientific discovery and democratize medical expertise *Chair: Melodie Christensen*				
09:30 – 09:45	Ray Meng Gao: New Frontiers in Machine Learned Quantum Chemistry				
09:45 – 10:00	Michele Ceriotti: Let them learn: AI models that master materials physics				
10:00 – 10:15	Ryutaro Uchiyama: AI-Driven Scaffolding of Open-ended Movement Exploration				
10:15 – 10:30	Truyen Tran: The New Scientific Method: Taste, Truth, and Thinking with AI				
10:30 – 11:00	TEA BREAK				
11:00 – 11:30	Bartosz Grzybowski: Can robots help us redefine chemical reactions? *Chair: Beatrice Soh*				
11:30 – 11:45	Adam Gormley: Polymer Biomaterials in a Self-Driving Lab				
11:45 – 12:00	Shyue Ping Ong: Physics, Scaling and Data in Foundation Potentials				
12:00 – 12:30	Karsten Reuter: When the Algorithms Take Over: AI for Experiment Planning and Control				
12:30 – 14:45	Poster Session #2 / Lunch				
14:45 – 15:00	AI FOR MATERIALS SCIENCE Linh La: A Disorder-Aware Multi-fidelity Framework for Robust Prediction of Superconducting Critical Temperature *Chair: Artem Maevskiy*	SELF-DRIVING LABS **Leong Shi Xuan: Toward Safe Autonomy in Self-Driving Laboratories** *Chair: Han Hao*	AI FOR CHEMISTRY Kye Sung Park: Learning Arrow Pushing for Reaction Space Prediction and Exploration *Chair: Benjamin Chen*	AI FOR BIOLOGY **Yatao Bian: Molecular Foundation Models: from Pretraining-Finetuning to LLMs** *Chair: Yimu Zhao*	AI FOR EARTH SCIENCE **Jeff Adie: NVIDIA Earth-2 and Generative AI for Climate and Weather** *Chair: Tapio Schneider*
15:00 – 15:15	Yuanchao Hu: Graph learning metallic glass discovery from Wikipedia	Christopher Hassam: Add, Mix, Heat, Filter - Repeat, Repeat, Repeat	Galymzhan Moldagulov: Hybrid Computational Strategy for Predicting Complex Ligand–Metal Architectures	Hongmin Chen: Instructing a Chatbot to Design Nucleic Acid Probes for Diagnostics	**Gianmarco Mengaldo: Hybrid Physics-AI Digital Twins of the Earth System**
15:15 – 15:30	Jingbei Bai: Machine learning reveals transferable rules for predicting grain boundary segregation	Hugo Kvanta: A Self-Driving Lab for Novel Energy Material Discovery	Victor Posligua: Predictive mass spectrometry from quantum-mechanical fragmentation and intensity modelling	Wanyu Lin; Haowei Hua: Local-Global Associative Frames for Symmetry-Preserving Crystal Structure Modeling	Juntao Yang: From Global to Local: AI-based Climate Downscaling for Southeast Asia
15:30 – 15:45	Guangcun Shan: Atomic-Level Interpretable Multimodal Graph Neural Network for Predicting Carbon Capture in Metal-Organic Frameworks	Tim Kodalle: Combining robotic deposition tools and advanced characterization to enable ML-guided material discovery	Maik Gabriel Niedziella: ReactionEye: Integrating GC–MS Data and Chemical Context for Multimodal Structure Elucidation in Reaction Screening	Yoshinori Hayakawa: Bridging LLM-based planning and workflow languages for automated, validated, scalable exploration of scRNA-seq analyses	George Turkiyyah: Synthetic Geology: Structural Geology Meets Deep Learning
15:45 – 16:00	Adrien Goldszal: Discovery of Sustainable Refrigerants through Physics-Informed RL Fine-Tuning of Sequence Models	Linden Schrecker: Printing kinetic data and microkinetic models in an automated lab	Alexander Ryabov: Towards Data-Driven Nonlocal Density Functionals: Deep Learning DFT with Attention to approach Chemical Accuracy	yuxuan Ren: From Molecules to Materials and Proteins: Flow Autoencoders as Lossless and Unified Tokenizers	Nguyen Minh: Physics-informed Deep Operator Networks for Real-Time Spatiotemporal Monitoring of Indoor Air Quality
16:00 – 16:15					

TIME	OLIVIA	SOPHIA	MOOR	MORRISON	HULLET
	Shuya Yamazaki: CSX Framework for Synthesis-Oriented Generative Materials Discovery	Maria Politi: An End-to-end, Autonomous Platform for Liquid-liquid Extraction Optimization	Ekaterina Skorb: Nanostructured Material Design via a Retrieval-Augmented Generation (RAG) Approach: Bridging Laboratory Practice and Scientific Literature	Junhan Wang: Latent World Models of Cell Painting Data for In Silico Phenotypic Screening	Huixuan Sun: AI-Enabled 3D Glare Assessment Framework for Urban Solar Planning
16:15 – 16:45	TEA BREAK				
16:45 – 17:00	ML ALGORITHMIC ADVANCES **Yongcun Song: Neural network methods for non-smooth PDE-constrained optimization** *Chair: Eun-Ah Kim*	AI FOR MATERIALS SCIENCE Stuart Miller: Building a Decision-Driven Materials Discovery Institute: Early Insights from MDRI *Chair: Santiago Miret*	SELF-DRIVING LABS **Peichen Zhong: Towards in silico prediction of solid-state material synthesizability** *Chair: Owen Melville*	AI FOR MATERIALS SCIENCE **Wen Jie Ong: Accelerating AI-Powered Chemistry and Materials Science Simulations with NVIDIA ALCHEMI Toolkit** *Chair: Karsten Reuter*	AI FOR CHEMISTRY **Benjamin Chen: CatPlat: A Physics-Grounded Data Engine for AI-Driven Materials Discovery** *Chair: Yanwei Lum*
17:00 – 17:15	Yueming Lyu: NeCLO: Neural Convolutional Learning Optimizer for Electromagnetics	Honghao Chen: CatMaster: An Agentic Autonomous System for Computational Heterogeneous Catalysis Research	Kiran Vaddi: Beyond Point Sampling: Autonomous Phase Mapping of Biologic Formulation Stability via Hierarchical and Manifold Active Learning	Jiangjie Qiu: AdsorbFlow: energy-conditioned flow matching enables fast and realistic adsorbate placement	Shuan Chen: SynTwins: A Retrosynthesis-Guided Framework for Synthesizable Molecular Analog Generation
17:15 – 17:30	Chun-Sung Jao: AI for Plasma Diagnostics in Laboratory Astrophysics: Reconstructing Invisible Fields from Proton Images	Dorye Luis Esteras: Exploration and simulation of emergent magnetic materials via AI-driven workflows	Shun Muroga: Self-Driving Labs for Nanomaterials Development for Energy Applications: Syn-thesis, Dispersion, and Composite Forming	Jiaqi Zheng, SEA Garena: Toward GPU-Native Electronic Structure Calculations	Jan Christopher Spies: Yield Prediction of Organic Reactions in Biased Datasets via Positive-Unlabeled Learning
17:30 – 17:45	Nagendra Nagaraja, QpiAI India: Quantum AI	Jaehwan Choi: Materealize: a multi-agent deliberation system for end-to-end material design and synthesis	Udo Bach: An Autonomous Discovery Platform for Inorganic Photovoltaic Absorbers Beyond Lead Halide Perovskites	Ultrafast Spectroscopy Meets Data-Driven Materials Discovery at the Institut Courtois, Université de Montréal	Balamurugan Ramalingam: Generative Design and Experimental Validation of Non-Fullerene Acceptors for Photovoltaics
17:45 – 18:00	Subhajit Dandapat: Transformers with Physics-informed encodings and Simulation-Based inference for robust Gravitational-Wave detection in Pulsar Timing Array data	Yizhe Chen: SemiMat: A Semi-Supervised Toolkit for Data-Scarce Materials Property Prediction	Holger RöHM: E-MAP – A Self Driving Lab for Solution Based Combinatorial Semiconductor Discovery	Nitish Govindarajan: The Open Catalyst 2025 (OC25) Dataset and Models for Solid-Liquid Interfaces	Amirreza Mottafegh: Adaptive Human-in-the-Loop Optimization Using Language-Guided Priors for Chemical Synthesis
20:00 – 22:00	CONFERENCE DINNER				

FRIDAY, JUNE 19

DAY 4 — AT A GLANCE

TIME	OLIVIA	SOPHIA	MOOR	MORRISON	HULLET
09:00 – 09:30	Torsten Hoefler: Can we build an AI Climate Scientist? *Chair: Simon Billinge*				
09:30 – 09:45	Alex Hammer: Beyond the Proof of Concept: Autonomous Electrocatalyst Discovery Within Industrial Constraints				
09:45 – 10:00	Felix Hanke: Orchestrating the Three-Body Problem of Machine Learning, Simulation, and Experiments in Materials Discovery				
10:00 – 10:15	Artem Mishchenko: Why Experimental Data is the Next Frontier for AI x Materials				
10:15 – 10:30	Qianxiao Li: Learning mesoscopic dynamics				
10:30 – 11:00	TEA BREAK				
11:00 – 11:30	Jacqueline Cole: Data-Driven Materials Science for Energy-Sustainable Applications *Chair: Mohamad Moosavi*				
11:30 – 11:45	Berend Smit: AI-driven discovery of nanoporous materials				
11:45 – 12:00	Steinn Sigurdsson: Surviving the Transition: Doing Science in an Age of AI Accelerated Discovery				
12:00 – 12:15	BREAK				
12:15 – 12:45	Carlo Vittorio Cannistraci: Brain-inspired sparse network science for next generation efficient and sustainable AI *Chair: Gavin Koon*				
12:45 – 13:00	Tapio Schneider: First Principles, Fast Algorithms: The Physics-AI Synthesis in Earth System Modeling				
13:00 – 13:15	AI4X Organizers: AI4X Rising Star Awardee Presentation				
13:15 – 14:45	LUNCH				
14:45 – 15:00	AI FOR MATERIALS SCIENCE **Seunghwa Ryu: Physics-Informed AI for Inference and Design under Data Scarcity** *Chair: Sonia Azimi Dijvejin*	AI FOR MATERIALS SCIENCE **Yizhou Zhu: When Machine Learning Force Fields Fail Expectations: Lessons We Learned from Solid Electrolyte Materials** *Chair: Wen Jie Ong*	SELF-DRIVING LABS **Keith A. Brown: Polymer Discovery through Modular Chemistry Plus Modular Automation** *Chair: Felix Hanke*	AI FOR MEDICINE AND HEALTHCARE **Melodie Christensen: Advancing Pharmaceutical Development Through AI/ML-Enabled Experimental Design** *Chair: Nasim Abdollahi*	AI FOR SOCIETY Julian Prieto: The Geopolitics of AI Driven Scientific Discovery: Uneven Geographies of Self Driving Laboratories *Chair: Kourosh Darvish*
15:00 – 15:15	Sergey Grebenchuk: Machine Learning-Assisted Search for Skyrmion-Hosting Heterostructures for Device Applications	Zheng Jie Liew: Learning Nonlinear Dissolution Trajectories in Binary Polymer–Solvent Systems	Andy Anker: Autonomous nanoparticle synthesis by design	Viktor Schlegel: MIRA: Medical Time Series Foundation Model for Real-World Health Data	Maryam Ebrahimiazar: Self Driving Discovery of Immersion Cooling Fluids for Data Center
15:15 – 15:30	Mathilde Franckel: High-throughput ML Screening of Doped Cathode Active Materials	Andy Paul Chen: Atomic Sudoku: Stochastic approaches for correlated disorder materials	Muye Xiao: Kinetic study of the aqueous Kolbe-Schmitt reaction enabled by automated reaction analysis	Lyubomir Kotopanov: From In Silico Design to Automated Synthesis: An AI-Driven Framework for Late-Stage Functionalization	Syed Momin Naqvi: Defending Federated Learning: Adaptive Integration of Differential Privacy, SMPC, and Byzantine Robustness
15:30 – 15:45			Yuanyuan Zhou: Deciphering the operando mechanism of Haber-Bosch process	Theo Tait: Agentic AI–Enabled Integration of a Hybrid System of Predictive Models for Accelerated Dir-	

TIME	OLIVIA	SOPHIA	MOOR	MORRISON	HULLET
	Xiangwen Wang: Discovery of flat-band 2D materials via physics-informed scoring and structure-based learning	Zhenzhu Li: Platonic representation of foundation machine learning interatomic potentials		ect-Compression Drug Product Development	Minh Tri Nguyen: The Economy of Reasoning: Incentivizing Epistemic Diversity in Decentralized Scientific Swarms
15:45 – 16:00	Liudmila Klimova: Materials informatics framework for accelerated discovery of high-refractive-index 2D materials	Litong Wu: The Zintl–Klemm Concept in the Amorphous State: A Case Study of Na–P Battery Anodes	Zhengzuo Liu: A Data-driven Closed-looped High-throughput Platform for Thermocatalyst Discovery	Sven Papidocha: From Model to Molecule: Rapid Discovery of Potent CDK2 Inhibitors Using Boltz-2	Dean Thomas: Securing Autonomous Chemical Robots Through Physical and Digital Containment
16:00 – 16:15	Yihao Wei: Beyond Known Archetypes: A Generative AI Framework for Inverse Design of Flat-Band Materials from Geometric Outliers	Martin Hoffmann Petersen: Importance of Electronic Entropy for Machine Learning Interatomic Potentials	Ailsa Edward: Development of a Platform for Sustainable Metal-Organic Framework (MOF) Synthesis, MABIL: MOF Automation using Biomass-Inspired Linkers	Daniel Yanes: A machine learning workflow to accelerate the design of in vitro release tests from liposomes	David T T Tran; Ernest E Y Chan: Edge-AI Driven Automation for Scalable E-Waste Recycling
16:15 – 16:45	TEA BREAK				
16:45 – 17:00	AI FOR MATERIALS SCIENCE **Atul Thakur: Simulation at GPU Speed: Reimagining Atomistic Simulation at Scale with NVIDIA ALCHEMI** *Chair: Alex Hammer*	SELF-DRIVING LABS **Kourosh Darvish: A digital twin for sim-to-real chemistry lab automation** *Chair: Artem Mishchenko*	AI FOR BIOLOGY Yijun Li: AFPFusionLM: A Hybrid Sequence–Structure Protein Language Model for Antifreeze Protein Function Prediction *Chair: Yongcun Song*	AI AGENTS AND LLMS FOR SCIENCE **Haizhao Yang: Modeling and Computation in the Space of Language: Symbolic and LLM-Based Approaches** *Chair: Aruhan Rui Shi*	AI FOR PHYSICS **Simon Billinge: Characterizing electronic and structural states of materials with ML** *Chair: Qianxiao Li*
17:00 – 17:15	**Martin Hoffmann Petersen: Best Poster: Computational Investigation and Generation of Site-Disordered Sodium Ion Cathode Materials**	Yang Choo: A Standard Physical Environment for Benchmarking AI-driven Cell Biology	Ryo Akiba: Multi-objective optimization for designing structurally similar proteins with dissimilar sequences	Qixiang Zhang: PieLoT — LLM-driven Toolbox for Theorem Proving Education	Tanja Duric: $2k_F$ instability and chiral spin density wave at the 1/9 magnetization plateau in the kagome antiferromagnets
17:15 – 17:30	Nikita Kazeev: LeMat-GenBench: A Unified Evaluation Framework for Crystal Generative Models	Tong Xie: MiST: Understanding the Role of Mid-Stage Scientific Training in Developing Chemical Reasoning Models	Fushuai Wang: End-to-end neural reconstruction of DNA structures from single-frame fluorescence images	Viktor Schlegel: BRIDGE: Bootstrapping Text to Control Time-Series Generation via Multi-Agent Iterative Optimization and Diffusion Modeling	Xianquan Yan: HSG-12M: A Large-Scale Benchmark of Spatial Multigraphs from the Energy Spectra of Non-Hermitian Crystals
17:30 – 17:45	Manuel Kober-Czerny: Using Time-Series Forecasting to Accelerate Materials Stability Assessments	Sayan Doloi: Democratizing Discovery: Ultra-Low-Cost Self-Driving Laboratories for Materials Science	Poompol Buathong: Better Protein Function Prediction by Modeling Survivorship Bias	Linus Ng: Beyond Semantic Similarity: A Two-Phase Non-Parametric Retrieval Workflow for Corporate Credit Underwriting	Zekun Shi, SEA Garena: Flow-Distorted Plane Waves
17:45 – 18:00	Ivan Trofimov: Symmetry-Aware Equivariant Network for Discovering SHG-Active Materials	Shreyas Pethe: Automated High Throughput Optimization for Halide Perovskite Memristors	Michal Kobiela: Risk-averse optimization of genetic circuits under uncertainty	Thi Ngoc Nguyen: ESS-MOTIFS: Discovering Rubric-Aligned Motifs for Cohort-Level Essay Assessment	Jonas Elsborg: Global Plane Waves From Local Gaussians: Periodic Charge Densities in a Blink

DAY 1

TUESDAY, JUNE 16

08:00 – 09:00 REGISTRATION

EARLY MORNING

09:00 – 10:30

CHAIR Shi Xuan Leong

09:00–09:15 Opening

Kostya Novoselov & Alán Aspuru-Guzik

09:15–09:45 Combining online characterization and synthetic robots – On the road to self-driving labs

Ulrich S. Schubert ✶ *AI for Materials Science*

09:45–10:15 The second AI revolution in fundamental science

Tommaso Dorigo ✶ *AI for Physics*

10:15–10:30 MaterialsCommons for Europe – SDLs and FAIR workflows for federated discovery of advanced materials

Tejs Vegge ✶ *AI for Materials Science*

10:30 – 11:00 TEA BREAK *sponsored by SEA Garena*

LATE MORNING

11:00 – 12:00

CHAIR Jacqueline Cole

11:00–11:30 Ada-Carbon: A self-driving laboratory to enable the lowest-cost pathway to scalable CO_2-to-fuels conversion

Curtis Berlinguette ✶ *AI for Materials Science*

11:30–11:45 Seeing the invisible in materials with AI
Maria K. Y. Chan ✶ *AI for Materials Science*

11:45–12:00 SPONSOR Accelerating Hit Optimization with Automated Parallel Synthesis
Lesley Schultz, Santha Santhakumar (TECAN & Acceleration Consortium)

12:00 – 12:15 BREAK

MIDDAY

12:15 – 13:15

CHAIR Kostya Novoselov

12:15–12:45 Unlocking Precision Medicine | The Digital Ecosystem Powering Tomorrow's Therapies
Laura Matz ✶ *AI for Medicine and Healthcare*

12:45–13:00 SPONSOR The Autonomous Materials Foundry: The Physical Infrastructure for AI-Driven Materials Discovery with Direct Atomic Layer Processing (DALP®) Technology
Maksym Plakhotnyuk, ATLANT 3D

13:00–13:15 Launch of AI for Science: Accelerating Discovery Through AI
Tan Chorh Chuan

13:15 – 14:45 LUNCH *sponsored by JEOL Asia Pte Ltd*

Self-Driving Labs

OLIVIA

Self-Driving Labs for Autonomous Experimentation and Discovery

CHAIR Adam Gormley

14:45–15:00 AI-driven LNP design for mRNA delivery
Bowen Li

15:00–15:15 Development of a benchtop self-driving laboratory for electrocatalyst deposition and evaluation
Shigeru Kobayashi

15:15–15:30 NIMO Controller: An accessible self-driving laboratory orchestrator based on the model context protocol
Naruki Yoshikawa

15:30–15:45 AutoMEA - an automated electrolyser device for self-driving labs
Calvin Phan

15:45–16:00 Integrating Multimodal Knowledge Mining and Autonomous Experimentation for Accelerated Electrosynthesis Discovery
Han Hao

16:00–16:15 IvoryOS: An Interoperable Platform and Community for Self-Driving Laboratories
Ivory Wenyu Zhang



Self-Driving Labs

SOPHIA

Automated discovery and closed-loop optimization in chemistry and polymers

CHAIR Ulrich S. Schubert

14:45–15:00 Learning Stochastic Polymer Dynamics at the Single-Molecule Level with High-Throughput Experiments
Beatrice Soh

15:00–15:15 High-index saddle dynamics for the automated mapping of reaction routes
Stephen Dale

15:15–15:30 PlateOpt: Bayesian Optimization for Organic Catalysis in Combinatorial Well Plates
Florian Boser

15:30–15:45 A Self-Driving Closed-Loop Workflow for Data-Efficient Kinetic Modeling and Op-timization of the Aldol Reaction
Xiao Li

15:45–16:00 A systematic effort toward establishing an automatic end-to-end synthesis workflow for small molecules
Chen Jie

16:00–16:15 Automation and AI-Powered Prediction in Chromatographic Separation
Wendi Cai



AI for Chemistry

MOOR

AI for Chemistry and Materials Discovery

CHAIR Berend Smit

14:45–15:00 Physical Unified Device Architecture for AI-Assisted CO_2 Electrocatalysis
Yanwei Lum

15:00–15:15 Accelerating Ammonia Decomposition Catalyst Discovery with AI
Mathilde Franckel

15:15–15:30 Towards ab-initio quality description of porous materials: Developing general Machine-Learned Potentials to simulate physical and adsorption properties of Metal-Organic Frameworks
Yue Yifei

15:30–15:45 Diffusion-Driven Generation of Novel Crystalline Materials with Target Optical Properties
Ivan Kruglov; Liudmila Klimova

15:45–16:00 Atom-in-molecule based quantum machine learning of defect formation energies
Alastair Price

16:00–16:15 AI-guided experimental design of zirconium MOPs with The World Avatar for sustainable photocatalysis
Patrick Butler



AI Agents and LLMs for Science

MORRISON

LLM Agents and Autonomous Scientific Discovery

CHAIR Tejs Vegge

14:45–15:00 Negative Space Learning: Where Survival is the Only Reward
Jennifer Dodgson

15:00–15:15 Large Language Model Agents Enable Autonomous Design and Image Analysis of Microwell Microfluidics
Ngoc Duy Dinh

15:15–15:30 Neurosymbolic Guardrails for World-Model Digital Twins: Securing AI-Driven Scientific Discovery and Autonomy
Samuel Addington

15:30–15:45 How Prompt Structural Framing and Cognitive Scaffolding Influence Performance in Generative AI Design?
Yitian Huang

15:45–16:00 Can We Automate Scientific Reasoning in Closed-Loop Experiments using Large Language Models?
Mengjia Zhu

16:00–16:15 Evolving collaborative research ideas with multi-agent grounding in lab-specific contexts and literature
Yu Chinen



ML Algorithmic Advances

HULLET

Bayesian Optimization for Autonomous Materials and Process Discovery

CHAIR Willi Gottstein

14:45–15:00 Neuromorphic Systems: Towards Sustainable AI
Luis Camuñas-Mesa

15:00–15:15 Directing Open-Ended Evolution in Artificial Life via Temporal Multi-Scale Structural Complexity
Andrey Ustyuzhanin

15:15–15:30 Self-Driven Process Optimization in Pneumatic 3D Printing: From Static Ensemble Learning to Autonomous Bayesian Method
Maxime Goulet

15:30–15:45 A Framework for Bayesian Optimization in Mixture Spaces
Paola Driza

15:45–16:00 Bayesian Optimization for the Inverse Problems in Materials Science
Hongbin Zhang

16:00–16:15 Meta Bayesian Optimization to Discover a Problem Worth Optimizing
Yuki Takezawa



16:15 – 16:45 TEA BREAK



AI FOR MATERIALS SCIENCE

OLIVIA

AI for Materials and Molecular Discovery

CHAIR Victor Posligua

16:45–17:00 Designing Materials That Can Be Made
Yousung Jung

17:00–17:15 Towards accelerating the discovery of efficient iridium(III) emitters using a novel database and machine learning based only on structural formulas
Sergei Tatarin

17:15–17:30 Data-scarce synthesis-by-design of ferroelectric Dion–Jacobson 2D hybrid organic–inorganic perovskites
Lulu Wang

17:30–17:45 SPONSOR SWITCH (EnterpriseSG) Talk
SWITCH

17:45–18:00 High-Throughput In-Device Screening of Printable Lead-Free Halide Perovskite Memristors via Machine Learning-Driven Optimization
Emha Bayu Miftahullatif



Self-Driving Labs

SOPHIA

Autonomous materials and chemistry optimization

CHAIR Keith A. Brown

16:45–17:00 Data-Driven Materials Discovery for Rechargeable Batteries: High-Throughput Experimental Platforms and Closed-Loop Autonomous Optimization
Shoichi Matsuda

17:00–17:15 Machine learning for in-situ composition mapping in a self-driving magnetron sputtering system
Sanna Jarl

17:15–17:30 When is Bayesian Optimization Beneficial? A Critical Assessment of Optimization Strategies in High-Throughput Organic Photovoltaic Manufacturing
Matthew Osvaldo

17:30–17:45 Constrained composite Bayesian optimisation for rational synthesis of polymeric particles
Fanjin Wang

17:45–18:00 Autonomous Optimization of Perovskite Solar Cell Thin Films via Robotic Spin-Coating and Bayesian Optimization
Lars Sonneveld



AI Agents and LLMs for Science

MOOR

Scientific Agents for Discovery and Simulation

CHAIR Andrey E Ustyuzhanin

16:45–17:00 How Autonomous Labs & AI Are Transforming Scientific Discovery
Santiago Miret

17:00–17:15 La Agente Optima – orchestrated Bayesian optimization and active learning for accelerated in-silico compound discovery
Marcel Mueller

17:15–17:30 El Agente Gráfico: Structured Execution Graph for Scientific Agents
Jiaru Bai

17:30–17:45 SciAgent: Containerized Code Generation for Scientific Computing with Verification
Shruti Badhwar

17:45–18:00 El Agente Forjador: Task-Driven Agent Generation for Quantum Simulation
Zijian Zhang



AI Agents and LLMs for Science

MORRISON

LLMs and Autonomous Agents for Scientific Discovery and Automation

CHAIR Ray Meng Gao

16:45–17:00 Reasoning in the Language of Materials
Mohamad Moosavi

17:00–17:15 A Universal Autonomous Agent for Atomistic Simulation and Benchmarking Its Capabilities
Fengxu Yang

17:15–17:30 DarkMatterFM: An Agentic Foundation Model for Multimodal Dark-Matter Inference with GPU-Accelerated Emulators
Ioana Zelko

17:30–17:45 MOOSE-Chem2: Exploring LLM Limits in Fine-Grained Scientific Hypothesis Discovery via Hierarchical Search
Zonglin Yang

17:45–18:00 DIGIBAT: Bridging the gap between physical automation and AI in energy research
Jingyu Feng



ML Algorithmic Advances

HULLET

Cross-domain ML for security and scientific imaging

CHAIR Gianmarco Mengaldo

16:45–17:00 Building Physical AI Systems: From Geometry and Physics to Scientific Discovery
Ivor W. Tsang

17:00–17:15 A Three-Level Feature Selection Framework for Android Malware Detection
Abdul Kadir

17:15–17:30 Exiaa: Explainable Injections for Adversarial Attack
Leonardo Pesce

17:30–17:45 MultiTaskDeltaNet: Change Detection-based Image Segmentation for operando ETEM with Application to Carbon Gasification Kinetics
Qian Yang

17:45–18:00 Code and Data are not all you need for reproducibility
Bohui lyu



DAY 2

WEDNESDAY, JUNE 17

EARLY MORNING

09:00 – 10:30

CHAIR Yong Tao Tan

09:00–09:30 **Learning Quantum Matter from Data: Data Centric AI for Scientific Discovery**
Eun-Ah Kim ✶ *AI for Physics*

09:30–10:30 **Editors Panel - Scientific Publishing in the AI Era**
Yanfei Zhu (Nature); Anna Rulka (Royal Society of Chemistry); Steve Cranford (Cell Press); Steinn Sigurdsson (arXiv); Nancy F. Chen (NeurIPS); Moderator: Alán Aspuru-Guzik (Acceleration Consortium / NVIDIA)

10:30 – 11:00 TEA BREAK

LATE MORNING

11:00 – 12:30

CHAIR Jennifer Dodgson

11:00–11:30 **Bridging natural and artificial intelligence with mixed-signal neuromorphic circuits**
Giacomo Indiveri ✶ *AI for Biology*

11:30–11:45 **CASCADE AI - An Agentic AI Variant-to-Disease Mechanism Discovery**
Ngiam Kee Yuan ✶ *AI for Medicine and Healthcare*

11:45–12:00 **Macroeconomic Modeling and Forecasting with AI Tools**
Aruhan Rui Shi ✶ *AI for Society*

12:00–12:30 **Building a Global Infrastructure for AI-Driven Innovation**
Jun Jiang ✶ *AI for Chemistry*

❖ 12:30 – 14:45 POSTER SESSION #1 / LUNCH ❖



AI FOR MATERIALS SCIENCE

OLIVIA

Autonomous AI for Materials Discovery and Synthesis

CHAIR Yeong Wai Yee

14:45–15:00 Machine learning for synthesis of real materials
Antonio Helio Castro Neto

15:00–15:15 Accelerating materials innovation through automated theoretical-experimental iterations empowered by AI-Chemist
Zhuoying Zhu

15:15–15:30 Accelerating Nanocarbon Dispersion Research via Machine Learning and Automated Experimentation
Hirokuni Jintoku

15:30–15:45 Automated Bulk Intermetallic Synthesis via Orchestrated Heterogeneous Laboratory Machines
Kensei Terashima

15:45–16:00 Exploration of Ternary Thin-Film Lithium Solid Electrolyte Composites Using the Digital Laboratory for Enhanced Lithium-Ion Conductivity
Kazunori Nishio

16:00–16:15 Closed Loop Inorganic Material Discovery with Design-Test-Make-Analyze Paradigm
Haiwen Dai



Self-Driving Labs

SOPHIA

Self-Driving Labs for Chemistry and Materials Optimization

CHAIR Yang Cao

14:45–15:00 Self-driving lab for viscous nanoemulsions
Nasim Abdollahi

15:00–15:15 Toward Generalizable, Data-Efficient Self-Driving Laboratories for Organic Materials
Martin Seifrid

15:15–15:30 An Integrated Platform for In Situ Electroanalytical–Driven Reaction Optimization
Timothy McClure

15:30–15:45 Designing of Microfluidic Concentration Generator Module for Self-Driving Fluid Mixing System
Jeongwook Lim

15:45–16:00 Resource-efficient Bayesian optimization for self-calibrating liquid handling
Owen Melville

16:00–16:15 ACHT-World: Causal World Models for Closed-Loop Self-Driving Laboratories
David Scott Lewis



AI for Chemistry

MOOR

AI-driven electrochemistry and catalyst discovery

CHAIR Yizhou Zhu

14:45–15:00 Machine Learning Accelerated Simulations of Electrochemical Interfaces
Pengfei Ou

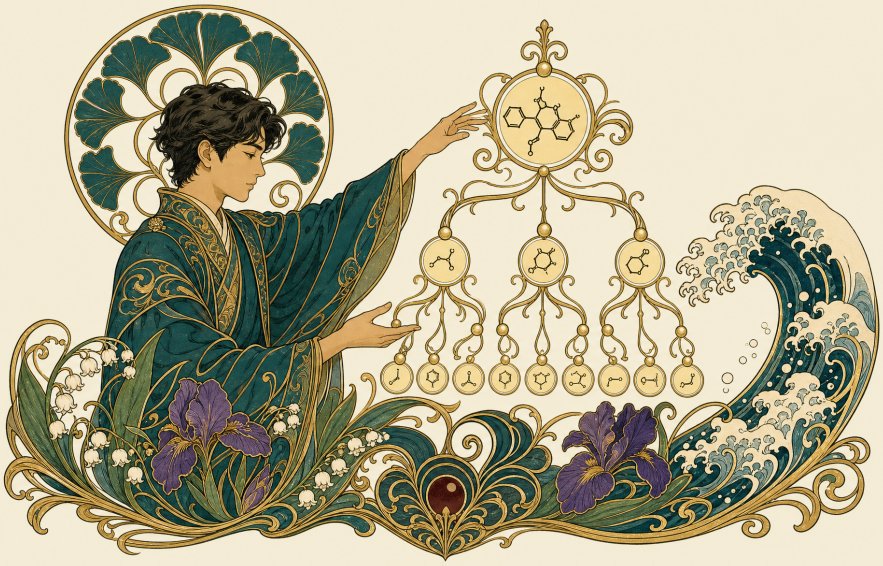
15:00–15:15 Active Learning Interatomic Potentials-Enhanced Molecular Dynamics for Grain Boundary Engineering in Antiperovskite Solid Electrolytes
Haobo Li

15:15–15:30 Autonomous Discovery of High-performance Ni–Mo Electrocatalysts for Green Hydrogen Production
Paolo Vincenzo Freiesleben de Blasio

15:30–15:45 Large Language Model Assisted Optimisation of Photocatalytic Hydrogen Production
Qi Jie Yeow

15:45–16:00 A reinforcement learning approach to generate equivalent circuit models for Electrochemical Impedance Spectroscopy
Yonatan Kurniawan

16:00–16:15 Benchmarking Foundation Potentials against Quantum Chemistry Methods for Predicting Molecular Redox Potentials
Yicheng Chen



AI for Medicine and Healthcare

MORRISON

AI for Healthcare, Therapeutics, and Clinical Decision Support

CHAIR Luis Camuñas-Mesa

14:45–15:00 Accelerating Biological Discovery Through AI, Robotics, and Human Organ Mimicry
Yimu Zhao

15:00–15:15 Inferring Oocyte Cytoplasmic Material Properties from Cytoplasmic Streaming Movies Using Physics-Informed Neural Networks
Alokendra Ghosh

15:15–15:30 Inferring the hidden and long-range dengue transmission routes in Singapore
Zhen Yuan Yeo

15:30–15:45 Event driven neural network on a mixed signal neuromorphic processor for detecting EEG based epileptic seizure
Giacomo Indiveri

15:45–16:00 Conceptualising Case Formulation as a Neurosymbolic AI Framework for Mental Health
Poorva Pandya

16:00–16:15 The Cognitive Clinical OS: Architecting Asynchronous Agentic Reasoning for Real-Time Decision Support
Malik Saif



ML Algorithmic Advances

HULLET

Neural Dynamics and Theoretical Deep Learning

CHAIR Carlo Vittorio Cannistraci

14:45–15:00 Thermodynamical Analogies in Deep Learning
Dmitry Vetrov

15:00–15:15 Towards Critical Branching Mechanism in Recurrent Neural Networks
Feixiang Ren

15:15–15:30 Order-chaos transition in deep neural network and its application to the training process
Ling Feng

15:30–15:45 Scalable learning of macroscopic stochastic dynamics
Mengyi Chen

15:45–16:00 Learning non-equilibrium mesoscopic dynamics with Onsager principle
Zhuoyuan Li

16:00–16:15 Learning Permutation-invariant Macroscopic Dynamics
Zhichao Han



16:15 – 16:45 TEA BREAK



AI for Materials Science

OLIVIA

AI for Materials Discovery and Property Prediction

CHAIR Seunghwa Ryu

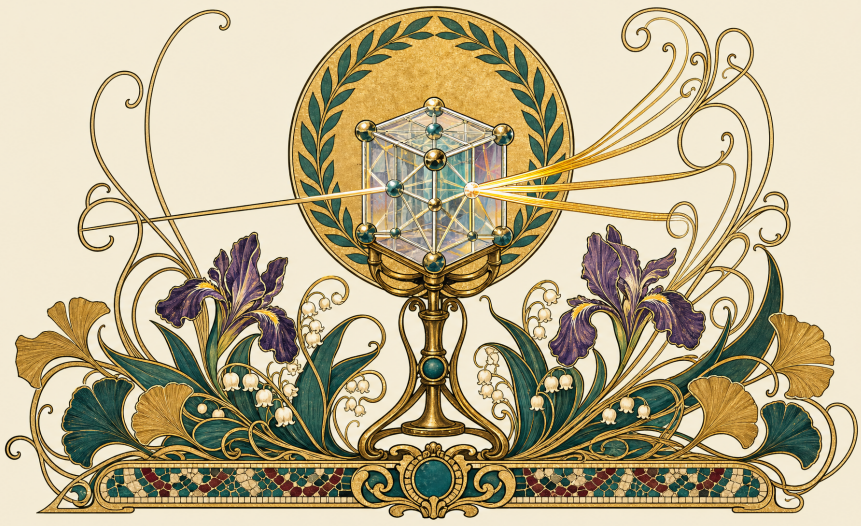
16:45–17:00 Machine Learning for 3D Printed Soft Robotics and Intelligent Systems
Yeong Wai Yee

17:00–17:15 A Multimodal Conditional JEPA for Composite Materials
Hangwei Qian

17:15–17:30 Test-Time Self-Evolution in Multi-Agent Systems for Materials Discovery
Bo Hu

17:30–17:45 Data-Driven Property Prediction for Memristor Resistive Switching Layers
Ben Rowlinson

17:45–18:00 EMOS: The Unified AI Platform for Electronic Materials Discovery
Atish Dixit



Self-Driving Labs

SOPHIA

Closed-Loop Autonomous Labs for Chemistry and Materials Discovery

CHAIR Shoichi Matsuda

16:45–17:00 Closed-Loop autonomous discovery of functional membranes and 2D Materials for resource recovery and energy applications
Daria Andreeva

17:00–17:15 Closed-loop Optimization of Mono-functionalization via Suzuki-Miyaura Reaction
Yuuya Nagata

17:15–17:30 Flow Chemistry as a Platform for Experimental Multi-objective Optimization of Heterogeneous Polymer Synthesis
Nicholas Warren

17:30–17:45 NIMO: Universal Middleware for Closed-Loop Materials Exploration
Ryo Tamura

17:45–18:00 MCP-Enabled LLM Agents for Closed-Loop Optimization in Real-Time Physical Experiments
Jiaen Yee; Hong Zhao Tan; DANNY Zekun Ren



AI for Society

MOOR

Responsible AI, Cultural Alignment, and Social Trust

CHAIR Truyen Tran

16:45–17:00 Beyond Alignment: Grounding AI in Society
Nancy F. Chen

17:00–17:15 Exploring Social Trust in AI
Sulfikar Amir

17:15–17:30 Align AI to our Aspirations, not our Flaws
Nikita Kazeev

17:30–17:45 Ethical Nail Salons: A community-governed and SDL-facilitated approach to mitigate occupational chemical hazards in nail salons
Reena Shadaan

17:45–18:00 AI & Culture Alignment: Interpretation over Measurement
Eric J. W. Orlowski



AI for Physics

MORRISON

Symmetry-Aware AI for Materials and Physics

CHAIR Shyue Ping Ong

16:45–17:00 Quantum Interactions in Materials: a New Frontier for AI
Marco Bernardi

17:00–17:15 Generative modeling and tensor-network
Yuehaw Khoo

17:15–17:30 Symmetry-Aware Deep Learning for Generalizable STEM Phase Classification
Jiadong Dan

17:30–17:45 Mapping diverse structures of liquid water and ice using variational autoencoders: A vector quantization approach to discover structural motifs in model latent spaces
Yue Yifei

17:45–18:00 VLM4Physics: Equation Discovery Using Multi-modal Inputs
Qianshu Ye



Unconventional Computing

HULLET

AI-Driven Unconventional Computing Hardware

CHAIR Giacomo Indiveri

16:45–17:00 CMOS-Integrated Silicon-Oxide Memristors: Reliability Characterization, SPICE-Based Circuit Simulation and potential application in neuromorphic computing
Fernando Aguirre

17:00–17:15 LLM-Powered Autonomous Agents for Spintronic Device Optimization: From Rule-Based to AI-Driven Design
Santhosh Sivasubramani

17:15–17:30 Design Methodologies for Skyrmion-Based Circuits and Systems in AI-Driven Applications: Bi-Directional Integration
Santhosh Sivasubramani

17:30–17:45 Ultra-low-energy skyrmion-based learning automata element for adaptive edge intelligence
Santhosh Sivasubramani

17:45–18:00 Spectrum-Aware Quantum Control beyond Classical Spectral Access
Jianlong Lu



DAY 3

THURSDAY, JUNE 18

EARLY MORNING

09:00 – 10:30

CHAIR Melodie Christensen

09:00–09:30 General-purpose AI systems from Google DeepMind designed to accelerate scientific discovery and democratize medical expertise
Vivek Natarajan ✶ *AI Agents and LLMs for Science*

09:30–09:45 New Frontiers in Machine Learned Quantum Chemistry
Ray Meng Gao ✶ *AI for Chemistry*

09:45–10:00 Let them learn: AI models that master materials physics
Michele Ceriotti ✶ *AI for Materials Science*

10:00–10:15 AI-Driven Scaffolding of Open-ended Movement Exploration
Ryutaro Uchiyama ✶ *AI for Biology*

10:15–10:30 The New Scientific Method: Taste, Truth, and Thinking with AI
Truyen Tran ✶ *AI Agents and LLMs for Science*

10:30 – 11:00 TEA BREAK

LATE MORNING

11:00 – 12:30

CHAIR Beatrice Soh

11:00–11:30 Can robots help us redefine chemical reactions?
Bartosz Grzybowski ✶ *AI for Chemistry*

11:30–11:45 **Polymer Biomaterials in a Self-Driving Lab**
Adam Gormley ✶ *Self-Driving Labs*

11:45–12:00 **Physics, Scaling and Data in Foundation Potentials**
Shyue Ping Ong ✶ *AI for Materials Science*

12:00–12:30 **When the Algorithms Take Over: AI for Experiment Planning and Control**
Karsten Reuter ✶ *AI for Chemistry*

❖ 12:30 – 14:45 POSTER SESSION #2 / LUNCH ❖



AI FOR MATERIALS SCIENCE

OLIVIA

Machine Learning for Materials Discovery and Properties Prediction

CHAIR Artem Maevskiy

14:45–15:00 A Disorder-Aware Multi-fidelity Framework for Robust Prediction of Superconducting Critical Temperature
Linh La

15:00–15:15 Graph learning metallic glass discovery from Wikipedia
Yuanchao Hu

15:15–15:30 Machine learning reveals transferable rules for predicting grain boundary segregation
Jingbei Bai

15:30–15:45 Atomic-Level Interpretable Multimodal Graph Neural Network for Predicting Carbon Capture in Metal-Organic Frameworks
Guangcun Shan

15:45–16:00 Discovery of Sustainable Refrigerants through Physics-Informed RL Fine-Tuning of Sequence Models
Adrien Goldszal

16:00–16:15 CSX Framework for Synthesis-Oriented Generative Materials Discovery
Shuya Yamazaki



Self-Driving Labs

SOPHIA

Autonomous labs for chemistry and materials discovery

CHAIR Han Hao

14:45–15:00 Toward Safe Autonomy in Self-Driving Laboratories
Leong Shi Xuan

15:00–15:15 Add, Mix, Heat, Filter - Repeat, Repeat, Repeat
Christopher Hassam

15:15–15:30 A Self-Driving Lab for Novel Energy Material Discovery
Hugo Kvanta

15:30–15:45 Combining robotic deposition tools and advanced characterization to enable ML-guided material discovery
Tim Kodalle

15:45–16:00 Printing kinetic data and microkinetic models in an automated lab
Linden Schrecker

16:00–16:15 An End-to-end, Autonomous Platform for Liquid-liquid Extraction Optimization
Maria Politi



AI for Chemistry

MOOR

AI for Chemical Reaction Prediction and Quantum Chemistry

CHAIR Benjamin Chen

14:45–15:00 Learning Arrow Pushing for Reaction Space Prediction and Exploration
Kye Sung Park

15:00–15:15 Hybrid Computational Strategy for Predicting Complex Ligand–Metal Architectures
Galymzhan Moldagulov

15:15–15:30 Predictive mass spectrometry from quantum-mechanical fragmentation and intensity modelling
Victor Posligua

15:30–15:45 ReactionEye: Integrating GC–MS Data and Chemical Context for Multimodal Structure Elucidation in Reaction Screening
Maik Gabriel Niedziella

15:45–16:00 Towards Data-Driven Nonlocal Density Functionals: Deep Learning DFT with Attention to approach Chemical Accuracy
Alexander Ryabov

16:00–16:15 Nanostructured Material Design via a Retrieval-Augmented Generation (RAG) Approach: Bridging Laboratory Practice and Scientific Literature
Ekaterina Skorb



AI for Biology

MORRISON

Foundation models and LLMs for biology, molecules, and materials

CHAIR Yimu Zhao

14:45–15:00 Molecular Foundation Models: from Pretraining-Finetuning to LLMs
Yatao Bian

15:00–15:15 Instructing a Chatbot to Design Nucleic Acid Probes for Diagnostics
Hongmin Chen

15:15–15:30 Local-Global Associative Frames for Symmetry-Preserving Crystal Structure Modeling
Wanyu Lin; Haowei Hua

15:30–15:45 Bridging LLM-based planning and workflow languages for automated, validated, scalable exploration of scRNA-seq analyses
Yoshinori Hayakawa

15:45–16:00 From Molecules to Materials and Proteins: Flow Autoencoders as Lossless and Unified Tokenizers
yuxuan Ren

16:00–16:15 Latent World Models of Cell Painting Data for In Silico Phenotypic Screening
Junhan Wang



AI for Earth Science

HULLET

AI for Earth System Modeling and Climate Forecasting

CHAIR Tapio Schneider

14:45–15:00 NVIDIA Earth-2 and Generative AI for Climate and Weather
Jeff Adie

15:00–15:15 Hybrid Physics-AI Digital Twins of the Earth System
Gianmarco Mengaldo

15:15–15:30 From Global to Local: AI-based Climate Downscaling for Southeast Asia
Juntao Yang

15:30–15:45 Synthetic Geology: Structural Geology Meets Deep Learning
George Turkiyyah

15:45–16:00 Physics-informed Deep Operator Networks for Real-Time Spatiotemporal Monitoring of Indoor Air Quality
Nguyen Minh

16:00–16:15 AI-Enabled 3D Glare Assessment Framework for Urban Solar Planning
Huixuan Sun



16:15 – 16:45 TEA BREAK



ML Algorithmic Advances

OLIVIA

Physics-Informed AI and Scientific Computing

CHAIR Eun-Ah Kim

16:45–17:00 Neural network methods for non-smooth PDE-constrained optimization
Yongcun Song

17:00–17:15 NeCLO: Neural Convolutional Learning Optimizer for Electromagnetics
Yueming Lyu

17:15–17:30 AI for Plasma Diagnostics in Laboratory Astrophysics: Reconstructing Invisible Fields from Proton Images
Chun-Sung Jao

17:30–17:45 SPONSOR Quantum AI
Nagendra Nagaraja, QpiAI India

17:45–18:00 Transformers with Physics-informed encodings and Simulation-Based inference for robust Gravitational-Wave detection in Pulsar Timing Array data
Subhajit Dandapat

AI for Materials Science

SOPHIA

AI-Driven Materials Discovery and Agentic Workflows

CHAIR Santiago Miret

16:45–17:00 Building a Decision-Driven Materials Discovery Institute: Early Insights from MDRI
Stuart Miller

17:00–17:15 CatMaster: An Agentic Autonomous System for Computational Heterogeneous Catalysis Research
Honghao Chen

17:15–17:30 Exploration and simulation of emergent magnetic materials via AI-driven workflows
Dorye Luis Esteras

17:30–17:45 Materealize: a multi-agent deliberation system for end-to-end material design and synthesis
Jaehwan Choi

17:45–18:00 SemiMat: A Semi-Supervised Toolkit for Data-Scarce Materials Property Prediction
Yizhe Chen



Self-Driving Labs

MOOR

Self-Driving Labs for Materials and Chemical Discovery

CHAIR Owen Melville

16:45–17:00 Towards in silico prediction of solid-state material synthesizability
Peichen Zhong

17:00–17:15 Beyond Point Sampling: Autonomous Phase Mapping of Biologic Formulation Stability via Hierarchical and Manifold Active Learning
Kiran Vaddi

17:15–17:30 Self-Driving Labs for Nanomaterials Development for Energy Applications: Syn-thesis, Dispersion, and Composite Forming
Shun Muroga

17:30–17:45 An Autonomous Discovery Platform for Inorganic Photovoltaic Absorbers Beyond Lead Halide Perovskites
Udo Bach

17:45–18:00 E-MAP – A Self Driving Lab for Solution Based Combinatorial Semiconductor Discovery
Holger RöHM



AI for Materials Science

MORRISON

AI for Chemistry and Materials Discovery

CHAIR Karsten Reuter

16:45–17:00 Accelerating AI-Powered Chemistry and Materials Science Simulations with NVIDIA ALCHEMI Toolkit
Wen Jie Ong

17:00–17:15 AdsorbFlow: energy-conditioned flow matching enables fast and realistic adsorbate placement
Jiangjie Qiu

17:15–17:30 SPONSOR Toward GPU-Native Electronic Structure Calculations
Jiaqi Zheng, SEA Garena

17:30–17:45 SPONSOR Ultrafast Spectroscopy Meets Data-Driven Materials Discovery at the Institut Courtois, Université de Montréal
Delphine Bouilly, Institut Courtois, Université de Montreal

17:45–18:00 The Open Catalyst 2025 (OC25) Dataset and Models for Solid-Liquid Interfaces
Nitish Govindarajan



AI for Chemistry

HULLET

AI for Chemistry: Molecular Design, Reaction Prediction, and Autonomous Synthesis

CHAIR Yanwei Lum

16:45–17:00 CatPlat: A Physics-Grounded Data Engine for AI-Driven Materials Discovery
Benjamin Chen

17:00–17:15 SynTwins: A Retrosynthesis-Guided Framework for Synthesizable Molecular Analog Generation
Shuan Chen

17:15–17:30 Yield Prediction of Organic Reactions in Biased Datasets via Positive-Unlabeled Learning
Jan Christopher Spies

17:30–17:45 Generative Design and Experimental Validation of Non-Fullerene Acceptors for Photovoltaics
Balamurugan Ramalingam

17:45–18:00 Adaptive Human-in-the-Loop Optimization Using Language-Guided Priors for Chemical Synthesis
Amirreza Mottafegh



20:00 – 22:00 CONFERENCE DINNER

Flower Field Hall, Gardens by the Bay, 18 Marina Gardens Dr, Singapore 018953



DAY 4

FRIDAY, JUNE 19

EARLY MORNING

09:00 – 10:30

CHAIR Simon Billinge

09:00–09:30 Can we build an AI Climate Scientist?
Torsten Hoefler ✶ *AI for Earth Science*

09:30–09:45 Beyond the Proof of Concept: Autonomous Electrocatalyst Discovery Within Industrial Constraints
Alex Hammer ✶ *AI for Materials Science*

09:45–10:00 Orchestrating the Three-Body Problem of Machine Learning, Simulation, and Experiments in Materials Discovery
Felix Hanke ✶ *AI for Materials Science*

10:00–10:15 Why Experimental Data is the Next Frontier for AI x Materials
Artem Mishchenko ✶ *Self-Driving Labs*

10:15–10:30 Learning mesoscopic dynamics
Qianxiao Li ✶ *AI for Materials Science*

10:30 – 11:00 TEA BREAK

LATE MORNING

11:00 – 12:00

CHAIR Mohamad Moosavi

11:00–11:30 Data-Driven Materials Science for Energy-Sustainable Applications
Jacqueline Cole ✶ *AI for Materials Science*

11:30–11:45 **AI-driven discovery of nanoporous materials**
Berend Smit ✶ *AI for Materials Science*

11:45–12:00 **Surviving the Transition: Doing Science in an Age of AI Accelerated Discovery**
Steinn Sigurdsson ✶ *AI Agents and LLMs for Science*

12:00 – 12:15 BREAK

MIDDAY

12:15 – 13:15

CHAIR Gavin Koon

12:15–12:45 **Brain-inspired sparse network science for next generation efficient and sustainable AI**
Carlo Vittorio Cannistraci ✶ *Unconventional Computing*

12:45–13:00 **First Principles, Fast Algorithms: The Physics-AI Synthesis in Earth System Modeling**
Tapio Schneider ✶ *AI for Earth Science*

13:00–13:15 **AI4X Rising Star Awardee Presentation**
AI4X Organizers

13:15 – 14:45 LUNCH

AI for Materials Science

OLIVIA

Machine Learning for Materials Discovery and Design

CHAIR **Sonia Azimi Dijvejin**

14:45–15:00 Physics-Informed AI for Inference and Design under Data Scarcity
Seunghwa Ryu

15:00–15:15 Machine Learning-Assisted Search for Skyrmion-Hosting Heterostructures for Device Applications
Sergey Grebenchuk

15:15–15:30 High-throughput ML Screening of Doped Cathode Active Materials
Mathilde Franckel

15:30–15:45 Discovery of flat-band 2D materials via physics-informed scoring and structure-based learning
Xiangwen Wang

15:45–16:00 Materials informatics framework for accelerated discovery of high-refractive-index 2D materials
Liudmila Klimova

16:00–16:15 Beyond Known Archetypes: A Generative AI Framework for Inverse Design of Flat-Band Materials from Geometric Outliers
Yihao Wei



AI for Materials Science

SOPHIA

Machine Learning for Materials and Interatomic Potentials

CHAIR Wen Jie Ong

14:45–15:00 When Machine Learning Force Fields Fail Expectations: Lessons We Learned from Solid Electrolyte Materials
Yizhou Zhu

15:00–15:15 Learning Nonlinear Dissolution Trajectories in Binary Polymer–Solvent Systems
Zheng Jie Liew

15:15–15:30 Atomic Sudoku: Stochastic approaches for correlated disorder materials
Andy Paul Chen

15:30–15:45 Platonic representation of foundation machine learning interatomic potentials
Zhenzhu Li

15:45–16:00 The Zintl–Klemm Concept in the Amorphous State: A Case Study of Na–P Battery Anodes
Litong Wu

16:00–16:15 Importance of Electronic Entropy for Machine Learning Interatomic Potentials
Martin Hoffmann Petersen



Self-Driving Labs

MOOR

Autonomous Discovery in Chemistry and Materials

CHAIR Felix Hanke

14:45–15:00 Polymer Discovery through Modular Chemistry Plus Modular Automation
Keith A. Brown

15:00–15:15 Autonomous nanoparticle synthesis by design
Andy Anker

15:15–15:30 Kinetic study of the aqueous Kolbe-Schmitt reaction enabled by automated reaction analysis
Muye Xiao

15:30–15:45 Deciphering the operando mechanism of Haber-Bosch process
Yuanyuan Zhou

15:45–16:00 A Data-driven Closed-looped High-throughput Platform for Thermocatalyst Discovery
Zhengzuo Liu

16:00–16:15 Development of a Platform for Sustainable Metal-Organic Framework (MOF) Synthesis, MABIL: MOF Automation using Biomass-Inspired Linkers
Ailsa Edward



AI for Medicine and Healthcare

MORRISON

AI for Drug Discovery, Pharma Development, and Clinical Data

CHAIR Nasim Abdollahi

14:45–15:00 Advancing Pharmaceutical Development Through AI/ML-Enabled Experimental Design
Melodie Christensen

15:00–15:15 MIRA: Medical Time Series Foundation Model for Real-World Health Data
Viktor Schlegel

15:15–15:30 From In Silico Design to Automated Synthesis: An AI-Driven Framework for Late-Stage Functionalization
Lyubomir Kotopanov

15:30–15:45 Agentic AI–Enabled Integration of a Hybrid System of Predictive Models for Accelerated Direct-Compression Drug Product Development
Theo Tait

15:45–16:00 From Model to Molecule: Rapid Discovery of Potent CDK2 Inhibitors Using Boltz-2
Sven Papidocha

16:00–16:15 A machine learning workflow to accelerate the design of in vitro release tests from liposomes
Daniel Yanes



AI for Society

HULLET

Autonomous Discovery and Society: Geopolitics, Security, and Decentralized Scientific Swarms

CHAIR Kourosh Darvish

14:45–15:00 The Geopolitics of AI Driven Scientific Discovery: Uneven Geographies of Self Driving Laboratories
Julian Prieto

15:00–15:15 Self Driving Discovery of Immersion Cooling Fluids for Data Center
Maryam Ebrahimiazar

15:15–15:30 Defending Federated Learning: Adaptive Integration of Differential Privacy, SMPC, and Byzantine Robustness
Syed Momin Naqvi

15:30–15:45 The Economy of Reasoning: Incentivizing Epistemic Diversity in Decentralized Scientific Swarms
Minh Tri Nguyen

15:45–16:00 Securing Autonomous Chemical Robots Through Physical and Digital Containment
Dean Thomas

16:00–16:15 Edge-AI Driven Automation for Scalable E-Waste Recycling
David T T Tran; Ernest E Y Chan



16:15 – 16:45 TEA BREAK



AI FOR MATERIALS SCIENCE

OLIVIA

AI for Materials Discovery and Property Prediction

CHAIR Alex Hammer

16:45–17:00 Simulation at GPU Speed: Reimagining Atomistic Simulation at Scale with NVIDIA ALCHEMI
Atul Thakur

17:00–17:15 Best Poster: Computational Investigation and Generation of Site-Disordered Sodium Ion Cathode Materials
Martin Hoffmann Petersen

17:15–17:30 LeMat-GenBench: A Unified Evaluation Framework for Crystal Generative Models
Nikita Kazeev

17:30–17:45 Using Time-Series Forecasting to Accelerate Materials Stability Assessments
Manuel Kober-Czerny

17:45–18:00 Symmetry-Aware Equivariant Network for Discovering SHG-Active Materials
Ivan Trofimov



Self-Driving Labs

SOPHIA

Autonomous and Self-Driving Laboratory Systems

CHAIR Artem Mishchenko

16:45–17:00 A digital twin for sim-to-real chemistry lab automation
Kourosh Darvish

17:00–17:15 A Standard Physical Environment for Benchmarking AI-driven Cell Biology
Yang Choo

17:15–17:30 MiST: Understanding the Role of Mid-Stage Scientific Training in Developing Chemical Reasoning Models
Tong Xie

17:30–17:45 Democratizing Discovery: Ultra-Low-Cost Self-Driving Laboratories for Materials Science
Sayan Doloi

17:45–18:00 Automated High Throughput Optimization for Halide Perovskite Memristors
Shreyas Pethe



AI for Biology

MOOR

AI for proteins, genetic circuits, and cellular biophysics

CHAIR Yongcun Song

16:45–17:00 AFPFusionLM: A Hybrid Sequence–Structure Protein Language Model for Antifreeze Protein Function Prediction
Yijun Li

17:00–17:15 Multi-objective optimization for designing structurally similar proteins with dissimilar sequences
Ryo Akiba

17:15–17:30 End-to-end neural reconstruction of DNA structures from single-frame fluorescence images
Fushuai Wang

17:30–17:45 Better Protein Function Prediction by Modeling Survivorship Bias
Poompol Buathong

17:45–18:00 Risk-averse optimization of genetic circuits under uncertainty
Michal Kobiela



AI Agents and LLMs for Science

MORRISON

LLMs, reasoning, and applied AI across education, finance, and modeling

CHAIR Aruhan Rui Shi

16:45–17:00 Modeling and Computation in the Space of Language: Symbolic and LLM-Based Approaches
Haizhao Yang

17:00–17:15 PieLoT — LLM-driven Toolbox for Theorem Proving Education
Qixiang Zhang

17:15–17:30 BRIDGE: Bootstrapping Text to Control Time-Series Generation via Multi-Agent Iterative Optimization and Diffusion Modeling
Viktor Schlegel

17:30–17:45 Beyond Semantic Similarity: A Two-Phase Non-Parametric Retrieval Workflow for Corporate Credit Underwriting
Linus Ng

17:45–18:00 ESS-MOTIFS: Discovering Rubric-Aligned Motifs for Cohort-Level Essay Assessment
Thi Ngoc Nguyen



AI for Physics

HULLET

AI for Quantum Materials and Electronic Structure

CHAIR Qianxiao Li

16:45–17:00 Characterizing electronic and structural states of materials with ML
Simon Billinge

17:00–17:15 $2k_F$ instability and chiral spin density wave at the 1/9 magnetization plateau in the kagome antiferromagnets
Tanja Duric

17:15–17:30 HSG-12M: A Large-Scale Benchmark of Spatial Multigraphs from the Energy Spectra of Non-Hermitian Crystals
Xianquan Yan

17:30–17:45 SPONSOR Flow-Distorted Plane Waves
Zekun Shi, SEA Garena

17:45–18:00 Global Plane Waves From Local Gaussians: Periodic Charge Densities in a Blink
Jonas Elsborg



APPENDIX

POSTER SESSIONS

173 accepted posters, grouped by research area

AI FOR CHEMISTRY — 19 POSTERS

№	TITLE	PRESENTER
16	Improving the univariate calibration approach with Bayesian modeling for IR reaction monitoring	*Jiayu Zhang*
43	Selective and Sustainable Oxidation of Allyl Alcohol in Water Using a TS-1 Catalyst in Continuous Flow: A Machine-Learning-Driven Approach	*Riko I Made*
44	Eliminating Cryogenic Constraints in Ipsenol Synthesis through Real-Time Reaction Landscape Mapping	*Charlotte Smith*
114	Impact of explicit long-range interactions on the accuracy of machine learning interatomic potentials in modeling molecular liquids	*Olga Chalykh*
153	BigSolDB 2.0, dataset of solubility values for organic compounds in different solvents at various temperatures	*Marina Kiseleva*
184	GoFlow: efficient transition state geometry prediction with flow matching and E(3)-equivariant neural networks	*Leonard Galustian*
198	iGRASP: A Modular Platform for Improved, Graph-Based Spectra Prediction	*Nick Wierich*
205	Future-Proofing Data for Catalyst Fingerprinting and Better Design Validation	*Wesley McNutt*
212	ChemSIE: From Document Based Records to Machine Actionable Experimental Data	*Itamar Wallwater*
271	An automatically generated reaction network for the synthesis of hBN using the Molecular High-Index Saddle Dynamics Search method	*Vitalii Sagan*
282	Multi-fidelity Bayesian optimisation for DFT-in-the-loop discovery of manufacturable homogeneous catalysts, auxiliaries, and ligands.	*Yong Lee*
288	Beyond Greedy Acquisition: A Distribution-Aware Active Learning Framework for Molecular Discovery	*Ruixuan Chen*
290	A Flexible, Code-Free, and Scalable Workflow for Structured Data Extraction from CO_2 Electrochemical Reduction Literature	*Haiwen Dai*
327	Smarter Electrolysis in Rock Reactors	*Joseph Chiong*

№	TITLE	PRESENTER
349	Automated Process Synthesis via Generative AI-based Dual-Loop Simulation and Optimization	*Yeong Woo Son*
353	Evaluating Chemistry-Guided Filtering Heuristics Using LLM-Extracted Reaction SMILES	*Chaewon Lee*
380	Predicting mechanisms and outcomes of complex radical cascades via a hybrid, network-QM-AI approach	*Kangjie Lin*
443	AI-Assisted Reaction Network and Catalyst Exploration for CO_2 Conversion	*Mikhail Polynski*
452	DPA4: A Generalist Foundation Model for the Era of On-Demand Interatomic Potentials	*Tiancheng Li*

AI FOR MATERIALS SCIENCE — 55 POSTERS

№	TITLE	PRESENTER
9	AI-driven computational workflows for scalable innovative materials design	*Stephan Roche*
27	LapidaryEngine: Feedback-Guided Iterative Text-to-Crystal Structure Generation	*Yusei Ito*
45	Identification of MOFs with Unique Pore Shapes Using Computer Vision	*Saad Aldin Mohamed*
47	aLLoyM: A Large Language Model for Alloy Phase Diagram Prediction	*Yuna Oikawa*
54	Unveiling Process–Structure–Property Coupling in CNT Fibers via Multimodal AI Analytics	*Daisuke Kimura*
59	Space-Group Identification from Multi-Phase Powder XRD via Latent Phase Modeling	*Tomoya Murata*
65	Deep Learning of Accurate Force Field of $Hf_xSi_{1-x}O_2$	*Yingtao Yang*
76	Machine learning analysis of literature dataset on the CO2 reduction toward prediction of high activity multi-elemental catalysts	*Umi Shin*
78	A Unified Diffusion Framework for the End-to-End Generation of Symmetry-Constrained Complex Molecular Crystals	*Wendi Cai*
84	Large Language Models in Materials Science: Assessing RAG Evaluation Frameworks through graphene synthesis	*Zen Han Cho*
97	Automation of the Polishing-Etching Process in Metallographic Observation	*Daijiro Hashimoto*
100	A shortcut towards simulating millions of atoms using machine learning potentials	*Linh La*
106	A Multi-Modal Deep Learning Platform for Cross-Domain Property Prediction in Chemical Process Design	*Mikhail Tsitsvero*

№	TITLE	PRESENTER
108	Multi-task Attention for Doped Thermoelectric Properties Prediction	*Leng Ze Tang*
110	Generative Symmetry in Crystal Modelling	*Jianghai Wang*
112	Data-driven discovery of novel materials for smart optoelectronics	*Liudmila Klimova*
116	Crystalline phase projection and identification from high temperature diffractograms using graph neural networks	*Léonard Imbert*
142	An Accurate Deep Learning Force Field for Dielectric and Ferroelectric $Hf_xZr_{1-x}O_2$ Solid Solutions	*Zhe Su*
143	A Comparative Study of Molecular Dynamics Approaches for Simulating Ionic Conductivity in Solid Lithium Electrolytes.	*Dounia Shaaban Kabakibo*
169	AI-Enabled Development of Cooling Device for High-Power Electronics	*Vassilis Christophides*
178	Mapping Materials Science: a multi-modal toolbox to curate broad synthesis procedure databases from scientific literature	*Mathilde Franckel*
189	AtomWorld: A Benchmark for Evaluating Spatial Reasoning in Large Language Models on Crystalline Materials	*Alexander Chen*
191	An Autoregressive Approach For Material Generation	*Niklas Dobberstein*
194	Recent developments and applications of the machine-learned moment tensor potentials	*Nikita Rybin*
217	A topological equilibrated configuration space analysis of nanoparticle systems	*Alexandros Keros*
225	Accurate and rapid measurement of fluid thermal conductivity	*Mohammad Zargartalebi*
229	Generalized convolutional many-body distribution functional representations	*Anatole Von Lilienfeld*
239	Toward Self-Driven Microscopy Exploration for the Characterization of Functional Materials	*Claudia Bazan*
249	Machine Learning-Based Surrogate Models for Performance Prediction of Triboelectric Nanogenerators	*Shashank Mishra*
261	SWORD: A compositional disorder-aware crystal representation for cross-dataset curation and disordered novelty assessment	*Yuayo Huang*
263	Computational investigation and generation of site-disordered sodium ion cathode materials	*Martin Hoffmann Petersen*
272	EGMOF: Efficient Generation of Metal-Organic Frameworks Using a Hybrid Diffusion- Transformer Architecture	*Yeonghun Kang*
278	Application of digitization and large language models for digital twins in permanent magnet materials	*Hongbin Zhang*
285	MatSeek: An Automated Knowledge-Driven Framework for Materials Research	*Huang Jianguo*

№	TITLE	PRESENTER
296	Rapid, Room Temperature Synthesis of a Biomass-Derived, Recyclable Copper Metal-Organic Framework Utilizing Automation for CO_2 Capture	*Daniel Davidson*
321	Using genetic algorithms to explore compositional space of perovskite thin film	*Jérôme Gautier*
332	Anomalyspy: A Generative Defect Localization in Semiconductor Packages, with X-Ray Microscopy	*Pawan Kumar*
348	Predictive Modeling for Quantitative Compositional Engineering of InZnHfO Thin-Film Transistors	*Jiho Lee*
351	Machine Learning-Based Optimization of SOC Windows for High-Performance μ-Si Anodes	*Taehoon Choi*
352	Quantum Annealing-Driven Active Learning Benchmark for Nanophotonic Design	*Serang Jung*
358	Model–Data Coevolution as the Basis of Stateful, Problem-Scoped Materials Databases	*Fengyu Xie*
360	Literature-Grounded LLMs for Predicting High Ionic Conductivity Solid-State Electrolytes	*Kunik Jang*
375	Expanding catalyst discovery across material classes by machine learning	*Junseok Moon*
376	An Explainable Conversational AI Framework for the Discovery of Cobalt Electrocatalysts in Industrial Water Electrolysis	*Jongyeop Baek*
379	Simulation-to-Experiment Transfer Learning for XRD-Based Autoencoder Modeling of SOEC Half-Cell Materials	*Hunmin Park*
381	TropicalField-Tandem: Physics-Informed Indoor→Outdoor Translation and Uncertainty-Aware Forecasting for Perovskite–Si Tandem Reliability	*Romika Sharma*
385	Label-Efficient Battery SOH Estimation via Domain-Aware Self-Supervised Learning	*Ji Young Yun*
387	Accelerating Catalyst Design via AI: High-Throughput Screening and Machine Learning Reveal Defect-Enhanced Activity in Pt-Au Nanoclusters	*Ilia Chepkasov*
388	AI-Assisted Architected Cementitious Microstructures for Durable and Low-Carbon Infrastructure	*Abhimanyu Goel*
393	MOFology: Ontologically-Grounded MOF Knowledge Graph and Prediction Framework	*Matthew Hart*
407	3D Microstructure Reconstruction of X70 Pipeline Steel from 2D EBSD Data Using SliceGAN	*Joonas Lahikainen*
415	Multiscale modeling of resistive switching in two-dimensional heterostructures	*Vitalii Kapitan*
435	A Hybrid Physics-Driven Neural Network Force Field for Liquid Electrolytes	*Junmin Chen*

№	TITLE	PRESENTER
441	Motif-driven scalable design of rutile multi-cation rutile oxides for oxygen evolution reaction	*Yiwen Yao*
444	LLM-Guided High-Throughput Discovery of Antifreeze Electrolytes Enabling −50 °C Stability and 99.5% Coulombic Efficiency	*Jing Jiang*

SELF-DRIVING LABS

44 POSTERS

№	TITLE	PRESENTER
39	Development of an automated system for ceramic powder process	*Daijiro Hashimoto; Woosuck Shin*
42	Dynamic Parameter Scanning: a Novel Method for Mechanistic Elucidation	*Dylan Pyle*
57	MaiML: A Common Data Format for Measurement and Analysis and Its Application to an Autonomous Experimental System	*Akira Aiba*
60	Robotic-arm-based self-driving laboratories powered by NIMO and IvoryOS	*Naruki Yoshikawa*
68	Affordable 3D Printed Automation for Self-Driving Laboratory: Expanding Access to High-Throughput Experimentation	*Sayan Doloi*
73	Autonomous Workflows and SHAP Interpretation of Deposition-Rates in Bipolar HiPIMS	*Manuel Kober-Czerny*
88	Automation of thermal ageing and tensile tests for adhesively bonded single lap joints	*Kazumasa Shimamoto*
118	On-the-fly reaction monitoring using correlated spectroscopies	*Jan GüNZL*
122	Electrochemical Feedback for Closed-Loop Facet Control in Pd Nanoparticles	*Shao Rong Choo*
157	ATLAS: accelerating materials discovery at Imperial College London	*Lana Lee*
190	Autonomous Search for Grinding Conditions using Robots and Bayesian Optimization	*Yuto Yotsumoto*
195	RAISE: A self-driving laboratory for interfacial property formulation discovery	*Aaron Clasky*
196	MicroMAP: A Material Acceleration Platform for the Synthesis of Organic Nanoparticle Dispersions	*Alexander Colsmann*
202	An automated gel screening platform	*Aaron Clasky*
203	Accelerating small organic molecules scale up with data-rich experimentation	*Ekaterina Trushina*
231	Challenging to formulation through autonomous experiments and consideration of digital twin framework application	*Kesaaki Minemura*

№	TITLE	PRESENTER
234	Towards Optimal Mixing: Enabling Autonomous Experimentation via Quantitative Emulsion Assessment	*Hitoha Sato*
244	Physical model-informed automated reaction optimization within a digital platform	*Shuyuan Zhang*
245	An Automated, Calibration-Free Platform for High-Throughput Reaction Screening and Data Analysis	*Manh Hung Tran*
267	DIY, Modular Automation Platform Built from Affordable Components for Directed Evolution and Molecular Biology, Toward Closed-Loop Workflows	*Takanori Uzawa*
275	Robotic Mechanochemical Synthesis of HKUST-1 with Process Monitoring	*Kazuki Ishizaki*
280	Scalable Low-Cost Laboratory Automation: A Digital Twin-Integrated Robotic Platform for Autonomous Liquid Handling	*Ali Shayesteh*
281	Bayesian optimization for self-driving liquid coating laboratory	*Jisoo Song*
286	A Provenance-First, AI-Ready Data Platform for Large-Scale Memristor Experiments	*Lai Gan*
292	Autonomous Discovery of Pareto-Optimal Gas-Diffusion Electrodes	*Zahra Azimi Dijvejin*
299	A low-cost, high-throughput solid dosing platform for self-driving laboratories	*Rui Zhang*
301	The Medicinal Chemistry Self-Driving Lab - Accelerating Hit Optimisation with a Direct to Biology Approach	*Stuart Green*
303	Robot-Enabled Biofabrication of Tissue Cultures with Micrometer-Scale Precision	*Daniel Hocevar*
305	Automated and Interpretable Experimental Platform for Process-Structure-Property Analysis via Raman Spectroscopy	*Takuya Miyajima*
306	Digitalizing Slurry Mixing for an Electrode Fabrication SDLs	*Jaehyun Oh*
307	Robotic Kneading for Organic Reactions: A Deterministic Platform for Data-Driven Synthesis in Semi-Solid Media	*Yuki Nishihori*
325	HELIOS - Holistic Experiment Learning Intelligent Orchestration System	*Sissi Feng*
326	Membrane Optimization for Electrochemical CO_2 Storage	*Jordan Rumscheidt*
336	Development of a Scalable High-Throughput Platform for Plasmid Transfection in 3D Mammalian Cell Culture	*Rosanna Jiang*
338	Reinforcement Learning to Increase Nuclear Fusion Efficiency	*Joseph Koh*
361	Accelerated Discovery and Characterization of Nanoscale-Covalent Organic Frameworks for Photocatalytic Water Splitting	*Ziheng Xiao*
373	Bayesian Optimization-Guided Experimental Design for Graphene-Reinforced Cementitious Composites	*Abhimanyu Goel*

№	TITLE	PRESENTER
391	LabDroid “Maholo”-Centered Automation and Autonomization of Life Science Experiments	*Akari Kato*
400	Audited Causal Discovery Agents for Brain Resilience and Alzheimer's Reversal	*David Scott Lewis*
402	PD-NCA AutoLab: Self-Organizing Neural Intelligence as a Testbed for Autonomous Science	*David Scott Lewis*
411	AI-Guided Optimization of EIS Measurements: Minimizing Low-Frequency Sampling for Data-Efficient Electrochemical Characterization	*Yonatan Kurniawan*
413	Transferable Impedance-Grounded Learning for Interfacial Degradation Across Energy Systems	*Hithesh Rai Purushothama*
434	Reinforcement Learning-Enabled Control of Single DNA Molecule Manipulation in Microfluidics	*Fuhai Zhou*
445	Accelerating Electrolyte Discovery via a Closed-Loop Physical AI Platform	*Vanesa Munoz Perales*

AI FOR EARTH SCIENCE — 8 POSTERS

№	TITLE	PRESENTER
50	Toward a Global SAR Foundation Model for SAR-to-Spectral-Indices Mapping	*Ziyi Song*
137	A Field-Deployable IoT-Edge-AI Framework for Landslide Prediction and Early Warning	*Amrita Joshi*
317	AI stretch-grid model for kilometre-scale weather prediction over deep tropics	*Ka Wing Chui*
340	AI in Life Cycle Assessment	*Alexei Lapkin*
342	Improving Value Chain Transparency in Bioprocess Life Cycle Assessment Using Surrogate Models	*Michail Vousvoukis*
378	Data-driven uncertainty-aware forecasting of sea ice conditions in the gulf of Ob based on satellite radar imagery	*Alexander Ryabov*
386	Dyna-STTN: Distilling Physical Dynamics into Spatio-Temporal Transformer Network for Weather Forecasting	*Jiafeiyang Dong*
395	Physics-informed local-global underground fluid flow modeling with multiple sinks	*Alexander Ryabov*

ML ALGORITHMIC ADVANCES — 7 POSTERS

№	TITLE	PRESENTER
15	A Modular and Interpretable Pipeline for Unsupervised Learning on Scientific Spatiotemporal Imaging Datasets	*Timothee Levilly*
117	Spectral Analysis of the Weighted Frobenius Objective	*Vladislav Trifonov*
186	From Visual Vocabulary to Grammar: An Interpretable Paradigm for Scientific Discovery in Spatiotemporal Data	*Zhen Yuan Yeo*
218	Sparse Global Mixing via Compact-Support Graph Kernels	*Himanshu Singh*
246	Electronic Circuit Optimization With Graph and Sheaf Neural Networks	*Eva Maria Hita Sogorb*
319	Scaling Multilingual E-Commerce with GenAI: Content Generation and Sentiment Analysis for Low-Resource Languages	*Kathakali Mitra / Harsh Khanna*
322	Conditional Diffusion for Storage Performance Modeling	*Aziz Temirkhanov*

AI AGENTS AND LLMS FOR SCIENCE — 10 POSTERS

№	TITLE	PRESENTER
14	A Multi-Agent LLM Framework with Hierarchical Citation Graph for Automated Survey Generation	*Duy Dung Le*
156	Beyond Statelessness: Engineering Subjective Cognition via Hierarchical Memory Consolidation and Tunable Agency	*Malik Saif*
210	A Multi-agent Framework for Physical Laws Discovery	*Bo Hu*
247	Black-box Membership Inference Attacks on Synthetic Text via N-gram Overlap	*Yidan Sun*
316	PERELMAN: Pipeline for scientific literature meta-analysis	*Daniil Sherki*
330	Quality-Diversity LLM for Generative Design	*Ariq Koh Boon Xiong*
389	When Designs Explain Themselves: Report Cards for Evolutionary LLMs	*Alex Siek*
390	IFC-QA: A Benchmark for Evaluating LLM Reliability over Industrial Building Information Model	*Anastasiia Volkova*
427	The Geometry of Reasoning Failure: Predicting Agent Errors from Semantic Scale Trajectories	*Andrey Ustyuzhanin*
432	MolViBench: Evaluating LLMs on Molecular Vibe Coding	*Jiatong Li*

AI FOR PHYSICS — 9 POSTERS

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30	Identifiable learning of dissipative dynamics	*Aiqing Zhu*
103	Learning to Image in Slepian-Pollack Basis – Achieving Super-resolution of Nanostructures	*Eng Aik Chan*
173	Divergence-Constrained Physics-Informed Neural Networks for Time-Domain Maxwell's Equations	*Zaifeng Yang*
223	OnsagerFlow: Learning mesoscopic dynamics from microscopic simulation	*Shiqi Wu*
256	Multi-Modal Classification of Extended 1D Cellular Automata	*Zhaoyun Chen*
276	Data-Driven Detection of Nonlinear Mode Interactions Using Post-Hoc Interpretable Deep Learning	*Bayan Abusalameh*
345	Partial-Physics Pretraining for Transfer-Learning in Computational Aerodynamics	*Benjamin Y. J. Wong*
399	Application of Automatic Differentiation and Optimization with PDE Constraints to Forward and Inverse Problems	*Alexander Ryabov*

AI FOR MEDICINE AND HEALTHCARE — 8 POSTERS

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5	Spatial Machine-Learning Prediction of Lung Function and Body Mass Index in Australian Cystic Fibrosis Patients	*Arul Earnest*
126	Post-PCI Cardiac Death Prediction via Synthetic Minority Augmentation and Stress-Tested Probability Quality	*Mikhail Lazarev*
248	A Connected Workflow to Streamline Tablet Manufacture and Dissolution Testing	*Maria Chang*
284	FHIR-Driven Medical Network Traffic Simulation for Multi-Departmental Healthcare Security Testing	*Miro Moffett*
367	ADMET Scoring Models for Real-World Drug Design	*Zihan Wang*
394	FedAdaPriv-CPU: Adaptive Differential Privacy with Frozen Backbone for Resource-Constrained Federated Medical Imaging	*Anusha Randhawa / Muhammad Hamza Zaman*
405	Toward TheraAgent: Evidence-Grounded, Self-Verifying AI for Oncology Treatment Recommendation	*Junhan Wang*
446	A Fairness Audit of Medical Imaging Foundation Models on a Multimodal Structured Clinical Benchmark	*Saketh Lingisetty*

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287	Single-Shot Phase Retrieval in Cryo–EM via Latent Conditional Diffusion Model	*xiaodong Yang*
347	Simulation-to-Real Alignment for Cryo-EM Image Modeling via Conditional GAN-Based Refinement	*Ziyue Jiang*
359	Flow-Matching-Based Posterior Sampling for Single-Shot Phase Retrieval in Cryo-EM	*Rongtao Zhang*
404	Evolving Robust Drug Candidates via Co-Evolutionary Artificial Life Simulators	*Junhan Wang*
425	Recent Progress in AI-Driven 3D (Bio)Printing for Tissue Engineering	*Mihaela-Raluca Dobrisan*
454	BioPrint-LKM: An evidence-grounded large knowledge model for bioprinting knowledge retrieval and parameter initialization	*Xi Huang*

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240	Democratizing Microscopy Training through Digital Surrogates	*Ali Shayesteh*
377	ZKBioVault: A Privacy-Preserving Biometric Authentication Framework for Fraud-Resilient Financial Identity Management	*Izza Sohail*
418	Impact of Disruptive Technologies on Value Creation and Capture: Comparing OTT and LLMs providers	*Maria Tsenzharik*

UNCONVENTIONAL COMPUTING — 2 POSTERS

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344	Chiropto-Neuromorphic Devices Based on a Photocatalytic Dye/Polymer Semiconductor Bulk Heterojunction for Circularly Polarized Light Detection and Memorization	*Boesung Kwon*
346	Enhancing Synaptic Plasticity and Multistate Retention of Organic Neuromorphic Devices Using Anion-Excessive Gel Electrolyte	*Jeongwoo Lee*