

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



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 <i>Chair: Shi Xuan Leong</i>				
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 <i>SPONSORED BY SEA GARENA</i>				
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 <i>Chair: Jacqueline Cole</i>				
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 <i>Chair: Kostya Novoselov</i>				
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 <i>SPONSORED BY JEOL ASIA PTE LTD</i>				
14:45 – 15:00	SELF-DRIVING LABS Bowen Li: AI-driven LNP design for mRNA delivery <i>Chair: Adam Gormley</i>	SELF-DRIVING LABS Beatrice Soh: Learning Stochastic Polymer Dynamics at the Single-Molecule Level with High-Throughput Experiments <i>Chair: Ulrich S. Schubert</i>	AI FOR CHEMISTRY Yanwei Lum: Physical Unified Device Architecture for AI-Assisted CO ₂ Electrocatalysis <i>Chair: Berend Smit</i>	AI AGENTS AND LLMS FOR SCIENCE Jennifer Dodgson: Negative Space Learning: Where Survival is the Only Reward <i>Chair: Tejs Vegge</i>	ML ALGORITHMIC ADVANCES Luis Camuñas-Mesa: Neuromorphic Systems: Towards Sustainable AI <i>Chair: Willi Gottstein</i>
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 Optimization of the Aldol Reaction	Ivan Kruglov; Liudmila Klimova: Diffusion-Driven Generation of Novel Crystal-line 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 <i>Chair: Victor Postigua</i>	SELF-DRIVING LABS Shoichi Matsuda: Data-Driven Materials Discovery for Rechargeable Batteries: High-Throughput Experimental Platforms and Closed-Loop Autonomous Optimization <i>Chair: Keith A. Brown</i>	AI AGENTS AND LLMs FOR SCIENCE Santiago Miret: How Autonomous Labs & AI Are Transforming Scientific Discovery <i>Chair: Andrey E Ustyuzhanin</i>	AI AGENTS AND LLMs FOR SCIENCE Mohamad Moosavi: Reasoning in the Language of Materials <i>Chair: Ray Meng Gao</i>	ML ALGORITHMIC ADVANCES Ivor W. Tsang: Building Physical AI Systems: From Geometry and Physics to Scientific Discovery <i>Chair: Gianmarco Mengaldo</i>
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 Iyu: 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 <i>Chair: Yong Tao Tan</i>				
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 <i>Chair: Jennifer Dodgson</i>				
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 <i>Chair: Yeong Wai Yee</i>	SELF-DRIVING LABS Nasim Abdollahi: Self-driving lab for viscous nanoemulsions <i>Chair: Yang Cao</i>	AI FOR CHEMISTRY Pengfei Ou: Machine Learning Accelerated Simulations of Electrochemical Interfaces <i>Chair: Yizhou Zhu</i>	AI FOR MEDICINE AND HEALTH-CARE Yimu Zhao: Accelerating Biological Discovery Through AI, Robotics, and Human Organ Mimicry <i>Chair: Luis Camuñas-Mesa</i>	ML ALGORITHMIC ADVANCES Dmitry Vetrov: Thermodynamical Analogies in Deep Learning <i>Chair: Carlo Vittorio Cannistraci</i>
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 Antiperovskite 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 Chemistry	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 <i>Chair: Seunghwa Ryu</i>	SELF-DRIVING LABS Daria Andreeva: Closed-Loop autonomous discovery of functional membranes and 2D Materials for resource recovery and energy applications <i>Chair: Shoichi Matsuda</i>	AI FOR SOCIETY Nancy F. Chen: Beyond Alignment: Grounding AI in Society <i>Chair: Truyen Tran</i>	AI FOR PHYSICS Marco Bernardi: Quantum Interactions in Materials: a New Frontier for AI <i>Chair: Shyue Ping Ong</i>	UNCONVENTIONAL COMPUTING Fernando Aguirre: CMOS-Integrated Silicon-Oxide Memristors: Reliability Characterization, SPICE-Based Circuit Simulation and potential application in neuromorphic computing <i>Chair: Giacomo Indiveri</i>
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 <i>Chair: Melodie Christensen</i>				
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? <i>Chair: Beatrice Soh</i>				
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 <i>Chair: Artem Mavvskiy</i>	SELF-DRIVING LABS Leong Shi Xuan: Toward Safe Autonomy in Self-Driving Laboratories <i>Chair: Han Hao</i>	AI FOR CHEMISTRY Kye Sung Park: Learning Arrow Pushing for Reaction Space Prediction and Exploration <i>Chair: Benjamin Chen</i>	AI FOR BIOLOGY Yatao Bian: Molecular Foundation Models: from Pretraining-Finetuning to LLMs <i>Chair: Yimu Zhao</i>	AI FOR EARTH SCIENCE Jeff Adie: NVIDIA Earth-2 and Generative AI for Climate and Weather <i>Chair: Tapio Schneider</i>
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 <i>Chair: Eun-Ah Kim</i>	AI FOR MATERIALS SCIENCE Stuart Miller: Building a Decision-Driven Materials Discovery Institute: Early Insights from MDRI <i>Chair: Santiago Mirer</i>	SELF-DRIVING LABS Peichen Zhong: Towards in silico prediction of solid-state material synthesizability <i>Chair: Owen Melville</i>	AI FOR MATERIALS SCIENCE Wen Jie Ong: Accelerating AI-Powered Chemistry and Materials Science Simulations with NVIDIA ALCHEMI Toolkit <i>Chair: Karsten Reuter</i>	AI FOR CHEMISTRY Benjamin Chen: CatPlat: A Physics-Grounded Data Engine for AI-Driven Materials Discovery <i>Chair: Yanwei Lum</i>
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? <i>Chair: Simon Billinge</i>				
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 <i>Chair: Mohamad Moosavi</i>				
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 <i>Chair: Gavin Koon</i>				
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 <i>Chair: Sonia Azimi Dijejin</i>	AI FOR MATERIALS SCIENCE Yizhou Zhu: When Machine Learning Force Fields Fail Expectations: Lessons We Learned from Solid Electrolyte Materials <i>Chair: Wen Jie Ong</i>	SELF-DRIVING LABS Keith A. Brown: Polymer Discovery through Modular Chemistry Plus Modular Automation <i>Chair: Felix Hanke</i>	AI FOR MEDICINE AND HEALTH-CARE Melodie Christensen: Advancing Pharmaceutical Development Through AI/ML-Enabled Experimental Design <i>Chair: Nasim Abdollahi</i>	AI FOR SOCIETY Julian Prieto: The Geopolitics of AI Driven Scientific Discovery: Uneven Geographies of Self Driving Laboratories <i>Chair: Kourosh Darvish</i>
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 Kotoponov: 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 <i>Chair: Alex Hammer</i>	SELF-DRIVING LABS Kourosh Darvish: A digital twin for sim-to-real chemistry lab automation <i>Chair: Artem Mishchenko</i>	AI FOR BIOLOGY Yijun Li: AFPFusionLM: A Hybrid Sequence–Structure Protein Language Model for Antifreeze Protein Function Prediction <i>Chair: Yongcun Song</i>	AI AGENTS AND LLMs FOR SCIENCE Haizhao Yang: Modeling and Computation in the Space of Language: Symbolic and LLM-Based Approaches <i>Chair: Aruhan Rui Shi</i>	AI FOR PHYSICS Simon Billinge: Characterizing electronic and structural states of materials with ML <i>Chair: Qianxiao Li</i>
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 Pethé: 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 CO₂-to-fuels conversionCurtis 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 Optimization 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 CO₂ 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

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

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

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

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

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 JEPAs 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 Kvantá

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

Poopool 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 Elsberg



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 _x Si _{1-x} O ₂	Yingtao Yang
76	Machine learning analysis of literature dataset on the CO ₂ 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	<i>Daniel Davidson</i>
321	Using genetic algorithms to explore compositional space of perovskite thin film	<i>Jérôme Gautier</i>
332	Anomalyspy: A Generative Defect Localization in Semiconductor Packages, with X-Ray Microscopy	<i>Pawan Kumar</i>
348	Predictive Modeling for Quantitative Compositional Engineering of InZnHfO Thin-Film Transistors	<i>Jiho Lee</i>
351	Machine Learning-Based Optimization of SOC Windows for High-Performance μ -Si Anodes	<i>Taehoon Choi</i>
352	Quantum Annealing-Driven Active Learning Benchmark for Nanophotonic Design	<i>Serang Jung</i>
358	Model-Data Coevolution as the Basis of Stateful, Problem-Scoped Materials Databases	<i>Fengyu Xie</i>
360	Literature-Grounded LLMs for Predicting High Ionic Conductivity Solid-State Electrolytes	<i>Kunik Jang</i>
375	Expanding catalyst discovery across material classes by machine learning	<i>Junseok Moon</i>
376	An Explainable Conversational AI Framework for the Discovery of Cobalt Electrocatalysts in Industrial Water Electrolysis	<i>Jongyeop Baek</i>
379	Simulation-to-Experiment Transfer Learning for XRD-Based Autoencoder Modeling of SOEC Half-Cell Materials	<i>Hunmin Park</i>
381	TropicalField-Tandem: Physics-Informed Indoor→Outdoor Translation and Uncertainty-Aware Forecasting for Perovskite-Si Tandem Reliability	<i>Romika Sharma</i>
385	Label-Efficient Battery SOH Estimation via Domain-Aware Self-Supervised Learning	<i>Ji Young Yun</i>
387	Accelerating Catalyst Design via AI: High-Throughput Screening and Machine Learning Reveal Defect-Enhanced Activity in Pt-Au Nanoclusters	<i>Iliia Chepkasov</i>
388	AI-Assisted Architected Cementitious Microstructures for Durable and Low-Carbon Infrastructure	<i>Abhimanyu Goel</i>
393	MOFology: Ontologically-Grounded MOF Knowledge Graph and Prediction Framework	<i>Matthew Hart</i>
407	3D Microstructure Reconstruction of X70 Pipeline Steel from 2D EBSD Data Using SliceGAN	<i>Joonas Lahikainen</i>
415	Multiscale modeling of resistive switching in two-dimensional heterostructures	<i>Vitalii Kapitan</i>
435	A Hybrid Physics-Driven Neural Network Force Field for Liquid Electrolytes	<i>Junmin Chen</i>

No	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

No	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	<i>Hitoha Sato</i>
244	Physical model-informed automated reaction optimization within a digital platform	<i>Shuyuan Zhang</i>
245	An Automated, Calibration-Free Platform for High-Throughput Reaction Screening and Data Analysis	<i>Manh Hung Tran</i>
267	DIY, Modular Automation Platform Built from Affordable Components for Directed Evolution and Molecular Biology, Toward Closed-Loop Workflows	<i>Takanori Uzawa</i>
275	Robotic Mechanochemical Synthesis of HKUST-1 with Process Monitoring	<i>Kazuki Ishizaki</i>
280	Scalable Low-Cost Laboratory Automation: A Digital Twin-Integrated Robotic Platform for Autonomous Liquid Handling	<i>Ali Shayesteh</i>
281	Bayesian optimization for self-driving liquid coating laboratory	<i>Jisoo Song</i>
286	A Provenance-First, AI-Ready Data Platform for Large-Scale Memristor Experiments	<i>Lai Gan</i>
292	Autonomous Discovery of Pareto-Optimal Gas-Diffusion Electrodes	<i>Zahra Azimi Dijvejin</i>
299	A low-cost, high-throughput solid dosing platform for self-driving laboratories	<i>Rui Zhang</i>
301	The Medicinal Chemistry Self-Driving Lab - Accelerating Hit Optimisation with a Direct to Biology Approach	<i>Stuart Green</i>
303	Robot-Enabled Biofabrication of Tissue Cultures with Micrometer-Scale Precision	<i>Daniel Hocevar</i>
305	Automated and Interpretable Experimental Platform for Process-Structure-Property Analysis via Raman Spectroscopy	<i>Takuya Miyajima</i>
306	Digitalizing Slurry Mixing for an Electrode Fabrication SDLs	<i>Jaehyun Oh</i>
307	Robotic Kneading for Organic Reactions: A Deterministic Platform for Data-Driven Synthesis in Semi-Solid Media	<i>Yuki Nishihori</i>
325	HELIOS - Holistic Experiment Learning Intelligent Orchestration System	<i>Sissi Feng</i>
326	Membrane Optimization for Electrochemical CO ₂ Storage	<i>Jordan Rumscheidt</i>
336	Development of a Scalable High-Throughput Platform for Plasmid Transfection in 3D Mammalian Cell Culture	<i>Rosanna Jiang</i>
338	Reinforcement Learning to Increase Nuclear Fusion Efficiency	<i>Joseph Koh</i>
361	Accelerated Discovery and Characterization of Nanoscale-Covalent Organic Frameworks for Photocatalytic Water Splitting	<i>Ziheng Xiao</i>
373	Bayesian Optimization-Guided Experimental Design for Graphene-Reinforced Cementitious Composites	<i>Abhimanyu Goel</i>

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

AI AGENTS AND LLMS FOR SCIENCE 🍷

10 POSTERS

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