

	7th July 2025				Updated 5th July 2025
	Tutorials				
Venue	Auditorium 1	Lecture Theatre 50	Lecture Theatre 51	Lecture Theatre 52	Lecture Theatre 53
9.00am		Accelerating Advanced Materials Discovery: Combinatorial Approaches with Direct Atomic Layer Processing (DALP®) Technology Maksym Plakhotnyuk Bonnie Tsim	AI for Weather and Climate Jeff Adia Gianmarco Mengaldo		
9.30am					
10.00am					
10.30am					
11.00am					
11.30am					
12.00pm		Lunch			
12.30pm					
1.00pm		Building Self-Driving Laboratories: A Practical Introduction for Experimental Researchers Mohammed Jeraal	Lunch		
1.30pm					
2.00pm					
2.30pm		Break	Critical Works on LLMs for Scientific Discovery: An Overview (P1)		
3.00pm			Zonglin Yang Yan Liu		
3.30pm			Break		
4.00pm		Enhanced AI-Driven Scientific Workflows for Accelerating Complex Materials Discovery Jose Hugo Garcias Andrei Voicu Tomut	Critical Works on LLMs for Scientific Discovery: An Overview (P2)		
4.30pm					
5.00pm					
5.30pm		Zonglin Yang Yan Liu			
6.00pm	End of Day				

	8th July 2025				
Venue	Auditorium 1				
8:50 am	Opening Address				
Session Chair	Kristen Persson				Session Chair
9:00 am	Machine learning force fields shows extreme generalisation Gábor Csányi				AI for Chemistry
9:40 am	ML Gradients for Computational Chemistry Rafael Gómez-Bombarelli				AI for Chemistry
10:00 am	Physics-informed digital twins of materials systems Boris Kozinsky				AI for Chemistry
10:20 am	Tea Break				
Session Chair	Rafael Gómez-Bombarelli				Session Chair
10:40 am	Building AI-Powered Infrastructure for Scientific Research Weinan E				AI for Science
11:20 am	Novel computing paradigms Marin Soljačić				Unconventional Computing
11:40 am	AI for MRO (Maintenance, Repair and Overhaul) Ric Parker				AI for Science
12:00 pm	Break				
Session Chair	Boris Kozinsky				Session Chair
12:20 pm	AI and autonomous laboratories for materials synthesis Gerbrand Ceder				Self-Driving Labs
1:00 pm	Fueling The Era of Data-Driven Materials Design and Synthesis Kristin Persson				AI for Chemistry
1:40 pm	Lunch				
	Parallel Sessions				
Venue	Auditorium 1	Lecture Theatre 50	Lecture Theatre 51	Lecture Theatre 52	Lecture Theatre 53
	AI for Materials Science	AI for Physics	AI Agents and LLMs for Science	Urban AI & Sustainability	AI for Medicine and Healthcare
Session Chair	Tian Xie	Yong Xu	Paul Smolensky	Wessel Bruinsma	Eleonore Vissol-Gaudin
2:40 pm	Generative Design of Inorganic Materials Kedar Hippalgaonkar	Physics-Informed Automatic Differentiation for Single-Shot Nanoscale 3D Imaging in In-Situ Transmission Electron Microscopy	Towards Mini Bang Theory: A Framework for Intelligence as Life Recognition Andrey Ustyuzhanin	Cozie and Kaggle: Crowdsourcing Data and Models for AI-driven Urban Heat and Energy Solutions Clayton Miller	From Generative AI to Enhanced Dementia Care: The Path to Early Detection and Intervention Jiayu Zhou
		Deepan Balakrishnan			
3:00 pm	Distance weighted self-attention for nonlocal density functional approximation by artificial neural network	PIED: Physics-Informed Experimental Design for Inverse Problems Apivich Hemachandra	LLM-based agent empowered with geometric, deep learning, data-oriented approaches and quantum chemistry to unravel synchrotron data of operando catalysis	MapReader: a framework for learning a visual language model for map analysis	BrainOOD: Out-of-distribution Generalizable Brain Network Analysis
	Kirill Kulaev				
3:15 pm	Elf autoencoder for unsupervised exploration of flat-band materials using electronic band structure fingerprints	Combining Flow Matching and Transformers for Efficient Solution of Bayesian Inverse Problems Danil Sherki	Construction and Application of Materials Knowledge Graph in Multidisciplinary Materials Science via Large Language Model Tong Xie	DesCartes: Hybrid Artificial Intelligence for optimal planning and decision making in urban systems Francisco Chinesta	Decoding Brain Waves: EEG Attention Detection Across Performance Levels
	Artem Mishchenko				
3:30 pm	Triviality metric for high-throughput detection of topological flat band materials	Algorithm unrolling for solving inverse problems in signal and image processing	Hybrid and Generative Models for Material Science Event Extraction Su Jian	Programmatic Reinforcement Learning for Trustworthy Microgrid Management Subrat Prasad Panda	Conversational Self-Play for Discovering and Understanding Psychotherapy Approaches
	Anupam Bhattacharya				
3:45 pm	Dis-CSP: Disordered Crystal Structure Predictions	Finite-difference least square methods for solving Hamilton-Jacobi equations using neural networks Alex Massucco	MatPilot: an LLM-enabled AI Materials Scientist under the Framework of Human-Machine Collaboration	Mapping Intelligibility: Hybrid AI, Sustainability, and "Wind Maps" of Singapore	Cross-dataset Evaluation of Dementia Longitudinal Progression Prediction Models
	Ruiming Zhu				

Programme for 8th July 2025 continues on the next page

4:00 pm	Tea Break				
	AI for Materials Science	Unconventional Computing	AI Agents and LLMs for Science	Self-Driving Labs	AI for Chemistry
Session Chair	Weinan E	Mario Lanza Martinez	Artem Maevskiy	Leonard Ng Wei Tat	Gábor Csányi
4:20 pm	Accelerating materials design with AI emulators and generators Tian Xie	Towards quantum AI advantage Dongling Deng	AI as a partner in scientific exploration Limsoon Wong	Building Lab of the Future Mimi Hii	Accelerating AI-Driven Chemical and Materials Discovery with NVIDIA ALCHEMI Wen Jie Ong
4:40 pm	Generation of Novel Stable Beautiful Materials Nikita Kazeev	Reconfigurable Nonlinear Computing in Silicon Wilfred G. van der Wiel	Mechanisms of Symbol Processing in Transformers Paul Smolensky	A knowledge foundation for symbolic AI in engineering Alexei Lapkin	AI-driven discovery and design of new materials and catalysts for sustainability Xiaonan Wang
5:00 pm	Generative model for enhancing reticular material discovery	Physical Hypercomputation: Non-Halting Dynamics in Material Substrates for Open-Ended Evolution goes to 'Unconventional computing Andrey Ustyuzhanin	Information fusion strategy based on language model and contrastive learning for knowledge retrieval of metallic materials	Accelerating the characterisation of molecular photoswitches for solar thermal energy storage	Harnessing Physics-inspired Machine Learning to Design Nanocluster Catalysts for Dehydrogenating Liquid Organic Hydrogen Carriers
	Theo Jaffrelot Inizan		Zhouran Zhang	Jacob Lynge Elholm	Tej S Choksi
5:15 pm	AI-empowered discovery of novel materials for smart electronic devices	5:20pm - 5:35pm Thermal Effects on Optoelectronics: A Graph Neural Network Approach	CogCommon: Enhancing Cross-Domain Knowledge Extraction with LLM-Assisted Commonality Discovery	Multispectral diagnostics of catalytic reactions in microfluidic systems	Comprehensive sampling of coverage effects in catalysis by leveraging generalization in neural network models
	Valentyn Volkov	Pol Benitez Colominas	Qian Hangwei	Bogdan Protsenko	Nitish Govindarajan
5:30 pm	Practical approaches for crystal structure predictions with inpainting generation and universal interatomic potentials	5:35pm - 5:50pm AI for carbon-based quantum materials	Towards Data-Driven Scientific Discovery	AutoFIS: Automated Bayesian Model Selection and Analysis for Electrochemical Impedance Spectroscopy	Machine Learning-Powered Exploration of Catalytic Reaction Networks for CO₂ Conversion into Value-Added Chemicals
	Peichen Zhong	Jiong Lu	Leo McKee-Reid	Daniel Persaud	Mikhail V. Polynski
5:45 pm	Apply DFT to DFT: Symmetry-preserved Generation of Crystalline Electron Densities	5:50pm - 6:05pm In-memory Subnet Computation for Area and Energy Efficient AI	Literature-based Hypothesis Generation: Predicting the evolution of scientific literature to support scientists		Redefining Catalysis Predictions Through Physics-Based Gaussian Model and Data-Driven Benchmarks: AuPd Alloy in Oxygen Reduction Reaction Catalysis for Fuel Cell Applications
	Yulin Cai	Zhao Shi, Yue Li	Pablo Sanchez Martin		Neeru Chaudhary
6:00 pm	End of Day				

	9th July 2025				
Venue	Auditorium 1				
Session Chair	Zhang Yang				Session Chair
9:00 am	Explainable AI for the Sciences Klaus Robert Müller				AI for Science
9:40 am	NVIDIA's Role in Supporting Scientific Computing Infrastructure Jack Wells				AI for Science
10:00 am	Scalable emulation of protein equilibrium ensembles with generative deep learning Yu Xie				AI for Biology
10:20 am	Tea Break				
Session Chair	Ron Dror				Session Chair
10:40 am	From Algorithm to Human Clinical Trials: Accelerating Drug Discovery and Development With Generative AI and Robotics Alex Aliper				AI for Biology
11:20 am	Compute-in-memory devices and architectures for efficient information processing Wei Lu				Unconventional Computing
11:40 am	The vast world of quantum advantage Hsin-Yuan Huang				Unconventional Computing
12:00 pm	KronosAI Yujie Huang				AI for Physics
12:20 pm	Break				
12:40 pm	Poster Session & Lunch				
	Parallel Sessions				
Venue	Auditorium 1	Lecture Theatre 50	Lecture Theatre 51	Lecture Theatre 52	Lecture Theatre 53
	AI for Materials Science	AI for Physics	AI for Chemistry	AI for Education & Policy	AI for Medicine and Healthcare
Session Chair	Isao Tanaka	Anatole von Lilienfeld	Chenru Duan	Eleonore Vissol-Gaudin	Ekaterina Skorb
2:40 pm	AI-based Hierarchical Representations of Materials for Structure-Property Prediction Abhishek Singh	Physics-Assisted Machine Learning for Wave Sensing and Imaging Xudong Chen	jystral: a Jax-based differentiable DFT framework for solids Industry Talk by SEA	Using AI to improve teaching and learning: a view from the trenches Ben Leong	Digital Healthspan Medicine Dean Ho
3:00 pm	Data-driven assessment of thermodynamic stability and search for competing phases: Application to the 2D Material Defect dataset	Super-resolution optical metrology and imaging of 3D nano-scale objects	No-Free-Lunch Theories for Tensor-Network Machine Learning Models	Exploratory investigation of electrodermal activity in learning from a large language model versus from curated texts	RetIRAG: A Retrieval-Augmented Generation Framework for Specialized Ophthalmology Applications
	Roman Eremin	Jin-Kyu So	Liwei Yu	Kenneth Y T Lim	Xu Ting
3:15 pm	Bridging Contextual Information in Deep Learning for Structural Defect Classification	Seeing the Invisible: Breaking the Diffraction Limit with Geometry-aware Deep Learning	Adapting hybrid density functionals with machine learning	Simulating Professional Workplaces: A Pedagogical Framework for Generative AI-Powered Role-Play for Competency-Based Education	MEDSAGE: Enhancing Robustness of Medical Dialogue Summarization to ASR Errors with LLM-generated Synthetic Dialogues
	Jiadong Dan	Wang Benquan	Alastair Price	Ng Sook Mun	Viktor Schlegel
3:30 pm	Fusion of quantum-mechanical and experimental data for phase diagram calculation	Simultaneous Optimization of Yield, Threshold, and Wavelength in Microring Lasers Using Bayesian Optimization	chemtrain: Learning deep potential models via automatic differentiation and statistical physics	AI regulations under the EU AI Act in critical urban systems	AI-Driven TCR Design: Leveraging Large Language Models for Personalized Cancer Immunotherapy
	Timofei Miryashkin	Mihir Rajendra Athavale	Paul Fuchs	Amelie Favreau	Zhou Jun
3:45 pm	Predicting defect formation energies in semiconductors using machine learning	Diffusion Model-Driven Optimization of High-Efficiency Wavelength-Scale Microring Lasers	Decoding kinetic selectivity in diffusion-limited solid state synthesis reactions through machine-learning accelerated molecular dynamics	AI and Evidence-Based Policymaking: Who Stays in the Human-AI Loop and Why?	Personalized dose selection platform for patients with solid tumors in the PRECISE CURATE AI feasibility trial
	Savvasanchi Aggarwal	Mihir Rajendra Athavale	Vir Karan	Jie Gao	Nigel Foo Hon Wei
4:00 pm	Tea Break				
	AI for Materials Science	AI for Physics	AI for World Domination	ML Algorithmic Advances	AI for Biology
Session Chair	Abhishek Singh	Tianbo Li	Nikita Kazeev	Weinan E	Alex Aliper
4:20 pm	Recommender system for discovery of new inorganic compounds Isao Tanaka	Deep learning density functional theory and beyond Yong Xu	How to Build AI Agent, How to Build Agentic AI, and How to Build Automatically? Liu Yang	Quantum Cognition Machine Learning -- a novel paradigm of machine learning, its theory and applications. Kharen Musaelian	Deep learning-based protein structure prediction with D-I-TASSER Zhang Yang
4:40 pm	Identifying and embedding transferability in data-driven representations of chemical space Stephen Gregory Dale	Quantum machine learning in chemical space Anatole von Lilienfeld	Adversarial Threats and Defenses in the Era of Large Language Models Luu Anh Tuan	Challenges for reliable forest monitoring with high resolution remote sensing and AI Emily Lines	AI for Structure-Based Drug Design Ron Dror
5:00 pm	Probing out-of-distribution generalization in machine learning for materials	Learning the Hamiltonian of Large, Disordered Atomic Systems	CryptoTrade: A Reflective LLM-based Agent to Guide Zero-shot Cryptocurrency Trading	Wells and context aware diffusion model for geologic cross section generation	ANTIPASTI: interpretable prediction of antibody binding affinity exploiting Normal Modes and Deep Learning
	Daniel Persaud	Chen Hao Xia	Qian Wang	Grigori Shutov	Kevin Michalewicz
5:15 pm	Embedding material graphs using the electron potential: application to material fracture	Crash testing machine learning force fields for molecules, materials, and interfaces: molecular dynamics in the TEA challenge 2023	Large Language Models for Cybersecurity: New Opportunities	Generative subgrid-scale modeling	Unsupervised Learning of Transient Structural Motifs of ssDNA Using Translationally and Rotationally Invariant Features
	Sherif Abdulkader Tawfik Abbas	Igor Poltavskiy	Dinil Mon Divakaran	Jiayi Zhao	Karls Kungsumutr
5:30 pm	Bridging the AI4Materials Innovation Gap — A Startup's Blueprint for Industrial Impact	Molecular Simulations with a Pretrained Neural Network and Universal Pairwise Force Fields	Bullying the Machine: How Personas Increase LLM Vulnerability Mohan Kankanhalli	Embedding Theoretical Baselines For Satellite Force Estimations	Prediction of the Future State of Photobioreactors Using Time Series Prediction Algorithm
	Yu Yang Fredrik Liu	Adil Kabylda		Benjamin Y J Wong	Wu Tianqi
5:45 pm	Finding Perovskite Composites With Preferable Features: Simple ML algorithms	Magnetic moment tensor potentials for investigating magnetic materials		Deep Topological Denoising: Autoencoder-Driven Noise Suppression for Atomic Force Microscopy data with Topological Data Analysis Validation	Generalization and Scoring in RNA 3D Structure Prediction: A Benchmarking Study
	Gurgen Kolotyan	Ivan S. Novikov		Ekaterina V. Skorb	Ivona Martinovic
6:00 pm	End of Day				

	10th July 2025				
Venue	Auditorium 1				
Session Chair	Terence O'Kane				Session Chair
9:00 am	Directions in Energy Efficient AI for Driving Earth Digital Twins Stan Posey				AI for Climate and Weather
9:40 am	Quantitative Investing in the Era of AI Revolution David Finkelstein				AI for Finance
10:00 am	From 2D to 3D: from semiconductors to cement Antonio Helio Castro Neto				AI for Materials Science
10:20 am	Tea Break				
Session Chair	Megan Stanley				Session Chair
10:40 am	Preparations for Next-Generation Weather and Climate Modelling at the Centre for Climate Research Singapore (CCRS) Chen Chen				AI for Climate and Weather
11:00 am	TBA Seok Min Lim				AI x Cybersecurity
11:20 am	Poster Session				
12:40 pm	Lunch				
	Parallel Sessions				
Venue	Auditorium 1	Lecture Theatre 50	Lecture Theatre 51	Lecture Theatre 52	Lecture Theatre 53
	AI for Materials Science	AI for Physics	ML Algorithmic Advances	AI for Biology	AI for Medicine and Healthcare
Session Chair	Leonard Ng Wei Tat	Khoo Jun Yong	Gianmarco Mengaldo	Yu Xie	
2:40 pm	Artificial Intelligence enabling disruptive Innovative Advanced Materials and Devices design & engineering Stephen Roche	The impact of Artificial Intelligence on precision Higgs Boson physics David Rousseau	Machine Learning-Based Predictive Control of Chemical Processes Zhe Wu	Playing the Long Game Towards Radical Life Extension Peter Fedichev	QAH-Net: a deep neural network for efficient and robust hologram reconstruction for off-axis digital holographic microscopy Kerem Delikoyun
3:00 pm	Machine learning of electronic charge densities in the simulation of electrochemical interfaces Salanne Mathieu	A trained Physics-Informed Neural Networks (PINNs) method for phase-field model in Allen-Cahn framework Song Le	Learning Macroscopic Dynamics from Partial Microscopic Observations Chen Mengyi	Variational Autoencoders Capture Plant Biomolecular Stress Information Anoop Patil	Enhancing Diagnostic Accuracy in Rare and Common Fundus Diseases with a Knowledge-Rich Vision-Language Model Meng Wang
3:15 pm	Virgo: neural network-accelerated prediction of physical properties in site-disordered materials Andy Paul Chen	Spin-1/2 kagome Heisenberg antiferromagnet: Machine learning discovery of the spinon pair-density-wave ground state Pinaki Sengupta	Learning Dynamics of Nonlinear Field-Circuit Coupled Problems with a Physics-Data Combined Model Shiqi Wu	Sparse Autoencoders Reveal Interpretable Structure in Small Gene Language Models Jie Zhang	Parallelized, Low-cost, and Real-time Machine Learning Model for Immune Cell Morphological Profiling Nicholas Ng
3:30 pm	Machine Learning-Driven Insights for Phase-Stable $\text{FAXCs1-xPb}(\text{IyBr1-y})_3$ Perovskites in Tandem Solar Cells Luo Ran	Utilizing Machine Learning for Identifying Quantum-Many-Body Phase Transitions Ron Ziv	Magnetic control of tokamak plasmas through deep reinforcement learning with privileged information Dmitry Sorokin	Effectiveness of Graph Neural Network Operators in Virulence Classification of Mouse-Influenza A Protein Interactions Kwoh Chee Keong	Expanding AI-Based Optical Urinalysis with Synthetic Data: A Large-Scale 849-Patient Study Igor Balashov
3:45 pm	Unsupervised Machine Learning for Phase Identification and Characterization of High-Resolution STEM EELS in Novel Battery Materials Yeo Zhen Yuan	Physics-informed neural network for single-shot phase retrieval in cryo-EM Yixiao Yang	Learning Non-Equilibrium Dynamics of Polymer Chains: A Data-Driven Approach Beatrice Soh	Flash optimization of drug combinations for <i>Acinetobacter baumannii</i> with iIdentif.AI-AMR Peter Wang	
4:00 pm	Tea Break				
	AI for Materials Science	ML Algorithmic Advances	AI Agents and LLMs for Science	Self-Driving Labs	AI for Chemistry
Session Chair	Stephen Roche	Xavier Bresson	Andrey Ustyuzhanin	Mimi Hii	Wen Jie Ong
4:20 pm	Discovering solid electrolytes through the analysis of machine-learned potential energy surfaces Artem Maevskiy	Constructing macroscopic dynamics using deep learning LI Qianxiao	MOOSE-Chem: Large Language Models for Rediscovering Unseen Chemistry Scientific Hypotheses Zonglin Yang	Beyond Automation: Self-Driving Laboratories as Engines for Next-Generation Photovoltaic Innovation and Scale-Up Leonard Ng Wei Tat	Generative Modeling on Sampling Rare Events in Chemistry Reactions Chenru Duan
4:40 pm	AI discovers new materials and phenomena - and natural intelligence explains them Artem Oganov	Physics-Constrained AI Emulation of Physical Processes in General Circulation Models Gianmarco Mengaldo	Development and analysis of largest, accurate and comprehensive Multicomponent (high entropy) alloy database using large language models Aravindan Kamatchi Sundaram	Rewards are all we need: building autonomous materials Sergei V. Kalinin	Solving the Problem of Sleeping and Lost Data in Chemistry with Artificial Intelligence Valentine P. Ananikov
5:00 pm	Datasets for Benchmarking Machine Learning Models for Accelerated Search of Fast Ionic Conductors Artem Dembitskiy	Multiple Descents in Deep Learning as a Sequence of Order-Chaos Transitions Feng Ling	Large Language Model for Automating the Analysis of Cryoprotectants Mariia Ashikhmina	Finding environmental-friendly chemical synthesis with AI and high-throughput robotics Le Duy Dung	Data-driven parametrization of molecular mechanics force fields for expansive chemical space coverage Tianze Zheng
5:15 pm	Health diagnosis and recuperation of aged Li-ion batteries with data analytics and equivalent circuit modeling Riko I Made	Dynamical systems' predictability using machine learning Yuxuan Yang	DARWIN 1.5: Large Language Models as Materials Science Adapted Learners Bram Hoex	Digital Exploration of Metal-Organic Polyhedra in The World Avatar Simon Rihm	NEXT-Mol: 3D Diffusion Meets 1D Language Modeling for 3D Molecule Generation Zhiyuan Liu
5:30 pm	Machine Learning Aided Atomistic Modeling of Solid State Electrolyte Interphase Formation for $\text{Li/Li}_7\text{P}_3\text{S}_{11}$ Bryant Li	Dynamical error metrics for machine learning forecasting Zhou Fang	Automated Benchmarking of LLMs: Applying Regression to Estimate LLM Accuracy Ben Leong	Transforming the Synthesis of Carbon Nanotubes with Machine Learning Models and Automation Yue Li	Gradient-guided discrete walk-jump sampling for biological sequence generation Zarif Ikram
5:45 pm	From Generative Models to Real-World Materials: Entalpic's AI-Driven Discovery Loop Alexandre Duval	Weighted Confidence Ensemble for Uncertainty Quantification in Physics-Informed Neural Networks Anshuman Pasupalak		Self-driving labs: how to tell the optimizer not to sample in an undesired region? Flore Mekki-Berrada	Leveraging Implicit Representations of Atomistic Foundation Model for Generation and Optimization of Molecules Yoon Ji Wei
6:00 pm	End of Day				

Venue		11th July 2025 Auditorium 1			
Session Chair		Teck Leong Tan		Session Chair	
9:00 am		Graph Transformers for Molecular Science -- Overcoming Limitations in Graph Representation Learning Xavier Bresson		ML Algorithmic Advances	
9:20 am		A Foundation Model for the Earth System: Air Pollution and Ocean Waves Wessel Bruinsma		AI for Climate and Weather	
9:40 am		Realizing Schrödinger's Dream with AI-Enabled Molecular Simulations Alexandre Tkatchenko		AI for Physics	
10:00 am		Tea Break			
Session Chair		Xujie Si		Session Chair	
10:40 am		The AI Mathematician Yang-Hui He		AI for Mathematics	
11:00 am		What kind of game is mathematics? Sergei Gukov		AI for Mathematics	
11:20 am		The electronic-structure genome of inorganic materials Nicola Marzari		AI for Materials Science	
11:40 am		AI X Blockchain Sunny Lu		AI for Finance	
12:00pm		Lunch			
Parallel Sessions					
Venue		Auditorium 1		Lecture Theatre 51	
		AI for Materials Science		AI for Physics	
Session Chair		Nicola Marzari		Alexandre Tkatchenko	
2:40 pm		Advances in Multi-component Alloy Design: From Interpretable Machine-Learning to Generative AI Teck Leong Tan		Designing an AI-Driven, Cross-Hardware Emulator for Noisy Quantum Computers with Gate-Based Protocols Khoon Jun Yong	
				Autocorrelation Matters: Understanding the Role of Initialization Schemes for State Space Models	
				Generative artificial intelligence and ethical considerations in health care: a scoping review and ethics checklist	
3:00 pm		Integrating graph neural networks with physics-informed loss function for mechanical response prediction of hollow concrete structures with morphed honeycomb configurations Wang Hanmo		Hyperspectral unmixing for Raman spectroscopy via physics-constrained autoencoders Dimitar Georgiev	
				Learning the deflated conjugate gradient method using gradient-based meta-solving	
				Federated Learning in Healthcare: A Benchmark Comparison of Engineering and Statistical Approaches for Structured Data Analysis	
3:15 pm		Composition driven machine learning for unearthing high-strength lightweight multi-principal element alloys Ng Chee Koon		A Symmetry-Aware Multimodal Transformer for Spin Hall Conductivity Prediction Ying Zhang	
				Phase Space Visualization and Neural Networks: Learning Hamiltonian Dynamics in the Duffing System	
				FAIM: Fairness-aware interpretable modeling for trustworthy machine learning in healthcare	
3:30 pm		Predicting the Chemical (Dis)order in Multicomponent Materials with High-Throughput Simulations and Representation Learning Jiayu Peng		Non-structured Solution-Processed Scintillators for Improved X-ray Imaging Xiaogang Liu, Zhen Mu	
				Efficient preconditioning for iterative methods with graph neural networks	
				Gastro-Health Project: Revolutionizing Personalized Nutrition and Health Forecasting Through Integrated AI Technologies	
3:45 pm		Minimizing the carbon footprint of 3D printing concrete: Leveraging parametric LCA and neural networks through multiobjective optimization Claudiane Ouellet-Piromondon		Topology-Preserving Deep Learning for Structural Integrity in Optical Semiconductor Characterization at Deeply Subwavelength Resolution Wang Benquan	
4:00 pm		Tea Break			
Session Chair		AI for Materials Science		Unconventional Computing	
		Valentine P. Ananikov		Wei Lu	
4:20 pm		Foundational Computational Polymer Properties Database: Bridging to Real-World AI Applications Ryo Yoshida		Quantum machine learning via photonics Fabio Sciarrino	
4:40 pm		Atomic Level Materials Engineering Kostya Novoselov		Memristor-based neuromorphic computation: status, challenges, and potential solutions Mario Lanza Martinez	
5:00 pm		Multi-objective synthesis optimization and kinetics of a sustainable terpolymer Balamurugan Ramalingam		Utility-Cost Ratio Maximization in Quantum Networks for Secure Quantum Key Distribution Jun Zhao	
5:15 pm		Classifying Petabytes of varying structural motifs in supercooled water Ervin Chia		Discovering Fault-Tolerant Quantum Circuits, and Quantum Error Correction Codes via Reinforcement Learning Remmy Augusta Menzata Zen	
5:30 pm		Metastable Polymorph Stabilization with Physics-based Descriptor Engineering and Machine Learning Dai Haiwen		AI Guided Multi-Objective Heterogeneous Chiplet Placement for Advanced Partha Pratim Kundu	
5:45 pm				The analysis and interpretation of quantum adversarial examples Shuangyue Geng	
6:00 pm		End of Day			