MONDAY – FRIDAY | OCTOBER 5TH – 9TH

PROGRAM OVERVIEW

Time & Room	Number	Title	Author(s)
MONDAY, OCTOBER 5th			
09:00-10:00, Lecture Hall N1		**Keynote 1**	**Tobias Hodel (University of Bern)**
10:10-10:30, Lecture Hall N1		**AI4Humanities&Social-Sciences Track**	**Supported by the TOPML Project funded by Carl Zeiss Foundation**
	AI4Sci79	**Generative AI in the Humanities: Theory, Culture, Methodology**	Fabio Ciotti (Università di Roma Tor Vergata)*
10:30-11:00 Coffee Break			
11:00-12:30, Lecture Hall N1	AI4Sci74	**Towards AI generated Philosophy through Autoformalization**	Maximilian Noichl (Utrecht University)*
	AI4Sci37	**Analyzing Historical Biographies with eXplainable AI**	Patrick Brookshire (Akademie der Wissenschaften und der Literatur | Mainz)*
	AI4Sci08	**Generative AI, Literary Studies, and the Plausibility of Interpretations**	Tim Lanzendörfer (Goethe University)*
	AI4Sci85	**Which kind of experts in what loops?**	Moritz Schaeffer (Johannes Gutenberg-Universität Mainz)*; Dominik Sobania (Universität Duisburg-Essen); Martin Briesch (Johannes Gutenberg-Universität Mainz); Franz Rothlauf (Johannes Gutenberg-Universität Mainz)
12:30-14:00 Lunch Break			
14:00-15:30, Lecture Hall N1	AI4Sci84	**From Science Fiction to Strategic Foresight**	Can-Elliot Sachs (LMU München)*; Linnetq Moxon (THI); Johanna Mauermann (JGU); Markus May (LMU); Jan Oliver Schwarz (THI); Christoph Bläsi (JGU)
	AI4Sci81	**Interpretability and Explainable AI for the Humanities and Social Sciences: From Plausible Stories to Testable Evidence**	Vera Schmitt (Johannes Gutenberg-Universität Mainz)*; Charlott Jakob (TU Berlin); Swarnadeep Bhar (Johannes Gutenberg-Universität Mainz); Raphael Fischer (Johannes Gutenberg-Universität Mainz)
	AI4Sci83	**Potentials and Dangers of Using AI for Politics**	Charlott Jakob (TU Berlin); Raphael Fischer (Johannes Gutenberg-Universität Mainz); Vera Schmitt (Johannes Gutenberg-Universität Mainz)*
	AI4Sci54	**Re-thinking and re-narrating „intelligence“ for inclusive AI-futures**	Angela Kölling (Mainz University)*
15:30-16:00 Coffee Break			
16:00-16:30, Lecture Hall N1	AI4Sci78	**ConflictBench: Benchmarking Scientific Conflict Reasoning for AI-Assisted Research**	Islam Mesabah (DFKI)*; Brian Moser (DFKI); Sebastian Vollmer (DFKI)
19:00-23:00		**Welcome Reception in Kurfürstliches Schloss Mainz, Forster Saal**	
		Opening Speech	**Christopher Bishop (Founder of Microsoft Research AI for Science)**
TUESDAY, OCTOBER 6th			
09:00-10:00, Lecture Hall N1		**Keynote 2**	**Claire Monteleoni (INRIA Paris)**
10:10-10:30, Lecture Hall N1		**DS: Explainable AI**	
	DS123	**The Explanandum Matters: On the Sensitivity of Shapley Feature Attribution to the Value Function in Classification**	Asma Ahmed Hashmi (LMU Munich)*; Peter Erber (LMU Munich); Patrick Kolpaczki (LMU Munich); Alireza Javanmardi (LMU Munich); Eyke Hüllermeier (LMU Munich)
10:10-10:30, Lecture Hall N2		**AI4Chemistry&Materials Track**	**Supported by the MAINCE Project funded by Carl Zeiss Foundation**
	AI4Sci16	**Overcoming Data and Validation Bottlenecks in Machine Learning Workflows for the Accelerated Discovery of Half-Heusler Thermo-electric Materials**	Shoeb Athar (Institute Charles Gerhardt Montpellier)*; Adrien Mecibah (Institute Charles Gerhardt Montpellier); Philippe Jund (Institute Charles Gerhardt Montpellier)
10:30-11:00 Coffee Break			
11:00-12:00, Lecture Hall N1		**Keynote 3**	**Alán Aspuru-Guzik (University of Toronto)**
12:10-12:30, Lecture Hall N1		**AI4Sci: AI4Chemistry&Materials**	
	AI4Sci23	**Machine Learning-Accelerated Discovery of Sustainable Redox-Active Polymers for Next-Generation Batteries**	Venkata Sai Subhash Ganti (University of Bayreuth)*; Lukas Wölfel (University of Bayreuth); Arla Diengdoh (University of Bayreuth); Tzvetan Mihaylov (Covestro Deutscheland Ag); Thomas Nevolianis (Covestro Deutscheland Ag); Jan Meyer (Covestro Deutscheland Ag); Christopher Künneth (University of Bayreuth)
12:10-12:30, Lecture Hall N2		**DS: Machine Learning**	
	DS028	**Co-Learning for Missing Arbitrary Modalities in Multi-modal Classification**	Francisco Mena (GFZ Helmholtz Center for Geosciences)*; Dino Ienco (INRIA, INRAE, University of Montpellier); Cassio Fraga Dantas (INRIA, INRAE, University of Montpellier); Roberto Interdonato (INRIA, CIRAD, University of Montpellier); Simon Besnard (GFZ Helmholtz Center for Geosciences)
12:30-14:00 Lunch Break			
14:00-15:30, Lecture Hall N1		**DS: Machine Learning**	
	DS096	**Invariant-Based Weight Sharing for Message Passing in Graph Neural Networks**	Florian Seiffarth (University of Bonn)*
	DS050	**How smoothing the affinity matrix affects neighborhood preser-vation in t-SNE**	Shirin Mohebi (Ghent University)*; Guillaume Bied (Ghent University); Jefrey Lijffijt (Ghent University)
	DS004	HyBiEn: Hybrid Bipolar Ensembles for Imbalanced Regression	Jelke Wibbeke (Carl von Ossietzky Universität Oldenburg)*; Rita P. Ribeiro (University of Porto); Sebastian Rohjans (Jade University of Applied Science); Andreas Rauh (Carl von Ossietzky Universität Oldenburg)
	DS124	GEMSS: A Variational Method for Discovering Multiple Sparse Solutions in Classification and Regression Problems	Kateřina Henclová (Datamole)*; Václav Šmídl (Czech Technical University in Prague)
	DS134	Size-Constrained Clustering via Bat Algorithm Optimization	Diego Vallejo-Huanga (Universitat Politècnica de València)*; Alexander Padilla (Universidad Politécnica Salesiana); Cesar Ferri (Universitat Politècnica de València); Fernando Martinez-Plumed (Universitat Politècnica de València)
	DS046	**DDCAE: A Dual-Decoder Convolutional Autoencoder for Joint Fault Scoring and Signal Restoration in Particle Accelerator Beam Diagnostics**	Charles Ndegwa (Universite Paris Saclay)*; Francesca Bugiotti (university Paris Saclay, Centrale Supelec); Barbara Dalena (CEA-Irfu, Saint-Aubin); Quentin Bruant (CEA-Irfu, Saint-Aubin); Valerie Gautard (CEA-Irfu, Saint-Aubin)
14:00-15:30, Lecture Hall N2		**AI4Sci: AI4Chemistry&Materials**	
	AI4Sci19	**End-to-End Uncertainty Quantification for Atomistic Machine Learning**	Matthias Kellner (EPFL)*
	AI4Sci28	**From Hansen Solubility Parameters to Deep Eutectic Solvents: A SMILES Foundation Model for Industrial Formulation Discovery**	Eswar Nagireddy (Sasol Chemicals)*; Florian Kretzschmar (SingularIT); Nikita Dalvi (Sasol Chemicals); Stefan Heyder (SingularIT); Arjan Gelissen (Sasol Chemicals); Mattis Hartwig (SingularIT); Allen Kelley (Sasol Chemicals)
	AI4Sci42	**Learning from Loss Landscapes: Stochastic Optimization for Molecular Energies**	Jennifer Leclaire (JGU Mainz)*; Andreas Hildebrandt (JGU Mainz)
	AI4Sci17	**Agentic Active Learning for Materials Discovery with Uncertainty-Gated Surrogate Simulation and First-Principles Labelling**	Massimilano Lupo Pasini (Oak Ridge National Lab)*; Zekun Chen (Lawerence Berkeley National Laboratory); Anubhav Jain (Lawrence Berkeley National Laboratory)
15:30-16:00 Coffee Break			
16:00-17:30, Lecture Hall N1		**DS: Benchmarking Methodologies**	
	DS055	**Design Choices That Matter: A Functional ANOVA Analysis for Remote Sensing Multi-Label Classification**	Maryam Gholami Shiri (Jozef Stefan Institute)*; Eva Tuba (Jožef Stefan Institute); Sašo Džeroski (Jožef Stefan Institute); Tome Eftimov (Jožef Stefan Institute); Ana Nikolikj (Jožef Stefan Institute)
	DS069	**Benchmarking Synthetic Time Series Generation for Privacy-Preserving Forecasting**	Luis Amorim (University of Porto)*; Vítor Cerqueira (University of Porto); Moisés Santos (University of Porto); Paulo Azevedo (University of Minho); Carlos Soares (University of Porto)
	DS097	**Topological Quality Assessment of Random Samples**	Alvaro Torras (Universidad de Sevilla); Jose M. Ramirez-Garcia (Universidad de Sevilla); Rocio Gonzalez-Diaz (University of Seville)*
	DS116	**Ordered-LRP: Structured Sparsity Patterns from Unstructured Pruning**	Guilherme Pereira (InescTec)*
16:00-17:30, Lecture Hall N2		**AI4Chemistry&Materials Track**	
	AI4Sci50	**MatSearch: Materials Substructure Search via Late Interaction of Atom-wise Embeddings**	Mark Spillman (Cusp.ai)*; Sina Samangooei (Cusp.ai); Sindy Löwe (Cusp.ai); Dario Coscia (Cusp.ai); Thomas Bridge (Cusp.ai); Hannah Openshaw (Cusp.ai); Felix Hanke (Cusp.ai)
	AI4Sci87	**Multi-agent Reinforcement Learning for insilico drug design.**	Kanishka Singh (Sanofi)*; Christoph Grebner (Sanofi); Gerhard Hessler (Sanofi)
	AI4Sci49	**Four-View Contrastive Learning for Metabolite Identification from Tandem Mass Spectra**	Manuel Ruiz Botella (Universitat Rovira i Virgili)*; Marta Sales-Pardo (Universitat Rovira i Virgili); Roger Guimerà (Universitat Rovira i Virgili)
	AI4Sci88	**Reasoning in Chemical Space: Structured Molecular Reasoning Models for Constrained Generation**	Sohvi Lukkonen (LIT AI Lab, Institute for Machine Learning, Johannes Kepler University Linz, Austria)*; Christoph Bartmann (LIT AI Lab, Institute for Machine Learning, Johannes Kepler University Linz, Austria): Johannes Schimunek (LIT AI Lab, Institute for Machine Learning, Johannes Kepler University Linz, Austria); Günter Klambauer (LIT AI Lab, Institute for Machine Learning, Johannes Kepler University Linz, Austria)
17:30-19:00, Poster Session		**Poster Session with: AI4Sci22, AI4Sci31, AI4Sci36, AI4Sci48, AI4Sci53, AI4Sci70, AI4Sci72 (see below)**	
WEDNESDAY, OCTOBER 7th			
09:00-10:00, Lecture Hall N1		**Keynote 4**	**Marwin Segler (Microsoft Research AI for Science)**
10:10-10:30, Lecture Hall N1		**AI4Chemistry&Materials Track**	
	AI4Sci89	**Data Quality as the Foundation of AI-Driven Drug Discovery**	Johannes Kirchmair (University of Vienna)*
10:10-10:30, Lecture Hall N2		**DS: Equation Discovery / Symbolic Regression**	
	DS084	**Symbolic Regression for Interpretable Time Series Regime Characterization**	Eduardo Passos (Faculdade de Ciências da Universidade do Portro)*; Ricardo Inácio (Faculdade de Engenharia da Universidade do Porto); Moisés Santos (Faculdade de Engenharia da Universidade do Porto); Carlos Soares (Faculdade de Engenharia da Universidade do Porto)
10:30-11:00 Coffee Break and Poster Session		**Poster Session with: AI4Sci22, AI4Sci31, AI4Sci36, AI4Sci48, AI4Sci53, AI4Sci70, AI4Sci72 (see below)**	
		Poster Session with: DS04, DS019, DS022, DS024, DS043, DS063, DS065, DS100, DS101, DS106, DS124, DS134, DS139	
11:00-12:30, Lecture Hall N2		DS: Machine Learning Applications	
	DS019	Reducing False Positives in Operational Remote Sensing: Lessons from Methane Plume Detection	Julia Wąsala (Leiden University)*; Joannes D. Maasakkers (SRON Space Research Organisation Netherlands); Holger Hoos (RWTH Aachen); Mitra Baratchi (Leiden Institute for Advanced Computer Science (LIACS))
	DS022	Discovering Stratified Learning Strategies for Student Subgroups with Exceptional Study Behavior: More Fine-grained Significance Categories in Regression Models	Dani Chambon (Technische Universiteit Eindhoven); Hilde Storms (Technische Universiteit Eindhoven); Teun van Gorcum (Technische Universiteit Eindhoven); Neha Bogavarapu (Technische Universiteit Eindhoven); Jan Ludwicki (Technische Universiteit Eindhoven); Wouter Duivesteijn (Technische Universiteit Eindhoven)*; Lieke van den Biggelaar (Technische Universiteit Eindhoven)
	DS024	Leveraging spatial transcriptomic through a heterogeneous graph-based method for spot-level cancer tissue classification	Veronica Buttaro (Università degli Studi di Bari Aldo Moro); Antonio Pellicani (Università degli Studi di Bari Aldo Moro)*; Annalisa Occhipinti (Teesside University); Claudio Angione (Teesside University); Gianvito Pio (Università degli Studi di Bari Aldo Moro); Michelangelo Ceci (Università degli Studi di Bari Aldo Moro)
	DS043	Discovering Latent Hydrological Regimes with Interpretable Mixture-of-Experts Surrogates	Francesco Paolo Folino (ICAR-CNR)*; Carmelina Costanzo (DIAm-UNICAL); Pietro Sabatino (ICAR-CNR); Luigi Pontieri (ICAR-CNR)
Lecture Hall N2		DS: LLMs and Automated Scientific Discovery	
	DS017	Teachers, Don't Leave Them MLLMs Alone: Stress Testing the Grading Wall	Ons zammel (Universidade do Porto Faculdade de Engenharia)*; Carlos Soares (Universidade do Porto Faculdade de Engenharia); Gerd Kortemeyer (ETH zurich); Fĺávia Carvalhido (Universidade do Porto Faculdade de Engenharia)
	DS052	On the Impact of Item Order and Questionnaire Popularity in LLMs	Simon Münker (Trier University)*; Simon Werner (Trier University); Achim Rettinger (Trier University)
	DS063	Has Someone Already Tested This? Construct-Level Hypothesis-Literature Matching	Lan Pan (Osnabrück University)*; Sebastian Musslick (Osnabrück University)
	DS065	TiLLMeOut: Time Series Large Language Models-based Outlier Detection	Fabrizio Angiulli (University of Calabria); Francesco De Luca (University of Calabria)*; Fabio Fassetti (University of Calabria)
	DS100	On the Effects of Reasoning Effort and Prompt-Based Diversification on Scientific Ideation Diversity	Yu Chinen (Laboratory for AI Biology, Center for Biosystems Dynamics Research, RIKEN)*; Haruka Ozaki (Laboratory for AI Biology, Center for Biosystems Dynamics Research, RIKEN)
Lecture Hall N2		**DS: Retrieval-Augmented Generation**	
	DS101	Mapping Similarity Spaces across Embedding Models with Synthetic Query Probing	Marcin Rozmus (Pegasystems); Peter van der Putten (Leiden University)*
	DS106	Contextual Chunk Augmen-tation for Biomedical RAG: Multi-Perspective Context Selection	Amsalu Fentie Jember (University of Bari Aldo Moro)*; Mario Alessandro Bochicchio (University of Bari Aldo Moro)
Lecture Hall N2		DS: Explainable AI	
	DS139	On the Fairness of Feature Attribution Explanations	Michele Fontana (University of Pisa); Francesca Naretto (University of Pisa)*; Anna Monreale (University of Pisa)
11:00-12:30, Lecture Hall N1		**AI4Chemistry&Materials Track**	
	AI4Sci52	**Bypassing Aggregation Noise in ChEMBL Using Context-Conditioned Transformers**	Michael Backenköhler (Helmholtz HIPS)*; Joschka Groß (Saarland University); Andrea Volkamer (Saarland University)
	AI4Sci56	**A (deep) learning jouney from point clouds to proteins**	Sofia Imperatore (TU Eindhoven)*
	AI4Sci47	**Robust Mechanism-of-Action Prediction in High-Content Microscopy Images through Test-Time Adaptation and Scaling**	Ana Sanchez-Fernandez (LIT AI Lab, Institute for Machine Learning, Johannes Kepler University Linz, Austria)*; Günter Klambauer (LIT AI Lab, Institute for Machine Learning, Johannes Kepler University Linz, Austria)
	AI4Sci66	**Towards Minimum Energy Pathways with Reinforcement Learning**	Jan Felix Kleuker (Leiden University)*; Aleksandra Bobrova (Leiden University); Thor van Heesch (University of Amsterdam); Rik Breebaart (University of Amsterdam); Thomas Moerland (Leiden University)
12:30-14:00 Lunch Break			
14:00-15:00, Lecture Hall N1		**Keynote 5**	**Chris Dallago (NVIDIA and Duke University)**
15:10-15:30, Lecture Hall N2		**DS: Continual, Transfer and Meta-Learning**	
	DS053	**Selective Time Series Forecasting via Metalearning**	Ricardo Inácio (Faculdade de Engenharia da Universidade do Porto)*; Vitor Cerqueira (University of Coimbra); Marília Barandas (Fraunhofer Portugal AICOS); Carlos Soares (Faculdade de Engenharia da Universidade do Porto)
15:10-15:30, Lecture Hall N1		**AI4LifeSciences Track**	**Supported by the AI Pilot of the State of Rhineland Palatinate**
	AI4Sci06	**Auditing Sybil: Explaining Deep Lung Cancer Risk Prediction Through Generative Interventional Attributions**	Bartłomiej Sobieski (University of Warsaw)*; Jakub Grzywaczewski (Warsaw University of Technology); Karol Dobiczek (Jagiellonian University); Mateusz Wójcik (Warsaw University of Technology); Tomasz Bartczak (Google); Patryk Szatkowski (Medical University of Warsaw); Przemysław Bombiński (Medical University of Warsaw); Matthew Tivnan (Harvard Medical School); Przemysław Biecek (University of Warsaw, Centre for Credible AI Warsaw University of Technology)
15:30-16:00 Coffee Break and Poster Session		**Poster Session with: AI4Sci22, AI4Sci31, AI4Sci36, AI4Sci48, AI4Sci53, AI4Sci70, AI4Sci72 (see below)**	
		Poster Session with: DS04, DS019, DS022, DS024, DS043, DS063, DS065, DS100, DS101, DS106, DS124, DS134, DS139	
16:00-17:30, Lecture Hall N2		**DS: Physics-Informed ML / Equation Discovery**	
	DS059	**Residuals Are Not Enough: Limits of Physics-Informed Pre-Training for Scientific Foundation Models**	Serge Kotchourko (University of Stuttgart)*; Amin Totounferoush (University of Stuttgart); Michael Mahoney (University of California, Berkeley); Steffen Staab (University of Stuttgart)
	DS109	**ELADO: Elliptic PDE Assessment Datasets for Operator Learning**	Frank Ehebrecht (Osnabrueck University)*; Toni Scharle (ROSEN Technology & Research Center); Martin Atzmueller (Osnabrueck University)
	DS114	**OANP: Operator Attentive Neural Processes for detecting unreliable predictions and and covariate shift**	Frank Ehebrecht (Osnabrueck University)*; Toni Scharle (ROSEN Technology & Research Center); Martin Atzmueller (Osnabrueck University)
	DS119	**Sparse Orthogonal Regression Technique: A Spectral Framework for Equation Discovery, Approximation, and Integration**	Sabin Roman (Jožef Stefan Institute)*; Ljupco Todorovski (University of Ljubljana); Saso Dzeroski (Jožef Stefan Institute)
16:00-17:30, Lecture Hall N1		**AI4LifeSciences Track**	
	AI4Sci07	**Towards Observable Continuous-Time Models for Causal Treatment Effect Estimation in Healthcare**	Maik Kschischo (University of Koblenz)*; Jennifer Wendland (University of Koblenz); Nicolas Freitag (University of Koblenz); Philipp Wendland (University of Applied Sciences Koblenz)
	AI4Sci34	**EVIDENT: Structuring Computational Trust for AI-Assisted Scientific Software in the Life Sciences**	David Teschner (JGU Mainz)*; Thomas Kemmer (JGU Mainz); Maximilian Sprang (Department of Dermatology, University Medical Center of the Johannes Gutenberg University Mainz); Stefan Tenzer (University Medical Center, Johannes Gutenberg University, 55131 Mainz, Germany); Andreas Hildebrandt (Institute of Computer Science, Johannes Gutenberg University, 55128 Mainz, Germany)
	AI4Sci35	**Open Tools for More Accessible and Transparent Biologically Informed Deep Learning**	David Selby (Deutsches Forschungszentrum für Künstliche Intelligenz)*; Daria Pavliuk (Deutsches Forschungszentrum für Künstliche Intelligenz); Gerrit Grossmann (Deutsches Forschungszentrum für Künstliche Intelligenz); Sebastian Vollmer (Deutsches Forschungszentrum für Künstliche Intelligenz)
	AI4Sci41	**Guideline Controlled AI for Clinical Decision Support**	Jonas Flechsig (Fraunhofer Institute for Industrial Mathematics)*
19:00-23:00		**Social Event in Altes Postlager**	
THURSDAY, OCTOBER 8th			
09:00-10:00, Lecture Hall N1		**Keynote 6**	**Gilles Louppe (University of Liège)**
10:10-10:30, Lecture Hall N2		**DS: Applications**	
	DS037	**Do Recipes Have Personas? Characterizing and Generating Creator Style in Attributed Procedural Graphs**	Lei Jiang (Microsoft)*
10:10-10:30; Lecture Hall N1		**AI4LifeSciences Track**	
	AI4Sci43	**Securing sequence design: a safety-centric analysis and expert consensus on governance for generative AI in biology**	Maximilian Sprang (University Medical Center of The Johannes Gutenberg University Mainz)*
10:30-11:00 Coffee Break and Poster Session		**Poster Session with: AI4Sci09, AI4Sci38, AI4Sci60, AI4Sci61 (see below)**	
		Poster Session with: DS017, DS029, DS038, DS045, DS048, DS052, DS083, DS147	
11:00-12:30, Lecture Hall N2		**DS: Hypothesis Generation / Causal Discovery**	
	DS035	**Learning to Guide Human Decision Makers with Vision-Language Models**	Debodeep Banerjee (University of Trento)*; Stefano Teso (University of Trento); Burcu Sayin (University of Trento); Rajib Pal (Bankura Sammilani Medical College And Hospital); Andrea Passerini (University of Trento)
	DS103	**Metadata-Driven Scientific Hypothesis Generation via Multi-Agent Symbolic–Neural Reasoning**	Fatimah Alotaibi (Virginia Tech)*; adithya kulkarni (Virginia Tech); Dawei Zhou (Virginia Tech)
	DS071	**From Exceptional Subgroups to Hypotheses: A Contrastive Analysis Approach**	Madalina Rogozan (Eindhoven University of Technology)*; Natalia Sidorova (Eindhoven University of Technology); Boudewijn van Dongen (Eindhoven University of Technology)
	DS038	What Drives LLM-Generated Hypotheses? Attribution-Informed Context Engineering for Scientific Discovery	Adnan Mahmud (University of Edinburgh)*; Gabriel Reder (University of Cambridge); Abbi Abdel Rehim (University of Cambridge); Amy Wilson (University of Edinburgh); Ross King (University of Cambridge)
	DS029	Actions Have Consequences: Detecting Outcome Performativity Using Intervention Testing	Brandon Gower-Winter (Utrecht University)*; Georg Krempl (Utrecht University)
	DS147	Discovering Latent Scientific Concepts through Discrete Representation Learning	Marjan stoimchev (JSI); Monu Verma (IU); Aveline Filliol (MSK); Maria Skamagki (MSK); Sara Flowers (MSK); Jacob Cohen (MSK); Zachary Azadian (MSK); Nancy Newlin (MSK); Mohamed Abdel-Mottaleb (IU); Saso Dzeroski (JSI)*; Paul Romesser (MSK); Scott Lowe (MSK); Nevenka Dimitrova (MSK)
11:00-12:30, Lecture Hall N1		**AI4LifeSciences Track**	
	AI4Sci45	**Constructing a Literature-Derived Functional Annotation Layer for Descending Neurons in the Drosophila Connectome**	Tokuma Hayashi (Universität Osnabrück)*
	AI4Sci51	**Toward an Adaptable Foundation Model for Unified Computational Drug Discovery**	Lisa Schneckenreiter (ELLIS Unit Linz, LIT AI Lab, and Institute for Machine Learning, Johannes Kepler University, Linz)*; Sohvi Luukkonen (ELLIS Unit Linz, LIT AI Lab, Institute for Machine Learning, Johannes Kepler University, Linz); Günter Klambauer (ELLIS Unit Linz, LIT AI Lab, Institute for Machine Learning and Clinical Research Institute for Medical Artificial Intelligence, Johannes Kepler University, Linz)
	AI4Sci71	**A Generalized Framework for Designing Complex Assemblies from Modular Components**	Soeren Brandt (Sail Biomedicines)*; Usman Mahmood (Sail Biomedicines); Mark Umbarger (Sail Biomedicines)
	AI4Sci77	**Benchmarking agentic solutions for automated immunogenomics data analysis**	Oleh Kovalyshyn (Kyiv School of Economics)*; Nadiia Kasianchuk (Kyiv School of Economics); Serghei Mangul (Jagiellonian University)
12:30-14:00 Lunch Break			
14:00-15:00, Lecture Hall N2		**DS: Agentic AI**	
	DS091	**DTOC: Dynamic Tool Output Compression for Adaptive Context Management in AI Agents**	Abhay Chaturvedi (Pegasystems); Shreya Bhattacharya (Pegasystems); Rashmika Gopalkrishnan (Pegasystems); Peter van der Putten (Leiden University)*
	DS092	**Same Outcomes, Different Journeys: Discovering Behavioral Divergence Between Humans and GUI Agents in Search Applications**	Maria Movin (Spotify; Stockholm University)*; Claudia Hauff (Spotify); Aron Henriksson (Stockholm Univeristy); Panagiotis Papapetrou (Stockholm University)
	DS111	**Evaluating Theory of Mind in Reasoning Models: Robustness over Reasoning**	Ian B. de Haan (Leiden University); Peter van der Putten (Leiden University)*; Max van Duijn (Leiden University)
14:00-15:00, Lecture Hall N1		**AI4Physics Track**	
	AI4Sci32	**Element Representations Shape Generalization in Materials Graph Networks**	Ran Zhao (KAUST)*; Kangming Li (KAUST)
	AI4Sci20	**Physics-Anchored Semigroup Consistency for Stable Long-Horizon Neural Operator Rollouts**	Muhammad Waasif Nadeem (RPTU Kaisers-lautern-Landau)*; Jephte Abijuru (RPTU Kaisers-lautern-Landau); Marius Kloft (RPTU Kaisers-lautern-Landau); Sophie Fellenz (RPTU Kaiserslautern-Landau)
15:00-16:00, Lecture Hall N1		**Keynote 7**	**Shirley Ho (New York University)**
16:00-16:30 Coffee Break and Poster Session		**Poster Session with: AI4Sci09, AI4Sci38, AI4Sci60, AI4Sci61 (see below)**	
		Poster Session with: DS017, DS029, DS038, DS045, DS048, DS052, DS083, DS147	
16:30-17:30, Lecture Hall N2		**DS: Life Science Applications**	
	DS040	**Few-Shot Biomedical Relation Extraction with Large Language Models: A Viable Alternative to Supervised Learning?**	Jakob Mraz (University of Ljubljana, Faculty of Computer and Information Science)*; Tomaž Curk (University of Ljubljana, Faculty of Computer and Information Science); Blaž Zupan (University of Ljubljana, Faculty of Computer and Information Science)
	DS030	**Benchmarking Literature Retrieval for a Model Organism: A Dictyostelium Case Study**	Yun Wang (University of Ljubljana)*; Gad Shaulsky (Baylor College of Medicine); Tomaž Curk (University of Ljubljana); Blaž Zupan (University of Ljubljana)
	DS057	**Not All Unlabeled Data Are Equal: Unlabeled Data Selection for Semi-Supervised QSAR Modeling with Large Chemical Repositories**	Oliver Majer (University of Ljubljana, Faculty of Mathematics and Physics); Sašo Džeroski (Jožef Stefan Institute); Jurica Levatić (Jožef Stefan Institute)*
16:30-17:30, Lecture Hall N1		**AI4Physics Track**	
		Particle Theory and AI	Tilman Plehn (Universität Heidelberg)
17:30-18:00, Lecture Hall N1		**DS 2026 / AI4Sci 2026 Business Meeting**	
FRIDAY, OCTOBER 9th			
09:00-10:30, Lecture Hall N1		**DS: Explainable AI**	
	D005	**Interpretable Rule-Based and Instance-Based Learning-to-Rank for Candidate Screening**	Andrea Iommi (University of Pisa)*; Cristiano Landi (University of Pisa); Antonio Mastropietro (University of Pisa); Riccardo Guidotti (University of Pisa)
	D016	**Model-Agnostic Counter-factual Explanations for Time-Series Classification via Prototype Movement**	Isak Samsten (Stockholm University)*
	D032	**When Nothing Matters: Extending Linear Models to Improve Interpretability and Faithfulness**	Martina Cinquini (University of Pisa)*; Francesco Spinnato (University of Pisa); Riccardo Guidotti (University of Pisa)
	D099	**On the Edit Path to GNN Decisions**	Florian Seiffarth (University of Bonn)*
09:00-10:30, Lecture Hall N2		**AI4Physics Track**	
	AI4Sci18	**Magnetism for AI and AI for magnetism: from skyrmion reservoirs to group-scale research acceleration**	Aditya Kumar (JGU Mainz)*
	AI4Sci26	**Agentic AI for Kerr Microscopy Experiments with Magnetic Skyrmions**	Kilian Leutner (Institute of Physics, Johannes Gutenberg University Mainz, Mainz)*; Yuean Zhou (Institute of Physics, Johannes Gutenberg University Mainz, Mainz); Thomas Brian Winkler (Institute for Molecules and Materials, Radboud University, Nijmegen); Robert Frömter (Institute of Physics, Johannes Gutenberg University Mainz, Mainz); Hans Fangohr (University of Southampton, Southampton); Mathias Kläui (Institute of Physics, Johannes Gutenberg University Mainz, Mainz)
	AI4Sci40	**Learning the NV-Visible Quotient of Equilibrium Quantum Magnetic Noise**	EL Mustapha Mansouri (Institute of Science Tokyo)*
	AI4Sci12	**Simulation-Based Fault Injection for AIEngine-Based ML Triggers**	Georgios Sotiropoulos (Karlsruhe Institute of Technology)*; Patrick Schwäbig (Rheinische Friedrich-Wilhelms-Universität Bonn); Foivos Paraskevas (Karlsruhe Institute of Technology); Marc Neu (Karlsruhe Institute of Technology); Tanja Harbaum (Karlsruhe Institute of Technology); Klaus Desch (Karlsruhe Institute of Technology); Torben Ferber (Karlsruhe Institute of Technology); Jürgen Becker (Karlsruhe Institute of Technology)
10:30-11:00 Coffee Break and Poster Session		**Poster Session with: AI4Sci25, AI4Sci30, AI4Sci39, AI4Sci68, AI4Sci69, AI4Sci73, AI4Sci76 (see below)**	
11:00-12:10, Lecture Hall N1		**DS: Continual, Transfer and Meta-Learning**	
	DS056	**Foundation vs. Specialized Models: Evaluating Catastrophic Forgetting in Continual Time Series Forecasting**	Nouha Karaouli (Univ Rennes, IRISA); Denis Coquenet (Univ Rennes, IRISA); Elisa Fromont (Université Rennes, IRISA/Inria Rennes)*; Martial Mermillod (Univ Grenoble-Alpes, LPN); Marina Reyboz (CEA)
	DS061	**Preserving Knowledge Legacy: Continual Learning on Heterogeneous Graph Attention Networks**	Francesco Scala (CNR-ICAR)*; Liliana Martirano (CNR-ICAR); Carmela Comito (CNR-ICAR); Sergio Flesca (UNICAL-DIMES); Luigi Pontieri (CNR-ICAR)
Lecture Hall N1		DS: Benchmarking Methodologies	
	DS045	On the Synthetic Evaluation of Time Series Clustering	Felix Iglesias (TU Wien)*; Tanja Zseby (TU Wien)
	DS048	Hidden-Context Drift Simulation for Realistic Stream Benchmarks	Yibin Sun (Victoria University of Wellington)*; Bernhard Pfahringer (University of Waikato); Heitor Murilo Gomes (Victoria University of Wellington); Albert Bifet (University of Waikato)
Lecture Hall N1		**DS: Equation Discovery / Symbolic Regression**	
	DS083	Likelihood-Free Bayesian Symbolic Regression for Discovery of Stochastic Differential Equations	Tim Schneider (University of Stuttgart)*; Daniel Tartakovsky (Stanford University); Wolfgang Nowak (University of Stuttgart); Steffen Staab (University of Stuttgart)
11:00-12:10, Lecture Hall N2		**AI4Physics Track**	
	AI4Sci10	**Plausible but Wrong: A Case Study on Agentic Failures in Astrophysical Workflows**	Shivam Rawat (Univeristy Bonn), Lucie Flek (University Bonn)
	AI4Sci21	**Towards an Autonomous AI Steward for Large-Scale Physics Experiments: Integrating Causal Diagnostics, RAG, and Conformal Prediction**	Oliver Noll (Helmholtz-Institut Mainz), Nicholas Tan Jerome (Institut für Prozessdatenverarbeitung und Elektronik (IPE, KIT))
	AI4Sci24	**A Robot Scientist for Drop Friction Measurements**	Jannis Brugger (TU Darmstadt), Yassin Riyazi (MPI for Polymer Research), Leonard Ries (MPI for Polymer Research), Mira Mezini (TU Darmstadt), Hans-Jürgen Butt (MPI for Polymer Research), Rüdiger Berger (MPI for Polymer Research), Stefan Kramer (JGU Mainz)
		AI4Chemistry&Materials Track Posters	
	AI4Sci22	**From Molecular Structure to Formulation-Relevant Properties: A Data-Driven Workflow for Surfactant Design**	Arjan Gelissen (Sasol Chemicals)*; Britta Jakobs-Sauter (Sasol Chemicals); Allen Kelley (Sasol Chemicals)
	AI4Sci31	**Coverage-Guided Data Pruning for Materials Learning**	Ran Zhao (KAUST)*; Kangming Li (KAUST)
	AI4Sci36	**From Drop Dynamics to Fluid Properties: An Image-Based Deep Learning Framework**	Yassin Riyazi (Max-Planck-Institut for Polymer research)*; Sajjad Shumally (Max-Planck-Institut for Polymer research); Leonard Ries (Max-Planck-Institut for Polymer research); Oleksandra Kukharenko (Max-Planck-Institut for Polymer research); Alice Allen (Max-Planck-Institut for Polymer research); Peter Stephan (TU darmstadt); Hans-Juergen Butt (Max-Planck-Institut for Polymer research); Ruediger Berger (Max-Planck-Institut for Polymer research)
	AI4Sci48	**CoCoGraph: A Collabo-rative Constrained Graph Diffusion Model for the Generation of Realistic Synthetic Molecules in Drug Discovery**	Manuel Ruiz Botella (Universitat Rovira i Virgili)*; Marta Sales-Pardo (Universitat Rovira i Virgili); Roger Guimerà (Universitat Rovira i Virgili)
	AI4Sci53	**Explaining What Matters: Faithfulness in Molecular Deep Learning**	Marcel Hiltscher (TU/e)*; Marc Bianciotto (Sanofi); Francesca Grisoni (TU/e)
	AI4Sci70	**Mimosa Framework: Toward Evolving Multi-Agent Systems for Scientific Research**	Martin Legrand (CNRS & Université Côte d'Azur & Centre Inria d'Université Côte d'Azur & 3iA Côte d'Azur); Tao Jiang
	AI4Sci72	**Chemical reaction extraction from chemical schemes: extension to Markush representation**	Ulrick Fineddie Randriharimanamizara (ICMUB UBE)*
		AI4LifeSciences Track Posters	
	AI4Sci09	**Estimating Demographic Attributes from Skin Lesion Images for Fairness Auditing in Dermatological AI**	Arib Yousuf (RPTU Kaiserslautern-Landau); Ko Watanabe (DFKI GmbH)*; Stanislav Frolov (DFKI GmbH); Aya Hassan (RPTU Kaiserslautern-Landau); Adriano Lucieri (DFKI GmbH); Andreas Dengel (DFKI GmbH)
	AI4Sci38	**A Novel Neural Network Model To Predict And Enable Prevention Of Honey Bee Colony Collapse**	Charles Brum (Stanford Online High School)*
	AI4Sci60	**The SAGE-Immune clock: Determining Sex-Specific Patterns of Immune Cell Aging**	Zhilin Zou (University Medical Center of the Johannes Gutenberg-University Mainz); Emre Kilic (University Medical Center of the Johannes Gutenberg-University Mainz); Mihai Netea (Radboud University Nijmegen Medical Centre); Maximilian Sprang (University Medical Center of the Johannes Gutenberg-University Mainz); Johannes Mayer (University Medical Center of the Johannes Gutenberg-University Mainz)*
	AI4Sci61	**On the Challenges of Maintaining Hierarchical Knowledge Bases for Clinical Decision Support**	Leandro Teixeira Crespo (Institute of Computer Science, Johannes Gutenberg University, Mainz; Institute of Medical Biostatistics, Epidemiology and Informatics (IMBEI), Mainz)*; Daan Apeldoorn (Institute of Medical Biostatistics, Epidemiology and Informatics (IMBEI), Mainz; IU International University of Applied Sciences, Düsseldorf); Felix Schuhknecht (Institute of Computer Science, Johannes Gutenberg University, Mainz); Andre Thevapalan (Institute of Medical Biostatistics, Epidemiology and Informatics (IMBEI), Mainz)
		AI4Physics Track Posters	
	AI4Sci25	**Precision autotuning for iterative solvers: An AMG case study**	Junhao Chen (Beijing University of Posts and Telecommunications); Qinmeng Zou (Beijing University of Posts and Telecommunications)*
	AI4Sci30	**AUTOFOAM: THE SELF-REFINING AUTONOMOUS OPENFOAM AGENT**	aditya a sesh (quasi ai)*; Arun Govind Neelan (Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique)
	AI4Sci39	**QuSafe Resolver: Grid-Validated Neural Safety Envelopes for Robust Qubit Control**	EL Mustapha Mansouri (Institute of Science Tokyo)*
	AI4Sci68	**Reweighted Hamiltonian Transport for Fixed Wavefunction Sampling in Variational Monte Carlo**	Moxian Qian (Johannes Gutenberg University Mainz)*
	AI4Sci69	**A Principled Probabilistic Machine Learning Framework for Optical Communication Channels**	SINA SEYFADINI KUHBANANI (Aston University)*; Felippe Alves (TELUS Digital Research Hub); David Saad (Aston University); Sergei Turitsyn (Aston University)
	AI4Sci73	**Physics-Informed Residuals Are Heavy-Tailed: Why MSE Loss Falls Short**	Jephte Abijuru (RPTU Kaiserslautern-Landau)*; Nadeem Muhammad Waasif (RPTU University Kaiseslautern-Landau); Sophie Fellenz (RPTU Kaiserslautern-Landau); Marius Kloft (RPTU Kaiserslautern-Landau)
	AI4Sci76	**Filter-Cone Certificates for Simulation-to-Reality Transfer in NV-Center Quantum Protocols**	EL Mustapha Mansouri (Institute of Science Tokyo)*; Keigo Arai (Institute of Science Tokyo)

Legend: AI4Humanities & SocialSciences · AI4LifeSciences · AI4Chemistry & Materials · AI4Physics · Discovery Science · Keynote · Break/Poster Session

Marker for Talk length: short talk **long talk**

Subject to change. Status: September 29, 2026