AI4AM 2026
ARTIFICIAL INTELLIGENCE FOR ADVANCED MATERIALS
May 18-21 • Madrid (Spain)

Tentative Program (as of 18/05/2026)

Tuesday May 19, 2026

08:00-08:45	**Registration**	
08:45-09:00	**Opening Ceremony**	
09:00-09:45	**Michele Parrinello** (IIT, Italy) The Material Science of Catalysis	P
09:45-10:15	**Aron Walsh** (Imperial College London, UK) Inverse Materials Design	K
10:15-11:00	**Coffee Break / Poster Session / Exhibition**	
11:00-11:20	**Saeed Jahromi** (Multiverse Computing & DIPC, Spain) Quantum-Inspired Tensor Networks for Materials Simulation and AI Applications	I
11:20-11:40	**Piero Altoe** (NVIDIA, Italy) Accelerating the Discovery Loop: Production-Ready Tools for GPU-Powered Materials Science	I
11:40-12:00	**Keith Butler** (University College London, UK) Learning the language of crystal chemistry: How methods from natural language can help discover new materials	I
12:00-12:15	**Andrew Salij** (Los Alamos National Laboratory, USA) Multi-objective Materials Discovery using Weighted Preference Optimization	O
12:15-12:30	**Valentyn Volkov** (XPANCEO, United Arab Emirates) Data-driven discovery of novel materials for smart electronic devices	O
12:30-12:45	**Claudio Cazorla** (ICREA (Institut Català de Recerca i Estudis Avançats), Spain) Uncertainty-Aware Machine Learning Discovery of Solid–Solid Phase Transitions in Inorganic Materials	O
12:45-13:00	**Ge Wang** (University of Science and Technology Beijing, China) LLM-Enabled MOFs Discovery: Bridging Rational Design and Laboratory Realization	O
13:00-14:00	**Cocktail Lunch (offered by AI4AM2026 organisers)**	
14:00-14:30	**Poster Session 1 / Exhibition**	
14:30-14:50	**Milica Todorovic** (University of Turku, Finland) Advances in active learning for materials optimisation	I
14:50-15:10	**Reinhard Maurer** (University of Warwick, UK) Machine Learning Surrogate Models of Electronic Structure	I
15:10-15:25	**Xinwei Wang** (Imperial College London, UK) Multi-fidelity machine learning interatomic potentials for charged point defects	O
15:25-15:40	**Julija Zavadlav** (Technical University of Munich, Germany) Machine Learning Potentials with Experimental Data in the Loop	O
15:40-15:55	**Burak Gurlek** (Max Planck Institute for the Structure and Dynamics of Matter, Germany) Transferable Machine-Learned Potentials for Vibrational Dynamics from Acene Crystals to Single-Molecule Host–Guest Systems	O
15:55-16:15	**Gabor Csanyi** (University of Cambridge, UK) Machine learned force fields: status and challenges in 2026	I
16:15-16:45	**Coffee Break / Poster Session**	
16:45-17:15	**Carla P. Gomes** (Cornell University, USA) Knowledge Centric AI for Scientific Discovery.	K
17:15-17:35	**Elmar Bonaccurso** (Airbus, France) Machine Learning for Optimized E2E Advanced Materials Lifecycle - Materials Design, Development, Analytics & Testing	I
17:35-17:50	**Simon Delacroix** (Ecole Polytechnique, France) High-throughput laser synthesis and active learning for optimization of luminescent materials	O
17:50-18:10	**Trevor David Rhone** (Rensselaer Polytechnic Institute, USA) Accelerating the discovery of van der Waals quantum materials using AI	I
18:10-18:30	**Tejs Vegge** (Technical University of Denmark, Denmark) MaterialsCommons and FAIR workflows for federated discovery of advanced materials	I
20:30	Conference Dinner	

Wednesday May 20, 2026

09:00-09:15	**Libor Vojacek** (Paul Scherrer Institute PSI, Switzerland) Polarons and charge-transfer excitations from grand-canonical neural networks	O
09:15-09:30	**Penghui Cao** (University of California, Irvine, USA) Neural network kinetics: exploring diffusion multiplicity and chemical ordering in compositionally complex materials	O
09:30-09:45	**Vincenzo Palermo** (CNR, Italy) Artificial Neural Network–Assisted Electrochemical Sensors for Reliable Biomarker Analysis in Complex Fluids	O
09:45-10:00	**Christopher Kuenneth** (University of Bayreuth, Germany) The Polymer Chemical Linguist: polyBERT´s Role in Next-Generation Polymer Informatics	O
10:00-10:20	**Jacqueline Cole** (University of Cambridge, UK) Data-driven Materials Science for Energy-Sustainable Applications	I
10:20-11:00	**Coffee Break / Poster Session / Exhibition**	
11:00-11:20	**Yousung Jung** (Seoul National University, South Korea) AI for Synthesizable Materials Discovery: From Prediction to Autonomous Design	I
11:20-11:40	**Rampi Ramprasad** (Georgia Tech, USA) AI-assisted design of functional polymers for a sustainable world	I
11:40-11:55	**Dorye L. Esteras** (ICN2, Spain) Modelling and simulation of magnetic materials via AI-driven workflows	O
11:55-12:10	**Irina Roslyakova** (GTT-Technologies, Germany) High-Throughput Materials Informatics Integrating Ab Initio, Machine Learning and CALPHAD Data	O
12:10-12:30	**Andrés Díaz Lantada** (UPM/IMDEA Materiales, Spain) AI-enhanced design for additive manufacturing of bioinspired, smart and living materials and devices	I
12:30-13:15	**Round Table:** AI for IAM in Europe, South Korea and USA	
13:15-14:00	**Cocktail Lunch (offered by AI4AM2026 organisers)**	
14:00-14:30	**Poster Session 2 / Exhibition**	
	Parallel Session - Seniors I - AI for Sustainable & Smart Materials	
14:30-14:45	**Rohit Batra** (IIT Madras, India) Automated Extraction of Multicomponent Alloy Data Using Large Language Models for Sustainable Design	O
14:45-15:00	**Joaquín Muñoz Rodríguez** (Bird & Bird LLP, Spain) Data Protection and Trade Secrets in AI-Powered Materials Databases: An Integrated Legal Framework	O
15:00-15:15	**Andrey Ustyuzhanin** (Constructor University, Germany) What Spin Glasses Teach Us About AI Architecture	O
15:15-15:30	**Daniel Marchand** (SINTEF, Norway) Evolutionary Coding Agents for Autonomous Optimization of Scientific Software and Metallurgical Design	O
15:30-15:45	**Ehsan Moradpur Tari** (University of Tartu Institute of Technology, Estonia) A correlation-based optimization model to recover lost and distorted data from scanning tunneling microscopy images based on density functional theory	O
15:45-16:00	**Sergio Gutiérrez Rodrigo** (Universidad de Zaragoza; Instituto de Nanociencia y Materiales de Aragón (INMA), Spain) Physics-Informed Neural Networks in Materials Science: a framework for optimization, symmetry identification, and inverse design	O
16:00-16:15	**Sai Gautam Gopalakrishnan** (Indian Institute of Science, India) Predicting ionic motion in solids using transfer learning	O
	Parallel Session - Seniors II - Machine Learning for Materials Modeling & Simulation	
14:30-14:45	**Christina Schenk** (IMDEA Materials Institute, Spain) Bayesian Calibration with Optimized Surrogate Models for Materials and Engineering	O
14:45-15:00	**Andrey Golov** (CIC Energigune, Spain) Machine-Learning Interatomic Potentials for the Investigation of Solid Electrolyte Interphase Formation	O
15:00-15:15	**Sergi Vela** (Institut de Química Avançada de Catalunya (IQAC-CSIC), Spain) AI-Driven Molecular Discovery through Automated Dataset Generation and Execution	O

15:15-15:30	**Bousige Colin** (Lab. of Multimaterials and Interfaces, Univ. Lyon1 / CNRS, France) Understanding the nucleation and growth of borophene on substrate using Machine Learning Tools	O
15:30-15:45	**Albert Bruix** (Universitat de Barcelona, Spain) Accelerating the structural and chemical characterization of nanostructured materials under reaction conditions with ML-guided Grand Canonical Global Optimization	O
15:45-16:00	**Richard Tran** (Entalpic, France) Exploring dopant effects on cathode synthesizeability and voltage stability with high-throughput ML	O
16:00-16:15	**Raffaele Cheula** (Aarhus University, Denmark) Graph models and fine-tuned machine learning potentials for microkinetic analyses in heterogeneous catalysis	O
Parallel Session - Seniors III - Data-Driven Innovation & Knowledge Graphs in Materials		
14:30-14:45	**Lukas Powalla** (Robert Bosch GmbH, Germany) Ontology Extraction for Electric Drive Materials Using AI Agents	O
14:45-15:00	**Natalia Bedoya** (Materials Center Leoben Forschung GmbH (MCL), Austria) ALPmat: A Platform for Collaborative AI-driven Advanced Materials Design	O
15:00-15:15	**Alexander Lobo** (BCG X AI Science Institute, USA) Hybrid AI–Physics Discovery of Ionic Liquids Under Industrial Carbon Capture Constraints	O
15:15-15:30	**Simon Stier** (Fraunhofer ISC, Germany) Towards Self-Organizing Research Data: Multi-Agent AI for Autonomous Knowledge Graph Operations based on Object-Oriented Linked Data	O
15:30-15:45	**Santiago Muiños Landin** (AIMEN Techology Centre, Spain) Generative AI for Materials Discovery and SSbD-Driven Material Selection: From Inverse Design to Knowledge Extraction for Faster Validation	O
15:45-16:00	**David Mercier** (Ansys Inc. Part of Synopsys, France) Unsupervised Spatial Machine Learning for Phase Clustering in Nanomechanical Maps with Kernel-Averaged Mechanical Mismatch	O
16:15-16:45	**Coffee Break / Poster Session / Exhibition**	
Parallel Session – Seniors IV - Deep Learning for Materials Characterization		
16:45-17:00	**Pierre Mignon** (Université Lyon1 - institut Lumière Matière, France) Simulation of STM Surface Images from 3D Atomic Structures. A Unet-based Convolutional Networks Tool.	O
17:00-17:15	**Javier Gomez** (ADVANCED MATERIAL SIMULATION SL, Spain) An LLM-Based Multi-Agent Framework for Assisted Finite Element Modelling Workflows	O
17:15-17:30	**Ivan Kruglov** (Emerging Technologies Research Center, XPANCEO, United Arab Emirates) OptiXNet: Symmetry-Aware Equivariant Network for Discovering SHG-Active Materials	O
17:30-17:45	**Emigdio Chavez Angel** (Catalan Institute of Nanoscience and Nanotechnology, Spain) Machine Learning-Assisted Detection of Water Contaminants Using Conventional Raman Spectroscopy	O
17:45-18:00	**Emanuele Telari** (Universitat de Barcelona, Spain) Charting nanocluster structures via convolutional neural networks	O
18:00-18:15	**Rachid Laref** (laboratoire UCCS, Université d´Artois, France) Accelerated Dimensionality Prediction of Lead Halide Perovskites via Wavelet Convolutional Neural Networks	O
Parallel Session – Seniors V - Machine Learning for Material Properties & Discovery		
16:45-17:00	**Zhenzhu Li** (Imperial Global Singapore, Singapore) Platonic representation of foundation machine learning interatomic potentials	O
17:00-17:15	**Malcolm Jardine** (Universitat de Barcelona, Spain) Leveraging Supervised Machine Learning to Predict Band Gaps of Modular Materials from Their Molecular Building-Blocks	O
17:15-17:30	**Pierre-Paul De Breuck** (Ruhr University Bochum, Germany) A generative material transformer using Wyckoff representation	O
17:30-17:45	**Onurcan Kaya** (ICN2, Spain) Revealing Structure-Property Relationships in Amorphous Boron Nitride Using Machine-Learned Potentials	O
17:45-18:00	**Eider Garate Perez** (Tekniker, Spain) Machine Learning Surrogates for Phase-Field Modeling of Dendritic Metal Solidification	O
18:00-18:15	**Pau Ferri Vicedo** (Instituto de Tecnologia Quimica, Spain) High-Throughput Transition-State Searches in Zeolite Nanopores with NNPs	O

Parallel Session – Seniors VI - Neural Networks & Predictive Modeling in Materials Science		
16:45-17:00	**Abigail Teitgen** (Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain) A Multitask Graph Neural Network Framework for Ames Mutagenicity Prediction	O
17:00-17:15	**David Nieto Simavilla** (ETSIME-UPM, Spain) GINNs: A GENERIC Informed Neural Networks methodology to learn thermodynamically sound rheological models	O
17:15-17:30	**Luiz Felipe Cavalcanti Pereira** (Universidade Federal de Pernambuco, Brazil) Machine learning-aided search of enhanced elastocaloric effect in graphene kirigami	O
17:30-17:45	**Nikita Orekhov** (XPANCEO, United Arab Emirates) Molecular dynamics with machine-learning potentials for describing defect dynamics in graphene and diamond	O
17:45-18:00	**Francisco Martin-Martinez** (King´s College London, UK) Embedded molecular representations for more efficient machine learning in molecular discovery and chemical property prediction	O
18:00-18:15	**Annica Heyne** (Federal Institute for Materials Research and Testing (BAM), Germany) Automated Optimization of the Electrodeposition of Alloy Thin Films using a Material Acceleration Platform (MAP)	O

Thursday May 21, 2026

Parallel Session – PhD Students I - Computational Materials Modelling & Simulation

08:30-08:40	**Efe Mehmet Peker** (Bundesanstalt für Materialforschung und-prüfung (BAM), Germany) Balance between precision and scalability: Kinetic Monte Carlo Simulation of Electrodeposition Processes	O
08:40-08:50	**Mirko Fischer** (University of Münster / Institute for Physical Chemistry, Germany) From Oligomers to entangled Polymers: How transferable are Machine Learning Interatomic Potentials?	O
08:50-09:00	**Rayen Ben Ismail** (University of Nottingham, UK) Towards Scalable Gallium Selenide Epitaxy on Graphene: A Multiscale DFT-KMC Framework for Optimizing Growth Conditions	O
09:00-09:10	**Alex Teruel** (Basque Center for Applied Mathematics, Spain) Screening Energetically Stable Structures in Solid-State Ionics Applications	O
09:10-09:20	**Aleksander Szewczyk** (TU Dresden, Germany) Data-Driven Exploration of Thermal and Elastic Properties in Covalent Organic Frameworks	O
09:20-09:30	**Viktor Svahn** (Uppsala university, Sweden) Limitations of cluster-trained MLIPs for liquid density and diffusivity	O
09:30-09:40	**Jonas Böhm** (ICMCB-CNRS, France) Predicting Crystal Structures and Ionic Conductivities in Li3YCl6−xBrx Halide Solid Electrolytes Using a Fine-Tuned Machine Learning Interatomic Potential	O
09:40-09:50	**Sara Shahbazi Fashtali** (Sapienza Università di Roma, Italy) Fine-Tuned Ab Initio–Trained MACE Model for Predictive Mechanical Modelling of Graphene Oxide	O
09:50-10:00	**Yunyu Zhang** (University College London, UK) A Multi-Scale Mixture of Experts Model for Structural Prediction of Cu Nanoparticles	O
10:00-10:10	**Cyprien Bone** (University College London, UK) Discovery and recovery of crystalline materials with property-conditioned transformers	O
10:10-10:20	**Elohan Veillon** (Université d´Artois, France) Fourier Transformers for Latent Crystallographic Diffusion and Generative Modelling	O

Parallel Session – PhD Students II - Machine Learning, Optimization & Predictive Properties

08:30-08:40	**Mary Tabut** (Sorbonne University, France) ML-SAPIE: An Autonomous Workflow Bridging High-Throughput DFT and Machine Learning for Surface Interface Discovery	O
08:40-08:50	**Manuel González Lastre** (Universidad Autónoma de Madrid, Spain) MAD-SURF: a general machine-learning interatomic potential for molecular adsorption on metal surfaces	O
08:50-09:00	**Haolin Wang** (University of Sheffield, UK) Benchmarking Bandgap Prediction in Semiconductors under Experimental and Realistic Evaluation Settings	O
09:00-09:10	**Stefaan Hessmann** (TU Berlin, Germany) Generative Pseudo-Force Fields for Structure Generation	O
09:10-09:20	**Mert Ozan** (Federal Institute for Materials Research and Testing (BAM), Germany) Machine learning aided, closed-loop optimization of electrodeposition processes in a Material Acceleration Platform	O
09:20-09:30	**Ge Lei** (Imperial College London, UK) From Prompt to Protocol: Fast Charging Batteries with Large Language Models	O
09:30-09:40	**Sheares Toh** (Imperial College London, UK) MAESTRO: An AI agent orchestrator for battery materials discovery	O
09:40-09:50	**Joana Cecibel Bustamante Pineda** (Federal Institute for Materials Research and Testing (BAM), Germany) Lattice thermal conductivity on argyrodite compounds Ag8TS6 (T= Si, Ge and Sn): Experimental and Theoretical approach	O
09:50-10:00	**Mathilde Franckel** (Imperial College London, UK) LeMat-Rho: High-Fidelity Charge Density Dataset for Machine Learning and Atomistic Materials Modelling	O
10:00-10:10	**Aakash Ashok Naik** (Federal Institute for Materials Research and Testing (Bundesanstalt für Materialforschung und -prüfung), Germany)	O

	Machine Learning driven insight into Bonding Heterogeneity Effects on Thermal Conductivity	
10:10-10:20	**Luke Keenan** (Trinity College DUblin, Ireland) Machine Learning Accelerators for Quantum Transport	O
10:20-10:30	**Junwu Chen** (EPFL, Switzerland) Generative Artificial Intelligence for Inverse Materials Design	O
10:30-11:00	**Coffee Break / Poster session / Exhibition**	
	Plenary Session	
11:00-11:20	**Roberto Luis Iglesias Pastrana** (Universidad de Oviedo, Spain) Helium Effect on Self-Healing at Tungsten Grain Boundaries Using a DFT-Based Machine Learning Interatomic Potential	I
11:20-11:35	**Kasper Tolborg** (Aalborg University, Denmark) Modelling the interplay between vibrations and disorder in crystalline materials	O
11:35-11:50	**Laura-Bianca Pasca** (University of Oxford, UK) Digital experiments for molecular passivation of hybrid perovskite surfaces	O
11:50-12:10	**Maria K. Chan** (Argonne National Laboratory, USA) MaterialEyes — Seeing the Invisible using Experiment, Theory, and AI	I
12:10-12:25	**Javier Heras Domingo** (Universitat de Barcelona, Spain) Multi-Modal Artificial Intelligence for Molecular Structure Identification using Infrared and Raman Spectroscopy	O
12:25-12:40	**Jolla Kullgren** (Chemistry - Ångström, Uppsala University, Sweden) Predictions and/or insight? - ML and physics-based NMR and IR spectroscopy for water in, and on, crystals	O
12:40-12:55	**Joseph Musielewicz** (Entalpic, France) TriForces: Augmenting Atomistic GNNs for Transferable Representations	O
12:55-13:15	**Miguel Marques** (Ruhr Universitat Bochum, Germany) Machine-learning materials science	I
13:15-13:35	**Maurice de Koning** (Instituto de Física Gleb Wataghin, Brazil) Deformation-trained Deep Potential model for superionic water ice: transferability from stress-strain data to phase equilibria	I
13:35	Closing & AI4AM2027 announcement	