AI4AM2025
ARTIFICIAL INTELLIGENCE FOR ADVANCED MATERIALS
April 08-10 • San Sebastián (Spain)

Tentative Program (as of 06/04/2025)

Tuesday April 08, 2025 (Plenary session)		
08:00-08:45	**Registration**	
08:45-09:15	**Opening Ceremony**	
09:15-10:00	**Gerbrand Ceder** (Berkeley University of California, USA) AI and autonomous laboratories for materials synthesis	P
10:00-11:00	**Coffee Break / Poster Session / Exhibition**	
11:00-11:10	**Wide Hogenhout** (European Commission, Belgium) European digital infrastructure for advanced materials	I
11:10-11:20	**Paolo Bondavalli** (European Innovation Council, Belgium) AI and advanced materials at EIC	I
11:20-11:30	**Tejs Vegge** (Technical University of Denmark, Denmark) Getting better materials faster with ML – a question of representation and distributed platforms	I
11:30-11:40	**Natalia Alexandra Konchakova** (HEREON, Germany) To Support Digital Maturity of Advanced Materials Communities	I
11:40-11:50	**Elisa Molinari** (Università degli Studi di Modena e Reggio Emilia, Italy) Community codes at the exascale for advanced materials	I
11:50-12:00	**Elena Novoselova** (Constructor Group, Germany) Constructor Tech: an enabling AI Platform for Innovation	I
12:00-13:00	**Round Table:** Towards a unified AI framework - methodological and infrastructural perspectives for EU Moderators: **Stephan Roche** (ICREA/ICN2, Spain) & **Elena Novoselova** (Constructor Group, Germany)	
13:00-14:00	**Cocktail Lunch (offered by AI4AM2025 organisers)**	
14:00-14:30	**Poster Session 1 / Exhibition**	
14:30-15:15	**Constructor Tech Workshop:** Transforming research - intelligent workflows for modern science **Stephan Roche** (ICREA/ICN2, Spain) Intelligent workflows for designing innovative advanced materials **Andrei Voicu Tomut** (ICN2, Spain) Demonstration of Scientific Workflow Applied to Disordered Quantum Materials	
15:15-15:45	**Kristin Persson** (Berkeley Lab, USA) Data-Driven Materials Design and Synthesis	K
15:45-16:15	**Yousung Jung** (Seoul National University, South Korea) Data-Enabled Synthesis Predictions for Molecules and Materials	K
16:15-17:00	**Coffee Break / Poster Session / Exhibition**	
17:00-17:15	**Piero Altoe** (NVIDIA, Italy) Revolutionizing AI-Driven Material Discovery Using NVIDIA ALCHEMI	O
17:15-17:30	**Ignacio Fernández Graña** (Pasqal, France) Material Discovery with Quantum-Enhanced Machine Learning Algorithms	O
17:30-17:45	**Elmar Bonaccurso** (Airbus Central R&T, Germany) Aircraft Paint System Optimization Workflow using a Combination of deterministic and data-driven Tools	O
17:45-18:00	**Martin Siron** (Entalpic AI, France) Addressing data quality issues and redundancies across chemistry databases for building better datasets for materials discovery: LeMat-Bulk	O
18:00-18:20	**Anatole von Lilienfeld** (University of Toronto, Canada) The magnificent 7: Simple rules for more efficient quantum machine learning in chemical space	I
20:30	**CONFERENCE DINNER** Restaurant PETRITEGI SAGARDOTE Petritegi Bidea, 8; Astigarraga, 20115, Gipuzkoa - more info Google Maps - Shuttle transfer info to be provided onsite	

Wednesday April 09, 2025 (Plenary session)

09:00-09:15	**Jesús Oroya** (Advanced Material Simulation, Spain) Optimizing AI-Enhanced Neural Network Subroutines for Plasticity in FEM	O
09:15-09:30	**Luis Martín-Moreno** (Instituto de Nanociencia y Materiales de Aragón, Spain) A Neural Network architecture for data-driven symmetry discovery and inverse design, with application to twistoptics	O
09:30-09:45	**Sergio Lucarini** (BCMaterials, Spain) Physics-informed neural networks for coupled Allen-Cahn and Cahn-Hilliard phase field problems	O
09:45-10:05	**Andrey Ustyuzhanin** (Constructor University, Germany) Novelty-Generating Materials as a Substrate for Open-Ended Computation	I
10:05-10:20	**Evgeny Blokhin** (Tilde MI & Materials Platform for Data Science, Estonia) Materials Platform for Data Science: A 10 Years Success Story	O
10:20-10:35	**Jörg Schaarschmidt** (Karlsruhe Institute of Technology, Germany) Advancing Digital Workflows in Material Science: Integrating AI into scientific workflows with the Material Digital Initiative	O
10:35-11:35	**Coffee Break / Poster Session / Exhibition**	
11:35-11:55	**Miguel Caro** (Aalto University, Finland) Predicting the atomic-scale structure of disordered materials with machine-learning potentials and experimental constraints	I
11:55-12:15	**Silvana Botti** (Ruhr University Bochum, Germany) Computational materials science with machine learning: from data to insights	I
12:15-12:30	**Leonardo Medrano Sandonas** (Dresden University of Technology, Germany) Advancing machine learning for organic material simulations with quantum accuracy	O
12:30-12:50	**Sanggyu Chong** (EPFL, Switzerland) Machine learning you can trust	I

Wednesday April 09, 2025 (Advanced Materials Program in Spain - AM@ESP)

09:00-09:15	**Ricardo Diez Muiño** (DIPC & Ikerbasque, Spain) Brief overview of the "Complementary R&D&I Plan for Advanced Materials" in Spain	
09:15-09:40	**Jordi Arbiol** (Institut Català de Nanociència i Nanotecnologia ICN2, Spain) Automated Atomic Scale Data Analysis and Modelling for (Scanning) Transmission Electron Microscopy	I
09:40-10:05	**María Carmen Asensio** (Universidad de Valencia, Spain) Accelerating Advanced Energy Materials Discovery with AI and Modern Characterization Tools	I
10:05-10:30	**Irene García Camacha** (Universidad de Castilla - La Mancha, Spain) Optimizing Hydrogel Synthesis for Customized Applications: An Interactive App for Practitioners	I
10:35-11:40	**Coffee Break / Poster Session / Exhibition**	
11:40-12:05	**Maciej Haranczyk** (IMDEA Materials, Spain) From Simulation to Autonomous Laboratory Preparation: ML-Driven Discovery of Porous Materials and Their Composites	I
12:05-12:30	**Luis Martín-Moreno** (Instituto de Nanociencia y Materiales de Aragón, Spain) Overview of the use of AI for Material Science at INMA.	I
12:30-12:55	**Pablo Piaggi** (CIC nanoGUNE, Spain) Understanding crystallization with atomistic machine learning and simulation	I
12:50-14:00	**Cocktail Lunch (offered by AI4AM2025 organisers)**	
14:00-14:30	**Poster Session 2 / Exhibition**	
	Parallel Session - PhD Students I	
14:30-14:40	**Mojan Omidvar** (Queen mary univeristy of london, UK) Accelerated Discovery of Perovskite Solid Solutions through unsupervised material fingerprints and Automated Materials Synthesis	O
14:40-14:50	**Kevin Alhada-Lahbabi** (INSA Lyon, France) Reinforcement Learning-Assisted Ferroelectric Domain Wall Design Using a Machine Learning PhaseField Surrogate	O

14:50-15:00	**Irea Mosquera-Lois** (Imperial College London, UK) Machine learning force fields for accurate defect calculations	O
15:00-15:10	**Onurcan Kaya** (Catalan Institute of Nanoscience and Nanotechnology, Spain) Revealing Structure-Property Relationships in Amorphous Boron Nitride Using Machine-Learned Potentials	O
15:10-15:20	**Lukas Volkmer** (University of Technology Dresden, Germany) Towards a data-driven multiscale framework for quantum-mechanical investigation of elastic properties of Al-Mg-Zr alloys	O
15:20-15:30	**Danish Khan** (University of Toronto, Canada) Adapting hybrid density functionals with machine learning	O
15:30-15:40	**Michael Alejandro Hernandez Bertran** (Istituto Nanoscienze, Consiglio Nazionale delle Ricerche CNR, Italy) Automated Workflows and Machine Learning models for X-ray spectra simulations: applications to Li-ion battery materials	O
15:40-15:50	**Adam Coxson** (University of Liverpool, UK) Deep Learning the Fock Matrix in the Atomic Orbital Basis for extended π-conjugated molecules within a Self-Consistent Framework	O

Parallel Session - PhD Students II		
14:30-14:40	**Ge Lei** (Imperial College London, UK) Unveiling 3D Geometries in LLMs: The Representation and Recall of Periodic Elements	O
14:40-14:50	**Sebastian Roca-Jerat** (Instituto de Nanociencia y Materiales de Aragón (CSIC-Universidad de Zaragoza), Spain) Neural-network wave functions for quantum many-body problems	O
14:50-15:00	**Amir Dahari** (Imperial College London, UK) Prediction of microstructural representativity from a single image	O
15:00-15:10	**Pol Sanz** (Institute of Chemical Research of Catalonia (ICIQ), Spain) Optimizing Active Learning Strategies for Neural Network Potentials in Catalyst Characterization Workflows	O
15:10-15:20	**Héctor Lobato** (Leartiker, Spain) Smart Design of Thermoplastic Vulcanizate Products: Linking Process to Performance via Machine Learning	O
15:20-15:30	**Adrien Moncomble** (Université Paris Cité - MPQ, France) aquaDenoising: AI-Enhancement of in situ Liquid Phase STEM Video for Automated Quantification of Nanoparticles Growth	O
15:30-15:40	**Sara Navarro** (Catalan Institute of Nanoscience and Nanotechnology, Spain) Developing Accurate Exchange-Correlation Functionals through Physics-Informed Machine Learning	O
15:40-15:50	**Pedro Julián Delgado Galindo** (IFMIF-DONES España, Spain) Modelling of complex Fe-C systems for radiation applications with MLIAPs	O
15:50-16:20	**Coffee Break / Poster Session / Exhibition**	
Parallel Session – Seniors I		
16:20-16:35	**Daniel Araya Matilla** (Advanced Material Simulation, Spain) AI-Enhanced Hybrid Modeling for Optimizing Polymeric Yarn Manufacturing Processes	O
16:35-16:50	**Clara Kirkvold** (University of Birmingham, UK) Leveraging reticular chemistry to develop topology-informed descriptors of nanoporous materials	O
16:50-17:05	**Cristiano Malica** (University of Bremen, Germany) Teaching oxidation states to neural networks	O
17:05-17:20	**Ivan Infante** (BCMaterials, Spain) Advancing Quantum Dot Simulations: from DFT insights to Machine Learning	O
17:20-17:35	**Yuting Li** (Khalifa University, United Arab Emirates) Machine Learning Assisted Discovery of Materials for Hydrogen Energy	O
17:35-17:50	**Ivor Lončarić** (Rudjer Boskovic Institute, Croatia (Hrvatska)) Modeling Molecular Crystals with Machine Learning Interatomic Potentials	O
17:50-18:05	**Jose Ignacio Aizpurua** (University of the Basque Country, Spain)	O

	Physics Informed Neural Networks for Thermal Insulation Material Ageing Estimation	
18:05-18:20	**Sai Gautam Gopalakrishnan** (Indian Institute of Science, India) Optimal transfer learning strategies for predicting material properties	O
18:20-18:35	**Evgeniya Kabliman** (University of Bremen / Leibniz Institute for Materials Engineering – IWT, Germany) Symbolic regression in material science and engineering	O
	Parallel Session – Seniors II	
16:20-16:35	**Davide Tisi** (EPFL, Switzerland) Transport mechanism of solid-state electrolytes via machine learning potentials at hybrid DFT level	O
16:35-16:50	**Lucas Garcia Verga** (Imperial College London, UK) Combining DFT and Machine Learning to Enhance the Screening of Oxygen Evolution Reaction Catalysts	O
16:50-17:05	**Jürgen Spitaler** (Materials Center Leoben Forschung GmbH, Austria) Active learning-based optimization of bainit steels based on probabilistic hybrid modelling	O
17:05-17:20	**Özlem Özcan Sandikcioglu** (Federal Institute for Materials Research and Testing (BAM), Germany) Autonomous exploration of new alloy chemistries using a Material Acceleration Platform (MAP)	O
17:20-17:35	**Sven Rogge** (Center for Molecular Modeling, Ghent University, Belgium) Exploring the opportunities in strain engineering: from introducing flexibility in rigid MOFs to classifying elusive amorphous states	O
17:35-17:50	**Ask Hjorth Larsen** (CAMD, Technical University of Denmark, Denmark) Automated high-throughput computational workflows with Taskblaster	O
17:50-18:05	**Jose Marquez Prieto** (Humboldt University of Berlin, Germany) NOMAD: A Distributed Platform for FAIR and AI-Ready Solar Cell Research	O
18:05-18:20	**Tilmann Hickel** (BAM Federal Institute for Materials Research and Testing, Germany) Data-driven design of hydrogen solubilities in metallic alloys	O
18:20-18:35	**Binh Duong Nguyen** (Forschungszentrum Juelich GmbH, Germany) Machine learning for automated categorizing various defect types in KOH-etched microscopy images of 4H-SiC wafers	O
	Wednesday April 09, 2025 (Lavoiser Discussions)	
14:30-15:00	**Nicola Marzari** (EPFL, Switzerland) The electronic-structure genome of inorganic materials	I
15:00-15:20	**Sonia Conesa Boj** (TU Delft, The Netherlands) Machine Learning from the Large Hadron Collider to van der Waals Materials	I
15:20-15:40	**Chiara Zanardi** (Ca´ Foscari University of Venice, Italy) How artificial intelligence can help in an unusual detection of ions in sweat by graphene oxide and hexacyanoferrate modified electrodes	I
15:40-16:20	**Coffee Break / Poster Session / Exhibition**	
16:20-16:40	**Minh Tuan Dau** (Université Côte d'Azur, CNRS, CRHEA, France) Towards data engineering and model selection in predictive regression of 2D materials properties	I
16:40-17:00	**José-Hugo Garcia** (ICN2, Spain) Equivariant AI-based models for accurate electronic Hamiltonians	I
17:00-17:15	**Shubhojit Banerjee** (UML, USA) Uncertainty-informed transferable deep learning potentials for simulating BeF2-LiF system	O
17:15-18:15	**Round Table:** AI for experimental and theoretical research	

Thursday April 10, 2025 (Plenary session)

09:00-09:20	**Ömer H. Omar** (University of Liverpool, UK) High-Throughput Virtual Screening of Existing Organic Chromophores for Materials Discovery	I
09:20-09:35	**Artem Maevskiy** (National University of Singapore, Singapore) Machine Learning for Accelerated Discovery of Superionic Solids	O
09:35-09:50	**Aurelie Champagne** (CNRS - ICMCB, France) Predicting Crystal Structures and Ionic Conductivity in Mixed-Halide Solid Electrolytes Using Machine Learning Potentials	O
09:50-10:10	**Janine George** (CMD@BAM, Germany) Data-Driven Materials Design	I
10:10-10:25	**Giovanni Vignale** (IFIM, Singapore) Orbital-free density functional theory for periodic solids: Construction of the Pauli potential	O
10:25-10:40	**Amara Hakim** (ONERA, France) Unlocking 3D Nanoparticle Shapes from 2D HRTEM images: classification and denoising at atomic resolution	O
10:40-11:35	**Coffee Break / Poster session / Exhibition**	
11:35-11:55	**Florian Marquardt** (FAU, Germany) AI discovering Strategies for Quantum Technologies	I
11:55-12:15	**Maria Fernandez-Serra** (Stony Brook University, USA) ML-Density and energy optimized exchange and correlation functionals for density functional theory	I
12:15-12:35	**Gian-Marco Rignanese** (UCLouvain, Belgium) Response properties of inorganic materials from high-throughput density-functional perturbation theory and machine-learning	I
12:35-12:50	**Stephen Dale** (IFIM, Singapore) Diagonalization without Diagonalization: A Direct Optimization Approach for Solid-State Density Functional Theory	O
12:50-14:15	**Lunch**	
14:15-14:30	**Emigdio Chavez** (Catalan Institute of Nanoscience and Nanotechnology, Spain) ML-driven Thermal Sensing Using FTIR Spectroscopy	O
14:30-14:45	**Andy Paul Chen** (Nanyang Technological University, Singapore) Crystal Site Disorder Analysis with Machine-Learned Atomic Potentials and Statistical Methods	O
14:45-15:00	**José Luis Montaño-Priede** (Centro de Física de Materiales, Spain) Synergistic Integration of Bayesian Optimization and Advanced Simulation Tools for Plasmonic Performance Enhancement	O
15:00-15:15	**Andreas Räder** (Fraunhofer Institute for Silicate Research ISC, Germany) OpenSemanticLab - Linked-Data-Platform with agentic AI workflows	O
15:15-15:30	**Seon-Hwa Lee** (POSCO Research Institute for Future Technology, South Korea) Leveraging Machine Learning to Navigate Complex Design Spaces in Battery Material Development	O
15:30-15:45	**Samuel John Cooper** (Imperial College London, UK) Li-ion battery design through microstructural optimization using generative AI	O
15:45-16:00	**María Camarasa-Gómez** (Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Spain) Optimizing DFT Hybrid Functionals for 2D Materials Using Genetic Algorithms	O
16:00	**Closing & AI4AM2026 announcement**	

Thursday April 10, 2025 (Lavoiser Discussions)

09:00-09:20	**Romain Gautier** (IMN, France) Machine Learning Design of Low-Dimensional Hybrid Metal Halides with Perovskite Structure Type	I
09:20-09:40	**Antonio Rossi** (IIT, Italy) AI-Driven Protocol for 2D Materials Growth: Integrating Adaptive Synthesis and Spectral Analysis	I
09:40-10:00	**Jan-Lucas Uslu** (Stanford University, USA) Maskterial: A Foundation Model for 2D Material Flake Detection from Optical Images	I

10:00-10:15	**Alexander Tyner** (NORDITA, Sweden) Generative adversarial networks for inverse design of two-dimensional topological insulators	O
10:15-11:00	**Coffee Break / Poster session / Exhibition**	
11:00-11:20	**Simon Dubois** (UCL, Belgium) Inference based model Hamiltonians balancing accuracy, interpretability and data efficiency	I
11:20-11:35	**Felipe Yamada** (INESC TEC, University of Porto, Portugal) Enhancing Bacterial Detection by Harnessing Graphene Transistors´ Latent Features with Deep Learning	O
11:35-11:50	**Li Chen** (TU Dresden, Germany) Towards the computational design of molecular olfactory receptors for digital odor detection	O
11:50-12:05	**Ganna Gryn´ova** (University of Birmingham, UK) New Techniques for Materials Space Exploration	O