AI4AM 2024
ARTIFICIAL INTELLIGENCE FOR ADVANCED MATERIALS
July 02-04 • Barcelona (Spain)

Tentative Program (as of 02/07/2024)

Tuesday July 02, 2024		
08:00-08:45	**Registration**	
08:45-09:00	**Opening Ceremony**	
09:00-09:40	**Kostya Novoselov** (NUS, Singapore) Innovative material design	P
09:40-10:10	**Anatole von Lilienfeld** (University of Toronto, Canada) Physics based machine learning for materials and compound space	K
10:10-11:10	**Coffee Break / Poster Session / Exhibition**	
11:10-11:30	**Gianaurelio Cuniberti** (TU Dresden, Germany) Machine Learning for Molecular Sensing	I
11:30-11:45	**Vincenzo Palermo** (CNR-ISOF, Italy) Multivariate sensing of sodium and potassium ions using Prussian blue, graphene oxide electrodes and machine learning	O
11:45-12:00	**Nicholas Hine** (University of Warwick, UK) Understanding Domain Reconstruction of Twisted Bilayer and Heterobilayer Transition Metal Dichalcogenides through Machine Learned Interatomic Potentials	O
12:00-12:15	**Antonio Rossi** (Istituto Italiano di tecnología (IIT), Italy) Adaptive AI-Driven Material Synthesis: Towards Autonomous 2D Materials Growth	O
12:15-12:30	**Marek Grzelczak** (Centro de Fisica de Materiales (CSIC-UPV/EHU), Spain) Machine Learning for Nanoparticle Synthesis	O
12:30-13:00	**Marin Soljacic** (MIT, USA) Some intersections of photonics and AI	K
13:00-14:00	**Cocktail Lunch (offered by AI4AM2024 organisers)**	
14:00-14:30	**Poster Session 1 / Exhibition**	
14:30-15:00	**Sergei V. Kalinin** (UT Knoxville and Pacific Northwest National Laboratory, USA) Machine Learning for autonomous microscopy: from physics discovery to atomic fabrication	K
15:00-15:15	**Ivan Cole** (RMIT University, Australia) Refining Molecular Characterization to allow machine learning of the effectiveness of corrosion inhibitors	O
15:15-15:35	**Giulia Cisotto** (University of Milan-Bicocca, Italy) Variational autoencoders-enabled high-fidelity reconstruction and effective anomaly detection in EEG data	I
15:35-16:15	**Coffee Break / Poster Session**	
16:15-17:15	**Constructor sponsored Session** - AI Trends in Advanced Materials, **Nick Dobrovolskiy**, Constructor Technology - Constructor Platform and Knowledge Models, **Egor Alekseev**, Constructor Technology - Foundation models for material science, **Andrey Ustyuzhanin**, National University of Singapore - Sparse representation for machine learning the properties of defects in 2D materials, **Kostya Novoselov, Nikita Kazeev**, Institute for Functional Intelligent Materials, NUS - AI-powered prediction of materials, **Stephan Roche**, Andrei Tomut, ICN2	
17:15-17:35	**Bingqing Cheng** (Institute of Science and Technology Austria (IST Austria), Austria) Ab initio thermodynamics	I
17:35-17:50	**Javier Heras-Domingo** (ICIQ, Spain) Unlocking the Potential of EXAFS: Machine Learning Approaches for Spectroscopic Data	O

Wednesday July 03, 2024

09:00-09:20	**Gabor Csanyi** (University of Cambridge, UK) A foundational atomistic model for materials	I
09:20-09:40	**Nicola Marzari** (EPFL, Switzerland) Machine learning electrochemistry	I
09:40-10:00	**Boris Kozinsky** (Harvard University, USA) Multiscale machine learning: from quantum chemistry to dislocation dynamics	I
10:00-10:30	**Karsten Reuter** (Max-Planck-Gesellschaft, Germany) Beyond Crystallinity and Throughput: Machine Learning Accelerated Materials Discovery for Energy Conversion and Storage	K
10:30-11:00	**Coffee Break / Poster Session / Exhibition**	
11:00-12:00	**IoP Publishing Round Table** discussion on opportunities and challenges in AI for Advanced Materials Panel members: Amanda Barnard / Boris Kozinsky / Anatole von Lilienfeld / Silvana Botti Innovation Landscape for AI4AM	
12:00-12:15	**Wolfgang Wenzel** (Karlsruhe Institute of Technology, Germany) Platform MaterialDigital – enabling the industrial material data space of the future	I
12:15-12:30	**Andrea Ferrari** (Cambridge Graphene Centre / University of Cambridge, UK) The Innovative Advanced Materials Initiative and the Innovative Advanced Materials for Europe partnership	I
12:30-12:40	**Kostya Novoselov** (NUS, Singapore) Industry as the relevant driving force of scientific developments	I
12:40-13:15	Round Table Future of Materials: Science, Technology and Solutions Panel members: Andrea Ferrari / Kostya Novoselov / Stephan Roche / Andrey Ustyuzhanin and Laurent Dedenis	
13:15-14:00	**Cocktail Lunch (offered by AI4AM2024 organisers)**	
14:00-14:30	**Poster Session 2 / Exhibition**	
14:00-14:30	**Machine Intelligence // Workshop** We invite you to attend our hands-on session, where we will guide you through a comprehensive data science project using a sample dataset and provide valuable insights and tools to elevate your research capabilities. You will gain practical experience with Initiating a Data Science Project, Data Wrangling with Python, Exploratory Data Analysis and Visualization, Machine Learning Model Training. After the workshop you will have a chance to get a certificate of completion if you register on Constructor Platform and hand-in your assignments. **Ekaterina Butyugina** (Constructor Academy, Switzerland)	
	Parallel Session - PhD Students – I (AULA MAGNA)	
14:30-14:40	**Aishwaryo Ghosh** (S.N. Bose National Centre for Basic Sciences, India) Application of machine learning for materials with targeted properties	O
14:40-14:50	**Luis Martin-Encinar** (University of Valladolid, Spain) A Deep Learning Approach of Surface Elastic Chemical Potential for Accelerating Simulations in Strained Films	O
14:50-15:00	**Sergey Pozdnyakov** (EPFL, Switzerland) Merits of unconstrained atomistic machine learning	O
15:00-15:10	**Pol Febrer** (Institut Catala de Nanociencia i Nanotecnologia (ICN2), Spain) Learning the density matrix, a symmetry rich encoding of the electron density.	O
15:10-15:20	**Andrei Tomut** (Institut Catala de Nanociencia i Nanotecnologia (ICN2), Spain) LatMatcher - AI-Powered Tool for 2D Material Stacking and Property prediction.	O
15:20-15:30	**Ivan Žugec** (Centro de Física de Materiales (CSIC-UPV/EHU), Spain) Understanding the photoinduced desorption and oxidation of CO on Ru(0001) using a neural network potential energy surface	O
15:30-15:40	**Ivan Pinto** (Institut Catala de Nanociencia i Nanotecnologia (ICN2), Spain) Automatic detection of W vacancies in WS2 through CNN	O
15:40-15:50	**Pedro Julián Delgado Galindo** (IFMIF-DONES España, Spain) Machine Learning Interatomic Potentials for Fusion Oriented Materials	O

Parallel Session - PhD Students – II (Room 011+013)		
14:30-14:40	**Kevin Alhada-Lahbadi** (INSA Lyon, France) Ultrafast and accurate prediction of polycrystalline hafnium oxide ferroelectric hysteresis using graph neural networks	O
14:40-14:50	**Cibrán López Álvarez** (Universitat Politècnica de Catalunya, Spain) Graph neural networks for prediction of abrupt phase transitions in energy materials: the case of solid-state cooling	O
14:50-15:00	**Pol Benítez Colominas** (Universitat Politècnica de Catalunya, Spain) Predicting thermal effects in optoelectronic properties of solid solutions with crystal graph neural networks	O
15:00-15:10	**Anas Siddiqui** (University of Warwick, UK) Machine-Learned Interatomic Potentials for Transition Metal Dichalcogenide Mo1-xWxS2-2ySe2y Alloys	O
15:10-15:20	**Onurcan Kaya** (Institut Catala de Nanociencia i Nanotecnologia (ICN2), Spain) A Systematic Analysis of Amorphous Boron Nitride Films using Gaussian Approximation Potentials	O
15:20-15:30	**Egor Shibaev** (Constructor University, Germany) Non-stoichiometric TMDC rapid energy prediction and stable configuration search	O
15:30-15:40	**Jialiang Tang** (University of the Basque Country, Spain) Exploring Ground States of Fermi Hubbard Model on Honeycomb Lattices with Counterdiabaticity	O
15:40-15:50	**Victor Trinquet** (UCLouvain, Belgium) Active Learning: Accelerating Discovery of Optimal Optical Materials through Synergistic Computational Approaches	O
15:50-16:00	**Junhao Cao** (CNRS, France) Denoising of 4D-STEM Dataset using Pix2Pix GAN and Artifact Reduction	O
16:00-16:30	**Coffee Break / Poster Session / Exhibition**	
Parallel Session – Seniors I (AULA MAGNA)		
16:30-16:45	**Kavita Joshi** (CSIR National Chemical Laboratory, India) Solid-state hydrogen storage: Decoding the path through ML guided experiments	O
16:45-17:00	**Gustavo Dalpian** (USP, Brazil) Learning from machine learning: the case of band-gap directness in semiconductors	O
17:00-17:15	**Cristiano Malica** (University of Bremen, Germany) Dynamics of oxidation states in transition metals of Li-ion battery cathodes	O
17:15-17:30	**Xavier Cetó** (Universitat Autònoma de Barcelona, Spain) Rapid field identification of illicit drugs based on electroanalysis assisted by machine learning	O
17:30-17:45	**Elias Polak** (University of Fribourg, Switzerland) Applying a Well-Defined Energy Density for Machine-Learned Density Functionals	O
17:45-18:00	**Andrey Ustyuzhanin** (Constructor University, Singapore) Towards invertible 2D crystal structure representation for efficient downstream task execution	O
18:00-18:15	**Nikita Kazeev** (Institute for Functional Intelligent Materials, National University of Singapore, Singapore) WyckoffTransformer: Autoregressive Generation of Crystals	O
18:15-18:30	**Zan Lian** (Institute of Chemical Research of Catalonia (ICIQ), Spain) Understanding the Dynamic Behavior of Oxide-Derived Copper in CO2 Reduction with Machine Learning Based Large-Scale Simulation	O
18:30-18:45	**Timoteo Colnaghi** (Max Planck Computing and Data Facility, Germany) The role of AI and ML in the development of a multiscale modeling suite for sustainable magnetic materials	O
18:45-19:00	**Konrad Eiler** (UAB, Spain) Guiding experimentalists with machine learning towards optimal Ni-W coatings for fuel cells	O
Parallel Session – Seniors II (Room 011+013)		
16:30-16:45	**Antonio Pena Corredor** (IRT Saint Exupéry, France) Physically informed machine learning algorithms for the mastering of additive manufacturing processes	O

16:45-17:00	**Ioan Bogdan Magdau** (Newcastle University, UK) Foundational MLIP: the Li-ion Battery	O
17:00-17:15	**Pablo Piaggi** (CIC nanoGUNE, Spain) Understanding crystallization from solution and at interfaces with ab-initio machine-learning models	O
17:15-17:30	**Tianbo Li** (IFIM-NUS, Singapore) Variational density functional theory using the JAX deep-learning differentiable framework	O
17:30-17:45	**Stephen Dale** (IFIM, Singapore) Transferable diversity – a data-driven representation of chemical space	O
17:45-18:00	**Adithya Nair** (L´institut de recherche sur les céramiques (IRCER), France) Convolutional neural network analysis of x-ray diffraction data	O
18:00-18:15	**Jordi Riu Vicente** (UPC, Spain) Reinforcement Learning based Quantum Circuit Optimization via ZXCalculus	O
18:15-18:30	**Mikhail Lazarev** (HSE, Russia) Symbolic regression for defects interactions in MoS2 and WSe2	O
18:30-18:45	**Marcin Plodzien** (ICFO – The Institute of Photonic Sciences, Spain) Attention-based neural networks for Quantum State Tomography	O

Thursday July 04, 2024

09:00-09:20	**Juan Carrasquilla Alvarez** (ETH Zurich, Switzerland) Language models for the simulation of quantum many-body systems	I
09:20-09:35	**Alexander Tyner** (NORDITA, Sweden) Machine learning guided discovery of spin-resolved topological insulators	O
09:35-09:50	**Zahra Khatibi** (Trinity College Dublin, Ireland) Evolutionary Recipe: Designing Single Molecule Magnets for Spintronics	O
09:50-10:05	**Artem Mishchenko** (The University of Manchester, UK) Deep Learning Electronic Fingerprints for Mapping Flat-Band Materials in 2D and 3D Databases	O
10:05-10:20	**Luiz Felipe Pereira** (Universidade Federal de Pernambuco, Brazil) Modelling heat transport in amorphous Ge2Sb2Te5 with a deep neural network interatomic potential	O
10:20-10:40	**Volker Deringer** (University of Oxford, UK) Data-driven advances in modelling and understanding amorphous materials	I
10:40-11:15	**Coffee Break / Poster session / Exhibition**	
11:15-11:45	**Amanda Barnard** (Australian National University, Australia) Higher-Order Pattern Recognition for Materials Informatics using Explainable Artificial Intelligence	K
11:45-12:05	**Kedar Hippalgaonkar** (Nanyang Technological University (NTU), Singapore) Property directed generative design of inorganic materials	I
12:05-12:25	**Maite Alducin Ochoa** (CFM, Spain) Accessing photoinduced reaction dynamics on surfaces with neural networks	I
12:25-12:45	**Kamal Choudhary** (NIST, USA) JARVIS-Leaderboard: Large Scale Benchmark of Materials Design Methods	I
12:45-14:15	**Lunch**	
14:15-14:30	**Cormac Toher** (The University of Texas at Dallas, USA) Predicting the synthesizability and properties of disordered materials by combining first-principles calculations with machine-learning	O
14:30-14:45	**Michael Alejandro Hernandez Bertran** (FIM / University of Modena and Reggio Emilia & Istituto Nanoscienze / CNR, Italy) An X-ray spectra simulations workflow based on machine learning: applications to Li-ion battery materials	O
14:45-15:00	**Ivan Kruglov** (Emerging Technologies Research Center, XPANCEO, United Arab Emirates) AI-guided screening of van der Waals materials with high optical anisotropy	O
15:00-15:15	**Gabriel Schleder** (Brazilian Nanotechnology National Laboratory (LNNano/CNPEM), Brazil) Performance Assessment of Universal Machine Learning Interatomic Potentials: Challenges and Directions for Materials´ Surfaces	O
15:15-15:30	**Martin Hoffmann Petersen** (Technical University of Denmark, Denmark) Quest for outperforming cathode materials for Sodium-ion batteries	O
15:30	Closing & AI4AM2025 announcement	