View symposium details

SYMPOSIUM E

Data-based methods and AI for the development and processing of advanced materials

Oral sessions : AMSTERDAM - GROUND FLOOR
Poster sessions : ETOILE - FIRST FLOOR

Symposium Organizers:

François WILLAIME, CEA, France

Mario MAGLIONE, ICMCB-CNRS Université de Bordeaux, France

Peter GUMBSCH (Main organizer), Karlsruhe Institute of Technology / Fraunhofer Institute for Mechanics of Materials IWM, Germany

Tejs VEGGE, DTU - Department of Energy Conversion and Storage, Denmark

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Monday May 25

E01 Thin films and nanomaterials I

Chairperson(s): MAGLIONE Mario

PORTELLA Pedro

View session abstracts

08:30	3376	Thin film combinatorial studies of functional magnetic materials **DEMPSEY Nora M. (Invited)**
09:00	2633	A Digital Infrastructure for Experimental Materials Discovery Enables Synthesis of Four Exotic Materials in Six Process Runs **BERTIN Eugène**
09:15	2744	Fabrication of rare-earth free magnets using a bottom-up approach : high throughput analysis combining machine learning and Small Angle X Ray Scattering **LACROIX Lise-Marie**
09:30	156	Accelerated Discovery of Low-Dimensional Materials via Universal Machine-Learning Interatomic Potentials **BAGHERI Mohammad**

Monday May 25

E02 Metals

Chairperson(s): MAGLIONE Mario

PORTELLA Pedro

View session abstracts

10:30	3064	Developing and managing workflows to enable AI-driven materials design **HICKEL Tilmann (Invited)**
11:00	2942	A Three-Stage Learning Framework for Segmentation of Advanced High-Strength Steel Microstructures and Mechanical Properties Intelligent Prediction **WU Wenwang**
11:15	3168	MLIP-enabled atomistic study of solute segregation to coherent and semi-coherent interfaces: case study of α-Fe/Fe3C **HOLEC David**
11:30	2833	Dislocation Identification in Materials Using Polyhedral Template Matching-Based DXA **VALENCIA Felipe**
11:45	1752	SMaRT stacking: Optimally layered electromagnetic shields with maximal green index printed via fused deposition modeling **CARDINAELS Ruth**

Monday May 25

E03 Semiconductors

Chairperson(s): HICKEL Tilmann

View session abstracts

14:30	1343	An AI-assisted methodological workflow for thin-film growth: GaN and InGaN case studies **BASTIMAN Faebian (Invited)**
15:00	2343	Density Functional Theory Calculations of the Bandstructure for Cubic Boron Arsenide **KING Alex**
15:15	2401	DFT-1/2 Combined with PAO: An Accurate and Cost-Efficient Method for Calculating Band Edges of Semiconductor Junctions **KIM Seungchul**
15:30	3341	E-MAP – An Autonomous Energy Materials Acceleration Platform for Combinatorial Semiconductor Screening **FISCHER Sven**
15:45	2815	Predictive Understanding and Design of Molecular Semiconductors through Physics-Based and Data-Driven Modelling **NEMATIARAM Tahereh**

Monday May 25

E04 Materials shaping

Chairperson(s): DEMPSEY Nora m.

View session abstracts

16:30	1679	Autonomous Workflows and SHAP Interpretation of Multi-Pulse HiPIMS **RODKEY Nathan (Invited)**
17:00	2917	AI-assisted Automated Bed Leveling for FDM 3D printing **GERHARDS Julien**
17:15	2305	Integrating life cycle assessment and machine learning for the green design of glucose-based bio-based aerogels **ZHOU Kejie**
17:30	2485	Inverse Design of Plasmonic Hydrogen Sensors Using Deep Learning **MARTVALL Viktor**
17:45	1651	Accurate prediction and physical interpretation of the glass transition temperature in chalcogenide glasses using a Deep Neural Network **BELCIU Miruna-Ioana**
18:00	1746	A robotic synthesis platform for acceleration of materials development **HASSAM Christopher**
18:15	2311	Combinatorial High-Throughput Spatial Atomic Layer Deposition (CHT-SALD) for Accelerated Optimization of Protective Oxide coatings on Silver Nanowire Electrodes **MUÑOZ-ROJAS David**

Tuesday May 26

E05 Thin films and nanomaterials II

Chairperson(s): PORTELLA Pedro

View session abstracts

08:30	782	From Laboratory Logs to Materials Knowledge: Operating an AI-ready Open Data Infrastructure for High-Throughput Experiments **MITTMANN Lena Angelika (Invited)**
09:00	674	AI-driven recognition of RHEED pattern features for MBE monitoring **GORSHANOV Vadim**
09:15	2536	Prediction of Electrochromic Properties for Sputtered WO3 thin films : Combination of Experimental and Machine Learning Approaches **ROUGIER Aline**
09:30	2490	High-throughput synthesis and characterization of material thin film libraries **DENNINGER Peter**
09:45	2428	Machine Learning-Assisted Analysis of Degradation Factors for Advanced EUV Pellicle **HUNG Yi-Cheng**

Tuesday May 26

E06 Perovskites

Chairperson(s): MAGLIONE Mario

View session abstracts

10:30	2997	Making and measuring billions of materials per day with light **GARNETT Erik (Invited)**
11:00	1894	Physics-informed time-series forecasting of perovskite photo-luminescence stability **SIOL Sebastian**
11:15	1522	Evaluating Ensemble Learning and Neural Networks Models for predicting the Bandgap and Heat of Formation of A2BB'X6 Double Perovskites **AKINPELU Shittu Babatunde**
11:30	2522	Interpretable Physics-Informed Bayesian Optimization in Photovoltaic Materials Acceleration Platforms **CHAKAR Joseph**
11:45	3285	Using genetic algorithms to explore the compositional space of perovskites **GAUTIER Jérôme**

Tuesday May 26

E07 Methods I

Chairperson(s): WILLAIME François

View session abstracts

13:45	3286	Unknown properties of known materials **MARZARI Nicola (Invited)**
14:30	2435	Interpretable Prediction of Perovskite Pseudocubic Lattice Constants with Kolmogorov-Arnold Networks **CHRAPPOVA Krystof**
14:45	2628	From FAIR Data to FAIR Models: Machine Learning Workflows Integrated with Research Data Infrastructures **NASSTROM Hampus**
15:00	2175	Exploring Complex Chemical Spaces with Guided Diffusion Model **BATURIN Vladimir**
15:15	3065	Building machine learning force fields: problem-specific databases still matter in the era of big models **ZHONG Anruo**
15:30	1160	PNcsp: A Periodic Number-Based Crystal Structure Prediction Method Enhanced by Machine Learning **ORAN Cem**

Tuesday May 26

EP02 Poster session 2

View session abstracts

16:30	01_1287	Study of the atomic and electronic structures of the CsPbBr3/SnO2 interface using machine learning potentials **REINSFELT David**
16:30	02_1371	Revolution in Molecular Dynamics Driven by Machine Learning and GPU Acceleration **XU Jian-Bin**
16:30	03_1430	Designing Materials for High-Performance Solid Oxide Electrochemical Cells Using Atomistic Simulations **JEONG Incheol**
16:30	04_152	Machine learning prediction for polymer glass transition temperature with combined fingerprints and SHAP interpretation **DAMAYANTI Krista**
16:30	05_1526	Fast-Track Catalyst Discovery: High-Throughput Screening For Formic Acid Dehydrogenation **MASLOV Andrea**
16:30	06_162	Graph Neural Network Prediction of Nonlinear Optical Properties **ALKABAKIBI Yomn**
16:30	07_1659	Stochastic 3D PEDOT Crystal Growth on Hydrophobic MoS2 for Physically Unclonable Anticounterfeiting Tags **KIM Jinho**

16:30	08_2122	MADGUI: A No-Code Active-Learning Interface for Bayesian Optimization of Materials Composition and Processing **LAMBARD Guillaume**
16:30	09_2365	How to guide structure-property prediction in Hard carbon Na-ion batteries using fine-tuning of MACE foundational model **USUGA Andres-Felipe**
16:30	10_2481	Defect-mediated ion diffusion in metal halide perovskites: from DFT-sensitive NEB benchmarking to machine-learned diffusion dynamics **DESWAL Priyanka**
16:30	11_2511	Progress on the Development of a Neuroevolution Potential for W-Cr-Y-Zr SMART Alloy **KERR Ryan**
16:30	12_3073	DIAMOND: Workflows for automated development of machine learning interatomic potentials **AMMOTHUM Kandy Akshay**
16:30	13_3114	Multi-Scale and Machine Learning Framework for Structure-Property Prediction in High Entropy Alloys **TAKOUTSIN Mikael**
16:30	14_3232	Reproducible container solutions for codes and workflows in materials science **ALMEIDA DE MENDONCA João Paulo**
16:30	15_3252	Design of high strength steels using machine learning **JAISWAL Rajani**
16:30	16_3283	Prediction of the formation energy of AB binary compounds of transition metals using machine learning **MADRID RODARTE Stephanie Citlali**
16:30	17_3302	Explainable Data-Driven Predictions for 2D Materials Using Computed and Experimental Data **ROWLINSON Ben Daniel**
16:30	18_482	Comparative photovoltaic and thermal stability analysis of lead-free MASnI3 and FASnI3 perovskite solar cells using deep learning and SCAPS-1D **DJEFFAL Faycal**
16:30	19_486	NEGF-Based Numerical–Machine Learning Analysis of Graphene Double-Gate FETs for Nanoscale Digital circuit Applications **DJEFFAL Faycal**
16:30	20_574	Bayesian Optimization of Hydrothermal Recipes for LiNi0.8Co0.1Mn0.1O2 (NCM811) Materials Toward Enhanced Capacity **MADIKA Benediktus**
16:30	21_593	Data Driven Design of Stable Energy Materials by DFT and Machine Learning: Promising Electrocatalysts **PARK Hwanyeol**
16:30	22_822	Validating universal machine learning potentials for high-entropy oxides using multi-edge X-ray absorption spectroscopy **KUZMIN Alexei**
16:30	23_910	Data-Based Correlation Between Conductometric and Gravimetric Methods for Ash Determination in Industrial Sugar Streams **AK Halime**

Wednesday May 27

E09 Batteries

Chairperson(s): GEORGE Janine

View session abstracts

08:30	1291	Study of sodium-ion batteries with graph neural networks **CATILLO Marco (Invited)**
09:00	1464	Data-driven discovery of oxide electrolytes for Na-ion all solid-state batteries **YADEGARIFARD Atefeh**
09:15	2852	Bridging order/disorder, ion dynamics and bonding fingerprints in complex oxide networks using first-principles data and in-house, universal and fine-tuned machine-learned interatomic potentials **FAMILIARI Antonio**
09:30	772	Physics-Aware Inverse Design of Battery Cathode Compositions from Electrochemical Targets **BADAKHSHAN Ali**

Wednesday May 27

E10 Synchrotron

Chairperson(s): MAGLIONE Mario

View session abstracts

10:30	2727	AI-Driven Multimodal Analysis and Autonomous Workflows at the ESRF BM32 Beamline **EYMERY Joel (Invited)**
11:00	795	Extending the capabilities of differential deposition for x-ray mirror surface improvment using deep-learning **BRAS Patrice**
11:15	3144	Towards Faster Synchrotron-Based Materials Characterization **CHAHINE Gilbert**
11:30	3224	BM02/D2AM, new High-throughput, software and AI tools in X-ray Diffraction for Material Science **BELLEC Ewen**
11:45	1333	Data-Based Neural-Network and Polynomial Interatomic Potentials to describe Femtosecond Laser Processing of Materials **GARCIA Martin**

Wednesday May 27

E11 Method II

Chairperson(s): VEGGE Tejs

View session abstracts

13:45	2924	Robust Data Generation, Heuristics and Machine Learning for Materials Design **GEORGE Janine (Invited)**
14:30	2866	MARK: AI Materials Scientist for Development of Nanomaterials **HAN Sang Soo**
14:45	3084	qNEP: A highly efficient neuroevolution potential with dynamic charges for large-scale atomistic simulations **BERGER Esmée**
15:00	3028	Ontological Standardization of Workflows for Interoperability in Materials Science **HERRERA CONTRERAS Cinthya**
15:15	1733	Representing and Learning Microstructures for Accelerating Energy Materials Design **WANG Yanming**
15:30	3192	High throughput synthesis of luminescent inorganic thin films by coupling spray-coating deposition and laser irradiation **SENE Amandine**

Thursday May 28

E12 Method III

Chairperson(s): UHRIN Martin

View session abstracts

08:30	2104	Closing the loop: Active learning for efficient materials and process optimization **LAMBARD Guillaume (Invited)**
09:00	950	Search for superconducting ternary hydrides at moderate and low pressures with EDDPs **CAUSSE Maelie**
09:15	3354	Computational predictions of new high entropy oxides **AAMLID Solveig S.**
09:30	550	Deep Learning-based prediction of self-energies from ab-initio Dynamical Mean-Field Theory for transparent conducting oxides **BANERJEE Hrishit**
09:45	1170	Data-Driven Prediction and Property Mapping of Mechanical Behavior in Resorbable Magnesium Alloys Using Machine Learning **NANDAL Vickey**

Thursday May 28

E13 Method IV / Experimental workflows

Chairperson(s): DRAXL Claudia

View session abstracts

10:30	2528	PerQueue: A Dynamical, Graph-Based Workflow Manager **Beck Peter (Invited)**
11:00	308	Uncertainty-Aware Machine Learning Discovery of Solid–Solid Phase Transitions in Inorganic Materials **CAZORLA Claudio**
11:15	542	A Multi-Scale Mixture of Experts Model for Structural Prediction of Cu Nanoparticles **ZHANG Yunyu**
11:30	886	Automated Analysis of 2D materials using machine learning based clustering algorithms **PLATT Frederik**
11:45	1119	From AI-Driven High-Throughput Synthesis of Reticular Materials to Generative AI for Structural Optimization **NGUYEN-DANG Tung**

Thursday May 28

E14 Method V / Perovskites

Chairperson(s): LAMBARD Guillaume

View session abstracts

13:45	3374	NOMAD – a platform for accelerating materials research **DRAXL Claudia (Invited)**
14:15	1195	Interpretable Bayesian-Network Modelling and High-Throughput Gradient Sputtering for Data-Driven Optimization of Zn(O,S) Buffer Layers in CIGS Solar Cells **WOLF Maximilian**
14:30	1047	Predicting Phase Diagrams and Local Symmetry Breaking in Mixed B-Site Halide Perovskites Using a Machine Learning Potential **NGOIPALA Apinya**
14:45	1281	Tailoring Surface Phase Transitions in FAPbI3 via Organic Molecules Using a Machine-Learned Interatomic Potential **DUTTA Sangita**
15:00	1657	Discovery of materials for solar thermochemical hydrogen combining machine learning, computational chemistry, experiments and system simulations **BAYON Alicia**
15:15	2478	Defect-mediated ion diffusion in metal halide perovskites: from DFT-sensitive NEB benchmarking to machine-learned diffusion dynamics **DESWAL Priyanka**
15:30	1816	Single peak fitting method for PXRD processing **IMBERT Léonard**

Thursday May 28

E15 Methods VI / Physical properties

Chairperson(s): LAMBARD Guillaume

View session abstracts

16:30	3254	Learning Physical Observables in Materials with Physics-Aware, Differentiable AI Models **UHRIN Martin (Invited)**
17:00	3042	Universal Geometric Scaling of the superconducting transition temperature in Cuprates, Pnictides, and Moiré Superconductors **KOBLISCHKA Michael**
17:15	2620	Accelerated determination of synthesizability windows from first principles **TADGE Finja**
17:30	3059	Mechanistic Insights into Sulfuric Acid Formation in the Atmosphere via First-Principles Simulations **KACHMAR Ali**
18:00	3364	Optimizing Zn-substituted Cobalt Ferrite Photoanodes for Wastewater Treatment: A Hybrid RSM-ANN Approach to Enhanced Photoelectrocatalytic Performance. **ELAADSSI Yassine**
18:15	1216	Intelligent Design of A2BC2Electrides: EnablingThermocatalytic Ammonia Synthesis and Electrocatalytic Hydrogen Evolution Reaction **WANG Zhiqi**

Friday May 29

E16 Degradation resistant materials

Chairperson(s): SCHUSTER Frederic

View session abstracts

08:30	3056	Accelerated discovery of corrosion resistant materials **BALBAUD Fanny (Invited)**
09:00	2914	Multi-Fidelity Gaussian Process Regression for modeling MOX nuclear fuel thermal properties **PICCINELLI Davide**
09:15	1820	Efficient Thermodynamic Methods for the Design of Nuclear Materials Under Irradiation **HOUZÉ Nicolas**
09:30	767	Accelerated Discovery of H, O interstitials in quinary highly concentrated solid solutions: A First-Principles Calculations and Machine Learning Approach **BARRETEAU Celine**
09:45	679	Advancing Nanoindentation Data Analysis: Towards Feature-Rich Explainable Machine Learning and Open Science **TROST Claus O. W.**